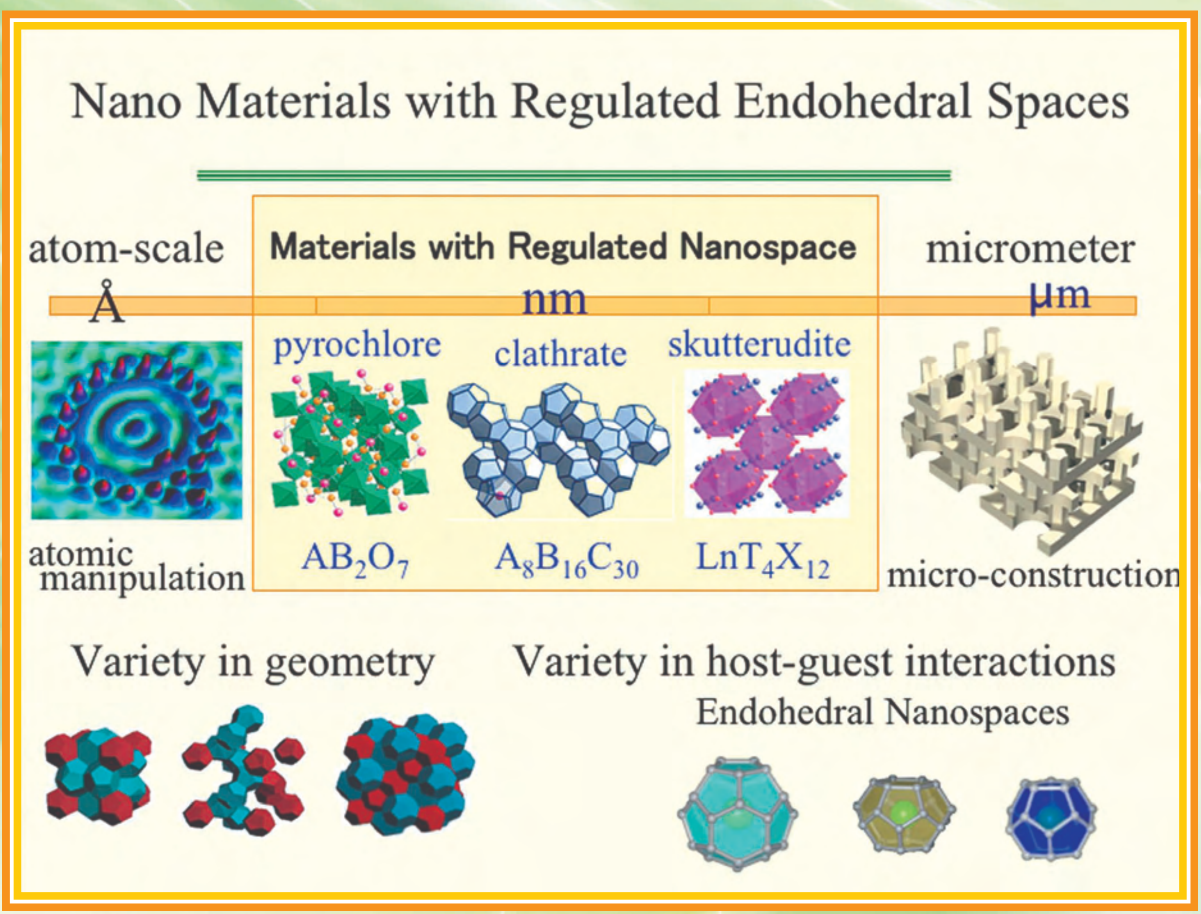
Volume 3

WPI-AIMR NEWS

September 12, 2008



World Premier International Research Center
Advanced Institute for Materials Research

Tohoku University

Cover: Nano Materials with Regulated Endohedral Spaces by K. Tanigaki, Professor of WPI-AIMR

Thanks to the development of micro/nano-fabrication technologies, it is now possible to form various structures in the microscopic area, and even, when using atom manipulation technologies such as STM or AFM, to form much smaller patterns by moving atoms one after another. However, in the physical microfabrication process, emerging defects may become a large obstruction upon observation of solid-state properties expected in the nano region. Moving atoms one-by-one to form a structure large enough to observe its solid-state properties requires a long period. Various nano space materials formed in the nanometer range through application of self-organization phenomenon are expected to constitute a new paradigm of material science that can provide possibilities for new solid-state researches as well as various applications.

表紙：種々のナノ空間を有する物質群　（WPI-AIMR　谷垣勝己教授　提供）

微細加工技術の進展により、現在では多様な微細領域の構造体が構築できるようになっている。また、STM や AFM などの原子操作技術を用いれば、原子を１個ずつ動かして微細なパターンを形成することも可能である。しかし、物理的な微細加工では発生する欠陥がナノ領域で発現する物性を観測する際に大きな障害となり生じる。また、原子を１つ１つ移動させて物性を観測するために十分な大きさを有する構造体を構築するためには、膨大な時間が必要となる。自己組織化現象を適用することにより、ナノメートル領域に形成される種々のナノ空間物質は、多様な構造とともに新しい物性研究の可能性を与える物質科学のニューパラダイムとなる事が期待される。

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Produced by the WPI-AIMR Communication Office

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Contents

Interviews

News Update

Research Prospect

WPI-IFCAM

Announcement

Appendix

Editor's note

We are excited to publish and distribute WPI-AIMR News Vol. 3 to our friends and colleagues on September 12, 2008, the first anniversary of the official announcement (September 12, 2007) of the five awardees of WPIRC (World Premier International Research Center).

It has almost been a year since WPI officially started on October 1, 2007 and we are now shaping up into a full-fledge research center in organization, personnel, and infrastructure with new advanced equipment and new buildings to house laboratories, offices and administration.

Although this program was initially set as a ten-year project, the first five-year critical review will be coming up soon, indeed in less than three years. Many, familiar with our program, commend our assembly of strong individual principal investigators and our flagship ideal of "fusion among various disciplines" is most welcome in the 21st century interdisciplinary science/ technology world. "Fusion" is indeed our buzz-word and goal. (My friend at Seoul National University wrote to me "the interdisciplinary graduate nano-science program is going to change its name to "Graduate School of Fusion Technology," while SNU is participating in a newly publicized "World Class University" Program in Korea.)

However, saying is one thing and doing is quite another, as everyone knows so well. Now we must deliver what we promised in our proposal, quickly and effectively. As noted in his interview by Professor Komatsu, in this volume, Professor Emeritus K. Sumino, a pioneer of semiconductor defect physics, pointed out that successful interdisciplinary work (fusion) requires an assembly of talented first-class researchers who greatly excel in their own disciplines and have open minds to unlimited possibilities.

The WPI Administration together with President Inoue are more than happy to assist the fellow researchers on their research endeavors in any way possible. After all that is the only purpose of this organization.

The results of the 39th International Physics Olympiad held in Hanoi, Vietnam, in July are listed in the News Update section. These showings will have a strong impact in future world-wide research, while the vast majority of people were preoccupied by the 2008 Beijing Olympics. I must confess that P. R. China did really well in both Olympics.

In this issue, we have listed our new WPI members, both research staff and supporting office staff who have joined us since October 1, 2007. Please welcome them all with open arms. – *Toshio Sakurai*

Interviews

Interview with Koji Sumino, Professor Emeritus of Tohoku University

Introduction:

Professor Koji SUMINO: Born in 1931. Started academic life in 1953 as a graduate student of the Physics Department at Tohoku University. Served as a research associate from 1956 to 1964, associate professor from l965 to 1973, professor from 1974 to 1995 and has been professor emeritus since 1995 at Tohoku University. Served also as an executive advisor to Nippon Steel Corporation from 1995 to 2000. His main research field has been crystal lattice defects and crystal plasticity, although his early work was mostly concerned with metals and alloys. He proposed a new type of interaction of dislocations with atomic ordering in alloys. He also put forward the concept of "surface dislocations" to describe the kinetics of the diffusionless migration of interfaces and applied it to twinning deformation and martensitic transformation. He received the Meritorious Prize from the Japan Institute of Metals in 1973 for his research on dislocations in metals and alloys. Changing his focus to crystal defects in semiconductors in around 1965, he investigated the dynamic properties of individual dislocations and the mechanical properties and strength characteristics of silicon, germanium and various compound semiconductors. He succeeded in describing macroscopically observable mechanical characteristics of semiconductors in terms of various collective behaviors of dislocations, taking account of the effect of impurities. He also greatly contributed to the progress of production technology for high quality silicon wafers used in large-scale integrated circuits through his basic research on defects in semiconductors.

Prof. Koji SUMINO

東北大学名誉教授　角野　浩二

Reflection on Lattice Defect Physics Research and Materials Technology

— Relationship between Fundamentals and Applications —

Komatsu: Professor Sumino, you are an authority in Japan on dislocation theory, and you have been involved in the development of the theory from its very beginning to maturity. Research on lattice defects is essential in understanding the physical properties of materials. Particularly in nanotechnology, lattice defects are unavoidable problems. Today, I would like to ask you about the relationship between fundamentals and applications from your experience, reflecting on how lattice defect physics has developed over time as an academic discipline.

Sumino: In the mid-1970s, the level of integration of silicon devices rapidly increased, and this resulted in growing demand for improved quality of silicon wafers for substrates. Controlling various lattice defects in crystals attracted attention as a key issue. In this historical context, as a specialist in crystal lattice defect physics, I became seriously involved in silicon material technology. I remember that there were active exchanges between fundamentals and applications, thus stimulating each other, and substantial advances were made in each of the two areas. I remember that we had vigorous discussions some 30 years ago. Now, I don’t feel the sense of vigor that existed in the exchanges between these areas anymore.

In this interview, I want to talk about what the exchange between basic research into lattice defects and silicon materials technology was like, which was active some 30 years ago, based on my experience. I will be happy if I can make some contribution to revitalizing disciplines in this field by recounting my experiences.

Komatsu: I hear that dislocation theory was born out of an understanding of the mechanical strength of metals. Why did you choose semiconductors as the topic of your research at some point?

Sumino: Strength characteristics, or the response of crystals to external forces, are typical physical properties of crystalline solids governed by the dynamic properties and behavior of dislocations. I entered this field of study in 1953 and changed my research field from metals and alloys to semiconductors around 1965.

Originally, I was not much interested in the strength characteristics of semiconductors, which are not industrial structural materials. Semiconductors were the only materials in which the velocity of individual isolated dislocations in crystals could be measured highly accurately as a function of temperature and stress. This is why I chose semiconductors.

The plastic deformation of crystals develops as high-density dislocations move in the crystal. Therefore, the strength characteristics of crystals are determined by how highly dense dislocations are introduced into the crystals under stress and what collective behaviors they exhibit. First, the kinetic properties of isolated dislocations in crystals of a material are measured. Then, the strength characteristics of the crystals, which are measured on a macro scale, are accurately determined. My aim was to carry out a quantitative analysis of the relationship between them, and thereby to investigate the details of various collective behaviors exhibited by dislocations during the deformation of crystals, and identify factors common to all materials that govern the mechanical strength of crystals. This study was not possible with materials other than semiconductors.

Our group started research with germanium, and expanded the scope of research to include silicon around 1970. All of the crystals used as samples were grown by the floating-zone (FZ) method and had high purity. We determined experimentally that the strength characteristics of semiconductor crystals are very strongly governed by three factors: 1. the deformation temperature; 2. the deformation rate; and 3. the density of dislocations (or dislocation sources) contained in the crystal before deformation. A phenomenon that was specific to semiconductors and not found in other materials was the rapid decrease in the strength of semiconductors with increasing density of the dislocations initially contained in the crystal. Once the above three factors were determined, the strength characteristics of the semiconductor crystals could be measured with good reproducibility.

We successfully demonstrated that all observation facts can be quantitatively described by correlating the temperature and stress dependence of the velocity of individual dislocations in these crystals with the dislocation multiplication mechanism. Consequently, the characteristics of the general collective behavior of dislocations during the deformation of crystalline solids were identified, and at this point the original purpose of my research was achieved.

Komatsu: So, instead of putting priority on the relationship of semiconductor crystals with production technology, you developed a basis for quantitatively understanding their strength characteristics. This was a benefit for the university, wasn’t it? Studies born out of this kind of intellectual curiosity are directly linked to production technology on the production floor.

Sumino: That’s right.

In carrying out research, I paid no attention to relationships with device technology. My research had nothing to do with that. But in the mid-1970s, unexpectedly I was often approached by the semiconductor industry.

At that time, one of the major issues in the device manufacturing technology community was controlling and preventing the occurrence of lattice defects (process-induced defects) during the device manufacturing process. The issues brought to me were related to the occurrence of dislocations during thermal cycling performed on silicon wafers.

I received the following information from the manufacturers’ engineers:

1. When a wafer is subjected to thermal cycling, dislocations and warping occur. The extent of dislocations and warping is not significant at low thermal cycles, but rapidly increases when the number of thermal cycles exceeds a certain value.
2. Dislocations and warping are much less likely to occur in silicon wafers grown by the Czochralski (CZ) process than in those grown by the FZ process, making CZ-silicon wafers stable against thermal cycling.
3. The advantage of CZ-silicon wafers over FZ-silicon wafers in mechanical strength is not that significant at low thermal cycles, but becomes rapidly significant when the number of cycles exceeds a certain value.

The manufacturers wanted me to investigate the reasons for this and give them effective guidelines to prevent the occurrence of dislocations in wafers and wafer warping. If you assume that the state inside a wafer is not affected by the number of cycles, you cannot explain the fact that the frequency of occurrence of dislocations and the extent of wafer warping rapidly increase when the number of thermal cycles exceeds a certain value. The cause is that in addition to the aforementioned fact that the mechanical strength of silicon crystals depends on the density of the dislocations initially contained in the crystals, dislocations occur locally in a wafer, move and increase to higher densities, and consequently the strength rapidly decreases with an increasing number of cycles. This was our conclusion. Also, we found that when a small mechanical stimulus is applied to the surface of a non-dislocated silicon crystal at room temperature using a needle, or fine powder, of diamond or carborundum, a fine non-crystalline region surrounded by dislocations is formed around the stimulus point.

We found that when subjected to a temperature over 500°C, such a fine non-crystalline region is transformed into a dislocated region with the same crystal orientation as that of the parent phase crystal, and that the thus introduced dislocations move under thermal stress, the number of dislocations increases, and the crystal is softened.

In other words, it became clear that silicon crystals believed to be non-dislocated at the stage of wafer fabrication and forming are transformed into dislocated crystals during thermal processing if surface treatment is not appropriate. I heard that after the publication of this study, wafer manufacturers changed their surface-treatment processing of wafers.

On the other hand, when FZ- and CZ-silicon crystals were tested in the normal strength test, there was no significant difference between them, as long as non-dislocated crystals were used as test samples. Therefore, we concluded that the difference in strength between the two types of silicon wafers is peculiar to deformation from thermal cycling.

The difference between FZ and CZ silicon is the difference in the concentration of oxygen impurities in it. So, we studied in detail what effects the difference in the concentration of oxygen impurities might have on dislocations. Our study found that oxygen impurities in solid solution has no effect on the motion of dislocations, and oversaturated oxygen concentrates in static dislocations at high temperatures and immobilizes them.

From this, we concluded that the strength stability of CZ-silicon wafers during thermal cycling is due to the fact that dislocations due to thermal stress are immobilized by oxygen impurities when the thermal stress is removed, and are inactive during subsequent thermal cycling.

As mentioned above, it became clear that issues involved in the occurrence of dislocations and warping due to thermal cycling of silicon wafers can be adequately addressed by properly taking into account the kinetic characteristics of the occurrence, motion and multiplication of dislocations in silicon and the effect of oxygen impurities on these processes. I heard that based on this knowledge, device manufacturers searched for the optimal conditions to control the occurrence of defects under the restrictions of the characteristics of the device manufacturing equipment and cost performance.

Komatsu: Could you tell me your idea on the relationship between fundamentals and applications?

Sumino: Let me explain the characteristics of knowledge required to answer the issues brought to us by the technology community. What was most required was a comprehensive and quantitative understanding of the microprocesses governing the deformation and mechanical strength of silicon crystals. It was not obtained from studies aimed at application to device technology.

In addition to a general understanding of the deformation of crystals, it was necessary to account for the effect of oxygen impurities on the activity of dislocations to understand the characteristics of wafer response to thermal cycling. Even if the phenomenon of the locking and inactivation of dislocations by oxygen impurities was found as an isolated finding, it would be impossible to obtain an overall view of the effects of oxygen impurities on wafer deformation. The findings would not have been effectively applied to technology.

Many phenomena are involved in technology. I would say that it is a self-evident truth that in order to create something new, a comprehensive and proper understanding of all phenomena involved in it is essential. I remember that it was Voronkov (Russian) who first succeeded in establishing a unified picture of grow-in defects in silicon crystals, which attracted significant attention in the 1990s. He had comprehensive knowledge of the characteristics and behavior of point defects. What is absolutely required of those involved in technological innovation is familiarity with related fields.

Recently, attempts have been made to develop devices using strained silicon. I think that controlling misfit dislocations is important. Basic knowledge of dislocations is essential here. If we can accurately understand temperature and stress changes during epilayer growth, we can predict how dislocations behave in the epilayers. I can imagine that by comparing such predictions with actual phenomena, we can understand the special relationship between the boundary structure and the occurrence of dislocations, and obtain important information for technological development. Probably, success in technological development depends on how we can establish comprehensive and systematic knowledge of activities of misfit dislocations during epilayer growth. What we need to this end is detailed knowledge of the various characteristics and behaviors of dislocations in silicon crystals.

I want to look back on the approaches the technology community made to me in the 1970s to 1980s. At the time, we contacted several engineering managers engaged in the development of silicon materials in corporations. They were from private companies, but contacted me as if they represented the industry. All of them had made remarkable achievements in technological development in their respective company, and looked absolutely confident in developing silicon materials.

They were not necessarily familiar with the field of lattice defects. But they were familiar with various technical issues and raised issues to me, as a lattice defect specialist, in a very appropriate manner. We received a lot of support in carrying out our research, but we were never told what to publish or what not to publish for the results of the study. We were never asked by particular companies to contribute to their technological development in return, either.

I sensed that, separate from their positions as corporate engineers, they sincerely hoped for the advancement of Japan’s silicon material technology. Thus, they were highly qualified engineers with deep insight.

In the mid-1980s, device manufacturers withdrew from research and development of silicon materials, and there were no experts on silicon materials left at device manufacturers. Issues such as quality control of silicon materials used in devices were left entirely in the hands of wafer manufacturers.

The reason behind this was that a huge additional capital investment was required for each increase in the integration level of devices, whereas the issue of increasing the crystal quality of silicon wafers was believed to be addressed by progressive improvements through practical experience at work, unless essential changes occurred in device structures.

As a result, it became the top priority for wafer manufacturers to produce wafers meeting specifications set by device manufacturers and expand sales, and the motivation to develop original technologies from a long-term perspective and to hold discussions was lost. This is how I feel.

Researchers in the field of basic research moved away from extensive research to investigate specific phenomena, using various research approaches, to gain an understanding from a broader perspective. Instead, they focused more on producing as many research papers as possible using the limited research approaches available to them. It was a natural consequence that basic research and applied technology stimulated each other less frequently and the exchanges between them decreased.

There is one thing I want to add. I hear that recently there is an increasing sense of deadlock in the silicon material technology community and an increasing number of experienced engineers are deciding to exit this field during organizational changes. I think that it is undesirable in terms of the psychological effect on young engineers entering this world. I think that appropriate action should be taken to give them hope for the future.

When a new fact is discovered, new ideas are developed based on it and a technological revolution occurs. This is a common occurrence. Engineers should always refine their skills and increase their knowledge of the science to prepare for a technological revolution to occur anytime.

Komatsu: Thank you for taking the time to tell us about the relationship between fundamentals and applications from your own research experience.

July 26, 2008 at Prof. Sumino's private room,
Transcript by Hiroshi Komatsu

東北大学名誉教授　角野浩二先生にきく
(Interview with Professor Koji Sumino－Japanese version)

格子欠陥物性研究と材料技術を振り返って

--------基礎と応用のかかわり-------

小松：角野先生は転位論の揺籃期から成熟期にわたって深く関わられた日本の第一人者です。材料物性の理解で｢格子欠陥｣の研究は欠くことができません。とくにナノテク技術は格子欠陥は避けて通れません。今日は一つの学問体系が出来上がる過程をたどりながら、基礎と応用のつながりをご体験からお話いただきたいとおもいます。

角野：1970 年代の半ば頃からシリコン・デバイスの集積度が急速に増大し、それとともに基板となるシリコン・ウェハーの品質の向上が要求されるようになりました。結晶に含まれる各種の格子欠陥を制御することが重要な課題としてクローズアップされたのです。そんな時代背景で結晶格子欠陥物性を専門とする私がシリコン材料技術と深い関わりを持つことになりました。

基礎と応用の間で活発な交流が行われ、双方が刺激しあってそれぞれの分野で大きな発展があったように記憶しています、あのころの生き生きとした交流の様子を思い出すと、30 年余りが経過した現在、これらの分野での交流の実態にあの頃の活気を感じることは私にはできません。

このインタビューでは格子欠陥の基礎研究と材料技術との間の交流が活発だった頃の状況を私の経験をもとに振り返ってみます。これがこの方面の学問や技術を活性化する上で何らかの参考になれば幸いです。

小松：金属材料の強度を理解することから転位論が生まれたと聞いていますが、ある時点から半導体を対象に選ばれたのはどのような理由からですか。

角野：転位のダイナミックな性質や挙動によって支配される結晶固体の典型的な物性はその強度特性、すなわち外部応力に対する結晶の応答です。私がこの分野に入ったのは 1953 年でしたが、1965 年頃研究対象をそれまでの金属や合金から半導体に移しました。

もともと、工業的な構造材料でもない半導体自体の強度特性にそれほど関心があったわけではありません。研究対象を半導体に移した理由は、それが結晶中の孤立した個々の転位の運動速度を温度や応力の関数として信頼度高く測定することが出来る唯一の物質だったからです。

結晶の塑性変形はその中で高密度の転位が運動することによって進行するので、その強度特性は、応力の作用の下で転位が結晶中にどのようにして高密度に導入され、さらに、それらがどのような集団的な運動挙動を示すかによって決定されます。同じ物質の結晶について、まず、その中の孤立した転位の運動特性を測定し、次いで、マクロな尺度で測定される結晶の強度特性を正確に調べる。そして、それらの間の関係を定量的に解析することにより、結晶が変形する際に転位が集団として示すさまざまな挙動の詳細を抽出し、それからすべての物質に共通な、結晶の強度を支配する因子を明らかにすることが私の狙いでした。これは半導体以外の物質では実行することが不可能な研究でした。

ゲルマニウムからスタートした私のグループの研究は 1970 年頃研究対象をシリコンに拡張しました。試料として用いた結晶はいずれも帯溶融（FZ）法で育成した純度の高いものでした。

これら半導体結晶の強度特性が次の３つの因子--- ①変形温度、②変形速度、それに③変形前の結晶に含まれている転位（あるいは転位発生源）密度----に非常に敏感に支配されることを実験的に確立しました。半導体に特有で他の物質に見られない現象は、その強度が最初結晶に含まれている転位の密度の増加と共に急激に減少することでした。以上３つの因子さえ決めればそれら結晶の強度特性は非常に再現性よく測定されました。

全ての観察事実が、これら結晶の中の個々の転位の運動速度の温度や応力に対する依存性、それに転位の増殖機構と結びつけて、定量的に記述できることを示すのにも成功しました。その結果、結晶固体が変形する際の転位の一般的な集団的運動挙動の特徴が明らかになり、この時点で私の当初の研究目的は達成されました。

小松：生産技術とのかかわりは二の次にして、学問的に半導体結晶の強度特性を定量的に理解する基礎を築けたのは大学のメリットですね。この知的好奇心から生まれた研究が現場の生産技術に直結する。

角野：そうです。それまでデバイス技術との関係など全く意識せず、それとは無縁な形で研究を進めてきた私でしたが、1970 年代の半ば頃、半導体産業界から急に積極的な働きかけを受けることになりました。

当時、デバイス製造技術界で大きな問題になっていたことの一つは、デバイス製造プロセス中に発生する格子欠陥（プロセス誘起欠陥）を制御・抑制することでした。私に持ち込まれた問題は、シリコン・ウェハーに繰り返し熱サイクルを施した際に起きる転位の発生と関係したものでした。

メーカー側の技術者から提供された情報は整理すると次のとおりです。

①ウェハーに熱サイクルを与えると転位の発生やそりが起きるが、それは熱サイクル数が少ない間は顕著ではないが、サイクル数がある値を越すと急に増大する。

②チョクラルスキー（CZ）法で育成したシリコンのウェハーでは FZ 法で育成したシリコンのそれよりもはるかに転位発生やそりが起きにくく、熱サイクルに対して安定である。

③そのような CZ シリコン・ウェハーの FZ シリコン・ウェハーに対する強度的な優位も、熱サイクルが少ない間はそれほど著しくはないが、サイクル数がある値を超えると急激に顕著になる、などです。

これらの理由を解明して、ウェハー中の転位やそりの発生を抑えるのに有効な指針を示してほしいとのことでした。

熱サイクル数がある値を超えると急に転位の発生やウェハーのそりが大きくなるという事実は、ウェハーの内部状態がサイクル数に対して不変であると考えたのでは説明することは出来ません。シリコン結晶の強度が最初結晶に含まれている転位の密度に敏感に依存するという、前に述べた事実と合わせて考えて、熱サイクル中に熱応力の作用によってウェハーの中で転位が局所的に発生し、運動し、増殖して、密度を増すために、強度がサイクル数の増加とともに急激に減少するのがその原因であると結論しました。

さらに、室温で無転位のシリコン結晶の表面にダイヤモンドやカーボランダムの微粉末や針によって軽い機械的刺激を与えると、その周りに転位を伴う微細な非晶質の領域が形成されることを見出しました。

このような微細な非晶質領域を 500℃以上の温度にもたらすと、母相結晶と同一の結晶方位をもつ有転位領域に変換されること、そして、そのようにして導入された転位は熱応力の下で運動し、増殖して結晶を軟化させることを突き止めました。

すなわち、ウェハーを加工・成型した段階で無転位であると信じられていたシリコン結晶は、表面処

理が適当でないと熱処理中に有転位結晶になってしまうことが明らかになったのです。この研究の発表後、ウェハー・メーカーでは、ウェハーの表面処理の工程を変えたと聞き及んでいます。

一方、FZ シリコン結晶と CZ シリコン結晶を通常の強度試験でテストすると、無転位結晶を試料とする限り、両者の間には有意の違いは認められません。従って、これら 2 種類のシリコンのウェハー強度の違いは熱サイクルによる変形に特有のものであることを結論しました。

FZ シリコンと CZ シリコンの違いはその中に含まれる不純物酸素の濃度の違いですから、それが転位に対してどのような効果を与えるかを私のグループでは詳細に研究しました。その結果、固溶状態にある不純物酸素は転位の運動に何の影響も与えないのに対して、過飽和状態にある酸素は高温で静止した状態にある転位に集積し、それを不動化してしまうことを見出しました。

このことから、熱サイクルの際の CZ シリコン・ウェハーの強度安定性は、熱応力化で発生してくる転位が、熱応力が働かなくなったときに不純物酸素によって不動化されてしまい、その後の熱サイクルでは活動できなくなることによるものであることを結論しました。

以上のようにして、シリコン・ウェハーの熱サイクルによる転位とそりの発生に絡む問題は、シリコン中の転位の発生、運動、増殖などの動力学的性質の特徴と、それらの過程に対する不純物酸素の効果を適切に考慮すれば、十分に対処できることが明らかになったのです。

こうした知識の上に、各デバイス・メーカーでは、デバイス製造設備の特性、コストパフォーマンスなどの制約の下で、欠陥発生を押さえるための最適条件の探索が行われたと聞いています。

小松：基礎的と応用についてのお考えをどうぞ。

角野：技術界から持ち込まれた問題に答えるために必要だった知識の特徴について考えてみましょう。何よりも必要だったのは、シリコン結晶の変形や強度を支配する微視的な過程の総合的、かつ、定量的な理解でした。それはデバイス技術への応用を目的とした研究によって得られたものではありませんでした。

結晶の変形現象の一般的な理解の上に、転位の活動性に対する不純物酸素の影響を考慮して、はじめて熱サイクルに対するウェハーの応答の特徴を理解することができたのです。仮に、不純物酸素による転位の固着・不活性化という現象が単発的に見出されたとしても、それだけではウェハーの変形に対する不純物酸素の効果に関する全般的描像を得ることは不可能で、それを技術に有効に応用することは出来なかったでしょう。

技術には多くの現象が関わっているので、何か新しいものを生み出すためには、それに関与するすべての現象を総合的に正しく理解することが不可欠であるという自明の理がこの場合に実証されたということでしょう。

思い返せば、1990 年代に大きくクローズアップされたシリコン結晶の成長欠陥に対して、最初に統一的な描像を確立することに成功したのも、点欠陥の性質や挙動に関する総合的な知識に明るかったロシヤ人の Voronkov でした。技術革新に取り組む者にとって絶対必要なことは、関係する分野の学問に精通していることです。

最近、歪シリコンを使ったデバイスを作ろうとする試みが行われていますが、ミスフィット転位の制御が重要となると思われます。ここでも転位に関する基本的知識が不可欠です。

エピ層の成長中の温度や応力の変化を正確に知ることができれば、その中で転位がどのような挙動をするかは予測することができます。そのような予測と実際に起きることを比較すれば、界面構造と転位発生との間の特殊な関係などが明らかになり、技術開発にとって重要な情報が得られると想像されます。技術開発の成否は如何にエピ成長の際のミスフィット転位の活動に対する総合的かつ系統的な知識を

確立できるかにかかっていると思われます。その際に必要なのは、シリコン結晶中の転位のさまざまな性質や動的挙動に関する詳細な知識です。

次に、1970年代から1980年代にかけての私に対する技術界からの働きかけについて回想してみます。

その頃、私は企業でシリコン材料の開発に携わっている技術責任者の何人かと接触を持ちました。それらの人たちはそれぞれ特定の企業に所属しているにも関わらず、あたかも業界を代表しているかのような感じで私に接してきました。いずれも各企業で技術開発に目覚しい成果を挙げた実績を持っており、シリコン材料の技術開発には絶対の自信を持っている様子が窺い知れるような人たちでした。

決して格子欠陥の学問に詳しくはありませんでしたが、技術的諸問題には精通しており、格子欠陥の専門家である私に対する問題提起の仕方が実に的を射ていました。私のグループの研究遂行上、ずいぶん便宜を図っていただいたこともありましたが、研究成果の発表に制約を求められるようなことは皆無で、特定の企業の技術開発への見返りを求められることもありませんでした。

彼らは企業人としての立場を離れて、真摯に我が国のシリコン材料技術の発展を思っていることが伝わってくる、高い見識と資質を持った技術者でした。

1980 年代の半ばになると、デバイス・メーカーはシリコン材料の開発研究から撤退し、シリコン材料に関するエキスパートはデバイス・メーカーからいなくなってしまいました。そして、デバイスに使うシリコン材料の品質のコントロールなどに関する問題は、専ら、ウェハー・メーカーの手に委ねられるようになりました。

その背景には、デバイスの集積度を上げるには、その度、新規に巨額の設備投資が必要になったことと、それに対して、シリコン・ウェハーの結晶品質の向上に関しては、デバイスの構造が本質的に変わらない限り、現場経験の積み重ねによる漸進的な進歩で十分対応できるとの判断があったのだろうと思われます。

結果的に、ウェハー・メーカーにとってはデバイス・メーカーが指定するスペックを満たすウェハーを製造し、販売を拡大することが至上命題となり、長期的視点から独創的な技術を開発したり、議論したりする機運が無くなってしまったように私には感じられます。

一方、基礎関係の研究者の間では、特定の現象をさまざまな研究手法を駆使して調べて、広範的な視点からの理解を得ようとする広がりをもった研究は少なくなり、手持ちの限られた研究手段を使って、出来るだけ数多くの論文を生産しようとする傾向が強まったようです。基礎研究を応用技術が互いに刺激しあうことは少なくなり、両者の間が疎遠になったのは、自然の流れでした。

最後に一言付け加えます。最近、シリコンの材料技術の世界では閉塞感が強まり、企業の組織変更などの機会に、自らの意思でこの世界を去っていく中堅の技術者が増えているのを耳にします。技術の伝承の上からも、新しくこの世界に入ってくる若い技術者への心理的影響の上からも、好ましいことではないと思われます。技術者に将来の希望を持たせるような何か適当な方策が考えられて然るべきではないでしょうか。

新しい事実の発見があれば、その上に新しい発想が生まれ、技術上の革命が起きることはよくあることです。何時そうなっても対処できるように、常に技術を磨き、科学に対する知識を高めて置くことが技術者の在り方だと私は思います。

小松：今日は基礎と応用の関連についてご自身の研究体験から貴重なお話をいただきありがとうございました。

（２００８年7月２６日、角野邸にて　小松　啓　記）

Prof. Katsumi TANIGAKI

主任研究者　谷垣　勝己

Interview with Professor Katsumi Tanigaki

A New World of Clustering Structures

Think Hard and Act Decisively; Failure is the Mother of Success

When I was small, there was no Internet and no computers games like today. Most of the time, children played outdoors. I was born in 1954 and during my childhood days, the possibilities of science sounded like a dream. People talked about space travel by rockets. But what interested me most were robots. Robots at that time seemed to be an unachievable dream, a fantasy. I imagined putting all kinds of artificial intelligence into a robot. Imagination has no limit or boundaries, especially when you know nothing about it. Today, with too much information and knowledge, it seems like everything is revealed and it is only a matter of whether you know it or not.

Playing outdoors often consisted of making simple toys out of wood or bamboo. Despite their simple structures, it was quite difficult to make them. Making one that was satisfactory enough required much trial and error and I spent hours elaborating them. This always came with many failures. I think this childhood experience formed the basis of my current experiments. On the other hand, I feel that students nowadays know a lot, but are very vulnerable to failure. They lack the strong will to keep on challenging to attain their goal, despite many failures. And they give up too easily. They tend to favor goals that are easily achieved and they are not very resilient in failure.

Looking back, I think I was always attracted to the electronics industry. At university, I majored in chemistry and after graduating, I started working in a company. It was 1975, and at that time, the oil and medical fields were the two most popular among university students looking for jobs because they offered good salaries, followed by the electronics industry. My professor referred me to an NEC laboratory and I visited the lab. Fortunately, I was offered a job immediately. So, I had ample time to devote to my dissertation without being disturbed by job hunting. However, NEC was not yet very well known then, and I remember my parents asking me, “What kind of a company is NEC?”

Fundamental research laboratories at the companies of that time had much larger budgets than universities and also owned a variety of equipment. It was the beginning of the fundamental research laboratory boom, the kickoff era, so to say, for fundamental research.

When I joined the NEC laboratory, other major Japanese company laboratories such as Hitachi, Mitsubishi and Toshiba were actively engaged in magnetic bubble memory research. Through various events and social meetings, I came to know many researchers working for different companies. I was engaged in magnetic bubble memory research for a total of around six years. My research subject was “nanoprocessing” of bubble memory and the key was how to miniaturize the memory. Cutting edge technology at that time could only miniaturize up to one micron. To enhance its accuracy, we used the very first equipment developed by the Japan Electron Optics Laboratory, currently known as JEOL. As it was the very first of its kind, its materials were exposed. This study became the breakthrough for me to enter the field of nanotechnology.

However, this research died out suddenly around the end of 1985 when IBM in the U.S. gave up bubble memory research.

Surprisingly after that, we young researchers were allowed to plan and do research on whatever we wanted. Thus, I switched from doing research into memory to looking for research themes, and I went out to look for research “seeds.”

At that time, the micro-fabrication accuracy of magnetic bubble memory was enhanced by one digit by using electron beam lithography with inorganic memory materials. However, clouds seemed to loom over compound semiconductors other than silicon, and I made a major decision to cut myself off from what I had been doing until then.

I was also interested in the effects of radiation upon microfabrication. I came to hear about a study by the Radiation Laboratory of Notre Dame University. So I applied for a sabbatical and with my own money, took off for the U.S.

When I came back, I was surprised when the Personnel Department told me that I was going to be fired. I was called in by the Fundamental Research Laboratory director Mr. Fujio Saito and went to see him, being anxious that I would be told the same thing. However, he only told me that he also experienced many challenges when he was young and encouraged me to try whatever I wanted to do. He supported me in various ways afterwards. He also advised me to study abroad for a few more years. But I declined his advice, because although research in Europe and America was far ahead of Japan in the 1950s, by the end of the 1980s, the gap had already narrowed significantly. If I were to go to the U.S., I might be able to upgrade my English communication skills, but what I really wanted to do was to make a molecular cluster thin film and for that purpose, I wanted an MBE. So I declined his advice to study abroad and told him that I wanted 40 million yen instead. Surprisingly, the money was granted, and to a youngster only in his mid-thirties! That was how I began my cluster research.

At that time, we young researchers at NEC shared a strong determination to be the ones to lead the fundamental research field. Many of my former NEC research colleagues now are in the frontline of research. To name a few off the top of my head, limited only to researchers working on crystals, I can think of Sumio Iijima (Meijo University), Taketoshi Hibiya (Keio University), Junji Matsui (Himeji Institute of Technology), Koichi Kakimoto (Kyushu University) and Fumio Shimura (Shizuoka Institute of Science).

In the meantime, I taught Japanese to foreigners free of charge. In exchange, I was able to learn English communication free of charge. At the NEC Tsukuba Laboratory, there were about 15 or 16 foreigners who came from the U.S., the U.K., France, India, Romania and other countries, which gave us an opportunity to communicate with people from different countries and to get to know different cultures. One of them is now a university professor in the U.S. Another was the daughter of Professor Hart of Oxford University. She came to Japan as an exchange student. As I had to speak English to teach Japanese, it gave me good practice in speaking English.

Looking back, there was a highly intellectual team with a good atmosphere at NEC Tsukuba at that time. We inspired each other both in terms of our research and our cultures. Those were the good old days.

Now, companies have a different standpoint. The relationship between universities and companies has reversed. I think that universities should, of course, engage in fundamental research, but also focus more on application studies and broaden their research fields. WPI can be a part of that. I expect Japanese researchers to have stronger aspirations and to take on more global challenges. The charisma that Japan used to have is now diminished. Japan now has less appeal to students from India and other Asian countries. Added to that, fewer Japanese students go abroad. WPI can contribute to a breakthrough in changing this situation. However, the younger generation has less intellectual hunger to begin with.

Students nowadays do not think within the framework of practical science and tend to stick to textbooks. They seem to think that there is an answer to everything. When you think this way, you cannot generate innovative new ideas. The answers that students present have very little sense of reality. When I say, “We don’t know, so let‘s try it,” the words seem to sound like a threat to them. Perhaps they do not think hard as often as my generation used to do. They are not resilient when being scolded and are extremely sensitive and vulnerable. There are fewer students who can take part in heated debates.

One of the missions of WPI is to nurture young researchers. I hope that it will not just be a means to grant funds for research, but that it will be an opportunity for young Japanese researchers to be inspired by foreign students and to eagerly absorb their good points.

Going back to the story of my research, my first study was on the formulation of the phthalocyanine thin film crystals using molecular beam epitaxy (MBE). This was the only molecule that could be regarded as a cluster back then in 1986.

It took a long time to obtain an ultra-high vacuum of over 10^{-8} Pa. At that time, there were three groups engaged in molecular semiconductor film formation research: the Hara group at RIKEN, the Maruyama group at the Institute for Molecular Science, and our group at NEC.

In academic circles, the Japan Society of Applied Physics was the society that I was most involved in. Among which, the most active society was the Organic Molecule/Bioelectronics Group established by the late Professor Masakazu Okada of Hiroshima University. This group now has over 900 members. When it was established, I was in my thirties. Professor Okada asked me to be its organizer. I declined immediately. “I want to devote myself to research, I do not want to waste my time on other things,” I told him. Even so, four years later, I was asked to be an organizer again. This time I accepted, and was an organizer for six years.

Since around that time, there were many new developments in molecular semiconductor studies. C_{60} was developed between 1989 and 1990, and became the theme of a study awarded the Nobel Prize. Inspired by that, I became more focused on clustered molecular semiconductors. MBE was very useful for that purpose. We had a very good engineer, who was very helpful in improving the equipment. He had only graduated from high school, but possessed an ability far exceeding that of the average college graduate. When he was faced with something he did not understand, he studied on his own and searched for solutions. He still works at NEC and is contributing greatly to their research. Engineers like him are crucial for research.

I repeatedly said that I did not need anyone working under me because I thought that teaching others would be a waste of time. However, two or three years after the Fundamental Research Laboratory was established, Mr. Hisatsune Watanabe, the laboratory director, came to my office one evening and asked me if I would like to have someone working under me. In the end, I got a new researcher. She turned out to be a major contribution to my research. She is still engaged in research at NEC’s laboratory in Tsukuba. By the time I left NEC, I had eight members of staff.

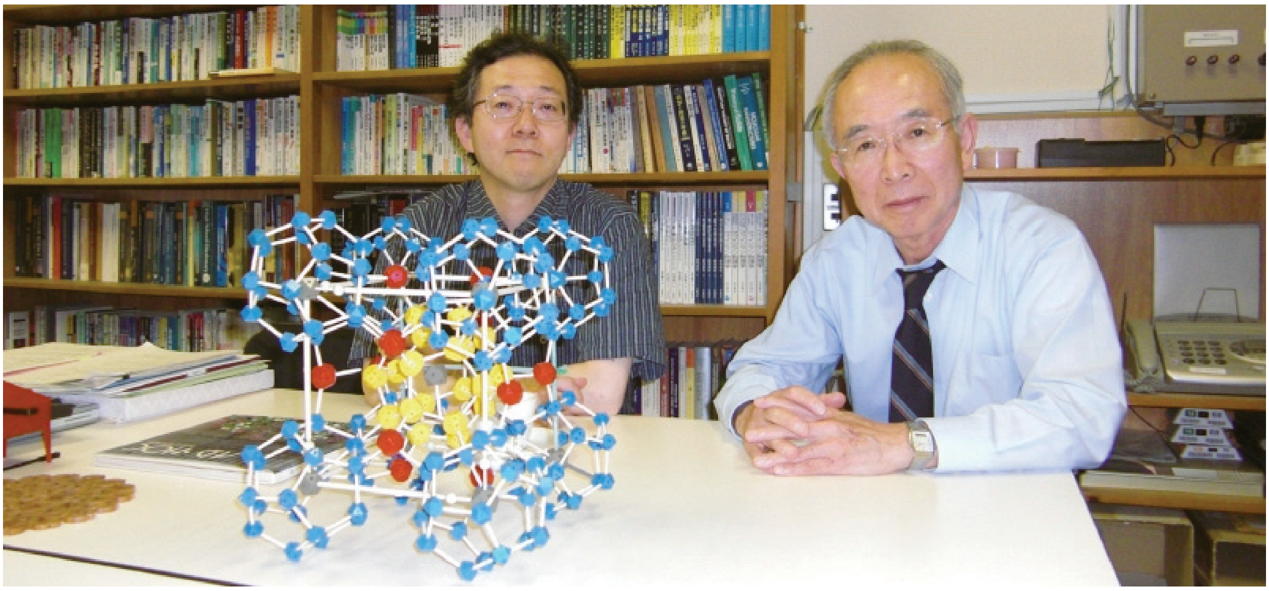
One special member of staff was Mr. Thomas Ebbesen. He is from Norway and is the son-in-law of the late Mr. Iwao Hayashi. He is the same age as me and we got along very well. We are still in contact with each other. I think and behave in a Japanese way and tend to be quiet even when I have something I want to say, but Thomas always stated his opinions straightforwardly. This was very helpful. We made a good team.

Around 1998, company research started to see a downturn. At that time, I was a research team leader. I was given the same pay and treatment as a general manager, but I did not like the managerial job. Then, I received an offer from a university and decided to leave NEC. My good research partner, Thomas, also left for France. He is now Professor and Director of the Nanotechnology Center at the University of Strasbourg. He and his wife, who is the daughter of the late Mr. Hayashi, have twin children.

Around 2001, fundamental research became not to be active like before. And this trend accelerated. Laboratory directors with science and engineering backgrounds used to think first what is best the lab. But that has changed and I had to spend more time on administrative procedures to raise research funds. To cope with the procedures demanded, not by the researchers but from the administrative department, I have to handle more paperwork.

When I was leaving NEC to take up the position of professor at the Graduate School of Science at Osaka City University, Mr. Rangu and Mr. Igarashi, who were NEC directors at that time, allowed me to take with me a truckload of the equipment I was using so that I could continue my research. Perhaps such generosity is unthinkable today. Thanks to that, I was able to carry on my research without any break. Six years later, when I received an offer from Tohoku University, I was allowed to take my equipment with me. I feel very grateful.

At that time, we were able to state our opinions openly and straightforwardly and often had heated debates. Even when it led to a quarrel, it sometimes ended up in a better understanding of each other. Company researchers are highly motivated. On the other hand, students have various demands and each one has to be treated in a different manner. They are extremely sensitive, and thus, I have to be very careful. What I regard as a mere discussion may be mistaken for a scolding. Perhaps if there were members of staff of different generations like in a family, it might help. Universities are based on the American system, in which each professor or associate professor forms an independent unit and has little contact with the others. This makes the accumulation and passing on of research experience difficult, especially for experimental research. I hope that the Ministry of Education and Science will reconsider and restructure this system. I think it is time to change the structure and allocate researchers according to their field of research. I think it would be better if a minimal unit consisted of one professor, one associate professor and one assistant professor, though two associate professors would be better. It is also important to nurture engineering administrators. The current system seems to be managed by people with liberal arts backgrounds who know little about actual research, thinking only with their heads. In the United States, unlike Japan, a large amount of money is spent on utilizing human resources with doctoral degrees.



Going back to research again, when the development of carbon clusters such as C_{60} brought attention to this field, I was able to keep up with the trend as I had established a basis from my previous research. Since around 1990, researchers were able to make compounds from silicon or germanium crystals which were until then unthinkable. Taking silicon as an example, it became possible to make clustered single crystals, not with the conventional diamond structure, but with different structures.

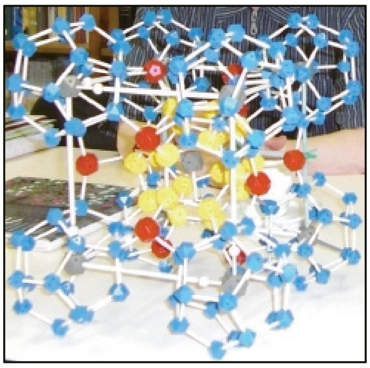


Figure 1

Figure 1 is an example of that model. It is a silicon polyhedron with a clustered structure and covalent bonds. And this is a perfect single crystal. Although it is formed 100% from silicon, it may also be possible to form it from carbon. Symmetry of the crystal is $Pm\bar{3}m$. The reason why it was not possible to form it from phthalocyanine before was because the molecules are in the form of plates and this tended to cause mismatches in the pile while blocking. But currently, it is possible to form many perfect cluster-structured crystals.

Moreover, there is a whole variety including polymorphisms. It is definitely like a Columbus' egg. Before, nobody thought it was possible and did not even venture to try it. A variety of new materials were created between 1991 and 2000. And the method of creation is by no means limited to MBE, but various other methods are currently being tried.

As you can also see from this crystal model, there is a hollow center in the unit cell. If you put an atom or a molecule in here, you can break its symmetry. When the symmetry is broken, a new property will emerge. For example, it may be possible to change independently electrical conductivity and thermal conductivity, which are normally correlated. This makes it possible to create a material with high electrical conductivity but extremely low thermal conductivity. This kind of material is very useful when converting heat into electricity. Previously, it was impossible to create this kind of material.

Unlike other inorganic semiconductors, in these clustered materials it may be possible to control holes and electrons with high accuracy. Thus, various new developments are expected. Flexible clusters are formed from light elements listed up to the third row of the Periodic Table. Unlike heavy metals, they turn out to be materials with lower environmental load.

I think my generation entered this field during the heyday of semiconductor research. We saw with our own eyes semiconductor technology developed to its limits. Now, the tide is turning towards new materials. Knowledge of chemistry will be very useful in the development of new materials.

I actually did organic composition for about three years during research into EL luminous molecular materials. Once a student at the Tokyo Institute of Technology named Saotome who was majoring in organic composition came to our lab. We were forming organic molecules which we had designed ourselves. Surprisingly, he found the routes one after the other very quickly. Inspired by him, I decided to study and train under his instructor, Professor Endo of the Tokyo Institute of Technology (who later became President of the Society of Polymer Science) and Mr. Takada (currently professor at the Tokyo Institute of Technology) for three years. Organic composition is similar to cooking. It requires a certain sense. In the end, I realized that I lack this sense. When a person with composition sense sees a target, they can easily picture a route to that goal. It takes only two or three days for a person with that kind of sense to form what would take me one year. It was very impressive. Mr. Saotome later moved on to the field of biology and is now engaged in bioscience research in Boston.

I have lived through very good times, having had the chance to move through a series of experiences from crystal forming to its processing. And as people did not pick so much on failures, I was able to devote myself to my research without worrying about other things.

WPI offers good opportunities. I hope we make it into a program that attracts and appeals to students from Europe and America.

I haven't talked about the old days for quite a while. It brought back a lot of memories and I guess I have talked a lot today. Nowadays, there is less dialogue between people. Before, on Saturdays, we used to study and work in the mornings, and afternoons were off. That system was pretty good. When the seminar was over, we went out to have a drink and had a good time. I feel that kind of atmosphere still remains in Sendai. And Sendai is not a large city. You can walk from one end of the city to the other. This is also good.

Time seems to flow slowly in Sendai. In Tokyo and Osaka, you feel that you are always being driven by something. I hope we continue to take good care of the wonderful nature and environment that Sendai offers us.

June 16, 2008, at Tanigaki Laboratory,
Department of Physics, Faculty of Science at Aobayama Campus,
Transcript by Hiroshi Komatsu

Nano Materials with Regulated Endohedral Spaces

atom-scale

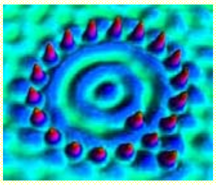
Materials with Regulated Nanospace

micrometer

Å

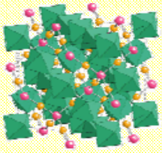
nm

μm



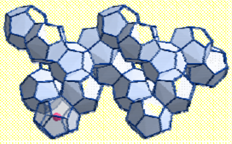
atomic manipulation

pyrochlore



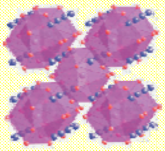
AB_2O_7

clathrate



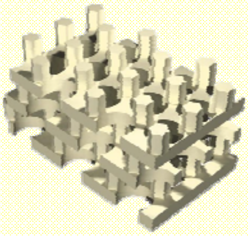
$A_8B_{16}C_{30}$

skutterudite



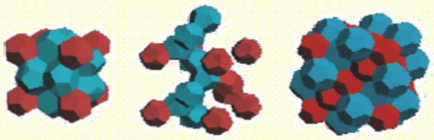
LnT_4X_{12}

micrometer



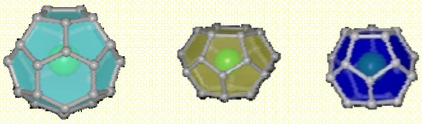
micro-construction

Variety in geometry

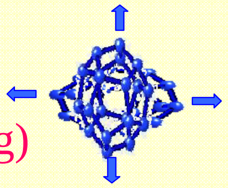


Variety in host-guest interactions

Endohedral Nanospaces

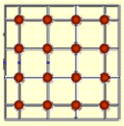


Nanonetwork Polyhedral Solids

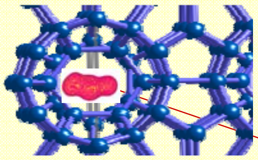


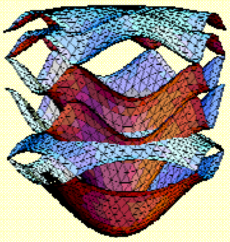
Intra-phonon

Aomic phonons (rattling)

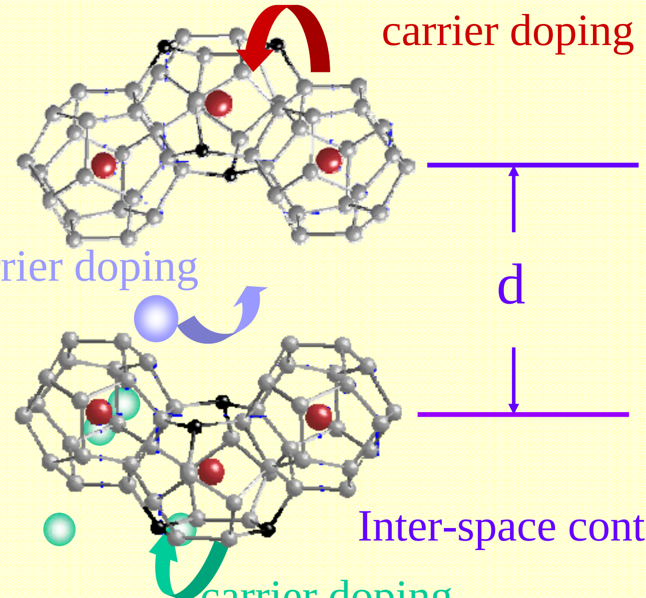


Lattice phonons





New electronic states



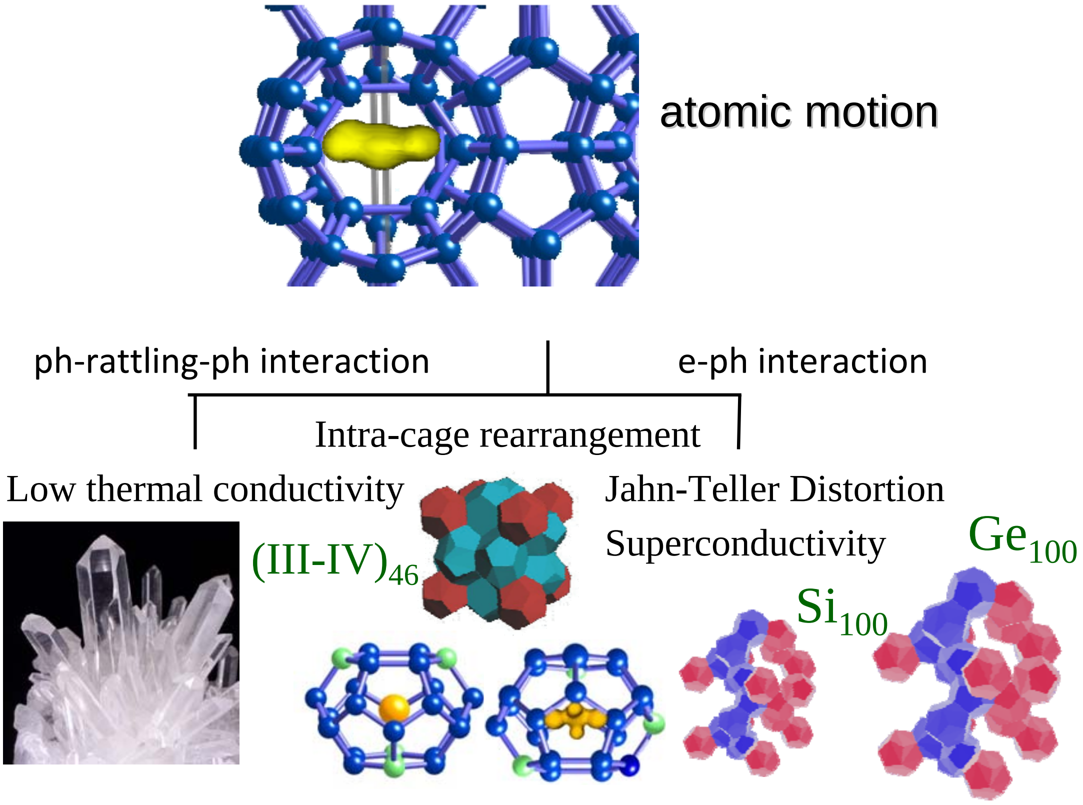
carrier doping

carrier doping

d

Inter-space control

carrier doping


atomic motion
ph-rattling-ph interaction
e-ph interaction
Intra-cage rearrangement
Low thermal conductivity
Jahn-Teller Distortion
Superconductivity
(III-IV)46
Si100
Ge100

WPI-AIMR　PI 谷垣勝己教授にきく
（Interview with Professor Katsumi Tanigaki－Japanese version）

------クラスター構造の新世界------

－熟慮断行、失敗は成功のもと－

子供の頃は今のようにコンピュータやゲームなどは無く、外で飛びまわって遊ぶことが主でした。私は１９５４年生れですが、当時は科学は憧れでした。宇宙ロケットの旅行などいろいろありましたが、中でもロボットにもっとも興味を惹かれました。ロボットは夢のユメでした。人工知能など自由に中に組み込むこともできるかもしれない。何もよく知らないから夢も大きくふくらませることができました。ところが、情報量が多すぎる今は何もかもわかっていて、それを知らないだけといった感じです。

外で遊ぶことの中には木や竹を切って、自分で細工し、杉（玉）鉄砲や竹トンボを作ったりすることがありました。作るのは意外にむつかしい。満足のゆくまで仕上げるにはいろいろな工夫が必要で、夢中になりました。遊び道具つくりに失敗はつきものです。その原体験が私の実験を支えていると思います。ところが、今の学生は頭デッカチで失敗に弱いようです。多少失敗があっても、目的の達成のためにはぶつかってゆくといった気力が薄く、すぐ止めます。どうしても、楽して結果が得られやすいものに流れてゆくなど、失敗に対する抵抗力が落ちています。

ふりかえると、私は一貫して電子産業に憧れていたと思います。大学では化学を勉強した後企業にゆきました。１９７５年当時は石油産業と医療関連は給料がよくて人気があり、電子産業はその次でした。先生の紹介で NEC の研究所を訪ねたところ、好運にも就職がすぐに内定し、落ち着いて研究論文をまとめることができました。もっとも、当時 NEC はよく知られていなかったので、親に『NEC ってどんな会社だ？』と聞かれたりしました。

当時の企業の基礎研究所は、大学よりも予算が１ケタから２ケタ多く、装置も色々ありました。基礎研究所ブームのはじまりで、まさに基礎研究のキックオフのときでした。

入所した時は磁気バブルメモリーの研究が日立、三菱、東芝など日本の大企業の研究所で盛んになされていました。懇親会などを通じていろんな企業の研究者と知り合うことができました。この研究をかれこれ６年ほどもやりました。私のテーマはバブルメモリーの「ナノ加工」で、メモリーをいかに微細化するかが研究の大きなカギでした。当時のトップ技術は１ミクロン止りでこの精度向上のため、部品がむき出しの日本電子製の１号機を使いました。このときの研究が「ナノテク」に参入するきっかけになりました。

しかし、米国の IBM が、バブルメモリーの研究に見切りをつけた１９８５年末頃から研究は急に立ち消えになりました。

その後なんと、若い人は自由に夢を描いて好きなことをやってよいということになったのです。記憶研から探索研になり、研究のシーズ（seeds）探しに向ったのです。

磁気バブルは無機材料によるメモリーで、微細加工精度を電子ビームで１ケタ上げることが出来ていました。しかし、シリコン以外の化合物半導体には陰りも見えていたので思い切ってこれまでのものから離れてみようと考えました。

さらにその頃は微細加工の時の放射線の影響も気になっていました。たまたま米国のノートルダム大学の Radiation Laboratory の研究を知り、休暇の手続きをして自分のお金で米国に出て行きました。

帰国して驚きました。人事係から「首だ」と言われたのです。基礎研究所長に会いに行けと言われて

覚悟を決めて所長の斎藤富士朗さんに会いました。ところが所長は、自分も若い時はいろんなことをやった。いいから好きなことをやれと言われ、その後、随分と支援していただきました。さらに、２年くらい外国留学して勉強することを勧められたのです。しかし留学は断りました。なぜかというと欧米の研究は５０年代には日本よりはるかに進んでいたのですが、８０年代末頃は差が小さくなっていました。米国留学で英会話は多少上手になるかもしれないが、それよりも分子のクラスター薄膜を作りたい。そのため、MBE の装置がほしかった。そこで留学は断り、その代り４０００万円ほしいといったら、なんとそのお金を出してくれました。まだ３０歳半ばの若者にです。それがクラスター研究のはじめです。

当時は自分たちで基礎研究をリードするぞという雰囲気が満ちていました。現在も第一線で活躍している NEC の出身者には、結晶関係に限ってもすぐ思いつくだけで、飯島澄男（名城大学)、日比谷孟俊（慶応義塾大学)、松井純爾（姫路工業大学)、柿本浩一（九州大学)、志村史夫（静岡理工科大学）の諸氏がいます。

英会話の方は、ボランティアで日本語を外国人に教えることで逆にタダで英会話を学習できました。当時のつくばの NEC では、米、英、仏、インド、ルーマニアなど１５～６人の外国人と国際的な交わりが普段に行われていて、互に異国のカルチャーを知る機会がありました。その中から今では米国で教授になった人もいます。オックスフォード大学のハート教授の娘さん（交換留学生）もいました。日本語を教えるのに英語を使いますので実地の会話のトレーニングになりました。

あとから考えると、あのころのつくばの NEC は研究にもカルチャーにも、良い頭脳集団があったことになります。良い時代でした。

今は企業の立場は変わっています。大学と企業の関係が逆になりました。大学は基礎をやるのはもちろんですが、もっと応用に眼を向けて、研究に拡がりがある方がよいと思います。まさに WPI はその一環となり得ます。日本から世界に打って出ようという気概がもっと成長するとよいですね。以前は日本にもカリスマ性がありましたが、最近では消えてきて、アジア、インドの学生を引きつけるものが少なくなっている。日本の若手も出てゆかない。WPI でも口火は切れるが、若手に知的な渇きがなくなっています。

最近は実学でなく教科書の中で生きている。全てに解があると思っている。これでは一定以上に新しいものは出て来ない。学生の答えに現実味が薄いです。わからないからやってみようというのは彼らには脅威に聞こえる。じっくり考えることが無くなっているのではないでしょうか。怒られることに対して抵抗力がなく、ものすごくナイーブです。白熱的な議論ができる学生が少なくなってきました。

WPI は若い人の育成も兼ねてはいるが、お金ではなく、外国の学生から刺激を得てよいところをどん慾に吸収することを望みます。

ところで研究に戻りますと、最初に手がけたのはフタロシアニンのクラスターの MBE による構築です。これが１９８６年当時知られていた唯一のクラスターと考えることのできる分子でした。

10^{-10}Pa を越える超高真空を得るには時間がかかりました。当時、実際に分子半導体成膜をやっていたのは理研の原グループ、分子研の丸山グループ、それに NEC の私の３グループでした。

学会では応用物理学会が中心で、中でも広島大学の故岡田正和先生の提唱で生れた「有機分子・バイオエレクトロニクス分科会」が活発で、会員は今では９００名を超えるようになっています。創立当時、私は３０代だったが岡田先生に幹事をやれと言われてすぐ断りました。私は研究をやりたい、無駄な時間を使いたくないと返事しました。しかし、４年あとには再度の依頼で幹事を引受けることになり６年間務めました。

その頃から分子半導体が伸びてきました。８９～９０年にかけて C_{60} が出てノーベル賞になった。それがヒントで、より力を集中してクラスター分子半導体をやるようになり、以前からの MBE の装置が大変役立ちました。その時、優秀な技術者がいて装置の改良などですごく助かりました。その人は高卒

ですが並の大卒が及ばない能力を持った人でした。わからないことは自分で勉強していました。今でもNECにいて重宝されています。このような技術者がいることはすごく大切です。

しかし一貫して、私は部下は不要と言っていました。教えることに使う時間がムダになると言っていました。ところが基礎研究所が出来て２～３年たった頃、渡辺久恒所長が夜中に研究室に入ってきて、部下を取らないかと言ってきました。結果的には女性の研究者をすすめられて、研究にプラスになりました。その方は今もつくばで研究しています。NECを出る時には部下は８名になっていました。

その中で異色だったのは故林厳雄さんの娘さんのご主人のエブソンさんです。その人はノルウエー人でした。私と同年齢でウマがよく合いました。今でもお付き合いしています。私は日本的で、言いたいことも我慢する方ですが、彼は全く遠慮せず、バンバン意見を言ってくれて、助かりました。良いコンビでした。

１９９８年頃になると企業の研究にも陰りがみられるようになりました。部長待遇の研究チームリーダであった私は管理する仕事が肌に合わないでいるとき、大学から誘いがあってNECを出ました。コンビだったエブソン氏も私と同時期にフランスへ移りました。彼は今ストラスブルグ大学のナノテクノロジーセンターの教授（センター長）をしています。林さんのお嬢さんとの間に双子に恵まれて。

２００１年頃には基礎研究が下火になり、NEC のみでなく日立なども企業の研究のトップには文系の人たちが増え、それを加速させました。かつて理系の代々の所長は研究所を守ってくれたのですが、しだいに研究費を得るための事務手続きに時間を取られることが多くなりました。研究者でなく事務方の要求で、作文書きが必要以上に増加しています。

大阪市立大学理学研究科へ教授として移る時、当時の上層部である覧具さん・五十嵐さんは、研究を続けられるように私が使っていた装置をトラック１台分も持たせてくれました。今では考えられないことかもしませんね。お陰で研究を中断することなく続けられました。数年後、東北大から声がかかった時、使っていた装置は移管することができました。私は大変感謝しています。

当時は言いたいことを本気で出せて、熱い議論ができた。ケンカもしたが、それで分かり合えたこともある。企業の研究者は強いモチベーションを持っている。しかし、学生は要求がいろいろで同じには扱えない。すごく傷つきやすいので気をつかいます。こちらは普通の議論をしているつもりでも、怒られていると勘違いされる。その時、家族のような世代構成のスタッフがいればよいのですが....。アメリカ式で教授、准教授がそれぞれ小さく独立していて、特に実験系では、研究の積み重ねや継承がむつかしい。このようなシステムは文科省も一度見直してほしいです。分野によって研究者の構成配置を考える時だと思います。教授、准教授、助教の１、１、１が最小の構成単位、できれば１、１、２がよいと思います。あとは、技官を育てることが大切です。現在は研究の実態を知らない文系の人が頭の中だけで考えているようです。米国は日本と違って膨大なお金を手配してポスドクを活用しています。

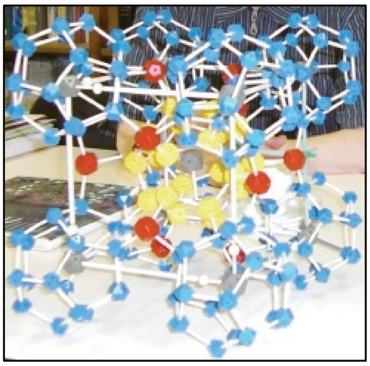


図 1

ふたたび研究の話に戻りますが、C_{60} などの炭素系のクラスターが出て、この方面に注目が集まった時、私はそれまでの研究を土台にすぐ対応できました。１９９０年頃からシリコンやゲルマニウムの結晶では思いもよらない化合物ができるようになった。例えばシリコンですが、これまでのようなダイヤモンド構造でなく、別の構造をもったクラスター状の単結晶ができるのです。

図１の模型がその例ですが、共有結合でシリコン多面体のクラスター構造を作っています。しかもこれは完全な単結晶です。１００％シリコンでできていますが、炭素などでも出来る可能性を持っています。結晶の対称性は $Pm\bar{3}m$ です。昔フタロシアニンでは出来なかったのは、分子が板状で、ブロック化するときに積み重なりの不整合が出来易かったからです。今ではこのようなきちんとしたクラスター構造の結晶が多数できるようになっています。しかも多型もあって多種多様です。まさに、

コロンブスの卵で、昔は初めから出来ないだろうとあきらめて、誰も試みなかったものです。C_{60} のフラーレンがヒントです。包接化合物の三次元版ともいえます。

１９９１年～２０００年の間にいろんな新物質が生み出されました。作り方も MBE のみでなく、加圧・減圧さまざまな試みがなされています。

この結晶モデルでもわかりますが、ユニットセルの中に中空があります。ここに原子や分子を入れることで対称性を破ることもできます。対称性が破れることで新しい物性が出現します。たとえば相関する電気伝導度と熱伝導度をそれぞれ独立に変えることもできます。電気伝導度が高くて熱伝導度が低い物質も可能です。これは熱を電気に変換するとき大変役立ちます。今までこのような材料は作れませんでした。温度差を大きくとることで熱の変換効率を向上させることもできます。

これらの、クラスター物質では、通常の無機半導体と異なり、ホールとエレクトロンの高精度の制御が可能となる可能性があり、今後多様な展開が期待されています。また、柔軟性のあるクラスターは周期律表の第３周期までの軽元素でつくられます。これは重金属と違って環境に負荷を与えることが少ないものになります。

考えてみると私たちの世代は半導体の隆盛期に研究に入り、その極限まで技術が展開するのを見たことになります。ここにきて新しい材料に向う気運が高まってきたのです。このような物質を開拓する上で化学の知識が大変有用になります。

実は私は EL の発光分子材料の研究をする目的で、有機合成を３年ほどやった経験があります。ある時、有機合成専門の早乙女君という学生が東工大から来ました。有機分子を自分で設計して作るのですが、短時間にその道筋を次々と見つけてしまうのです。これに刺激されて東工大のその学生の遠藤先生（のち高分子学会会長）と高田先生（現東工大教授）に弟子入りして、３年トレーニングを受けました。しかし、有機合成には料理と同じでセンスがいります。結局、自分にはこのセンスが欠けていると思いました。合成のセンスのある人はターゲットを見たら、そこに至る経路を次々と描けるのです。よくできる人は、私が１年かけて作るものを２、３日で作ってしまう。すごいです！早乙女君はその後生物学に移って、今では米国のボストンでバイオサイエンスをやっています。

結晶作りから加工までを一貫して体験できる、大変よい時代を過しました。失敗を大目に見てくれたので、のびのび研究できました。

WPI は良い機会ですが、欧米の学生が自発的に来たくなるようなものにしたいですね。

今日は久々に昔話をしましたが、つい若い時を想い出し長話をしてしまいました。今は対話が欠けることが多いです。昔の土曜日は今ありませんね。けっこう良かったです。ゼミのあと、皆で飲み会をしながらパーとやりました。仙台はまだそんなことができる雰囲気が残っていますね。街を端から端まで歩けるのもいいです。

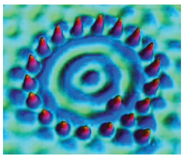
仙台は時間がゆっくり流れています。東京や大阪は何かに追われている感があります。この良い自然環境を大事にしたいですね。

（２００８年6月１６日、青葉山理学部物理学科　谷垣研究室にて　小松　啓　記）

ナノ固体物性とデバイス基礎理学

原子領域

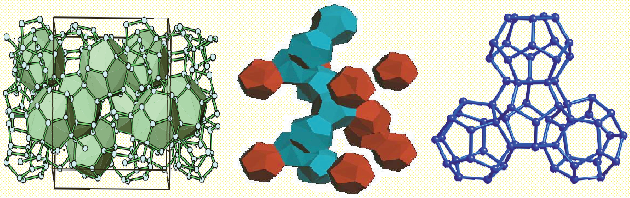
Å



原子操作

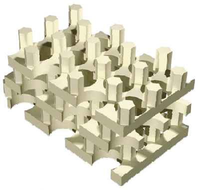
nm領域

ナノ領域の閉じ込め空間



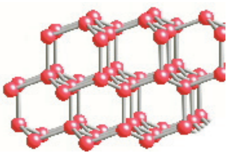
マクロ領域

μ m



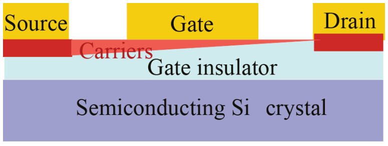
微細加工技術

シリコン結晶



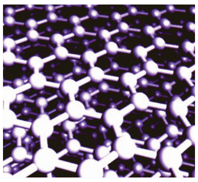
sp^3–ネットワーク

FET

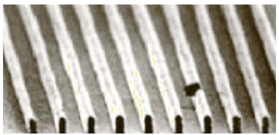


薄膜成膜

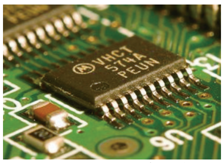
グラファイト結晶



sp^2-ネットワーク



微細加工



集積回路

News Update

WPI-AIMR Annual Workshop 2009

We cordially invite all WPI-AIMR members and our friends to the WPI-AIMR Annual Workshop 2009 to be held at Miyagi Zao Royal Hotel(http://www.daiwaresort.co.jp/zaou/) from March 1 to March 6, 2009.

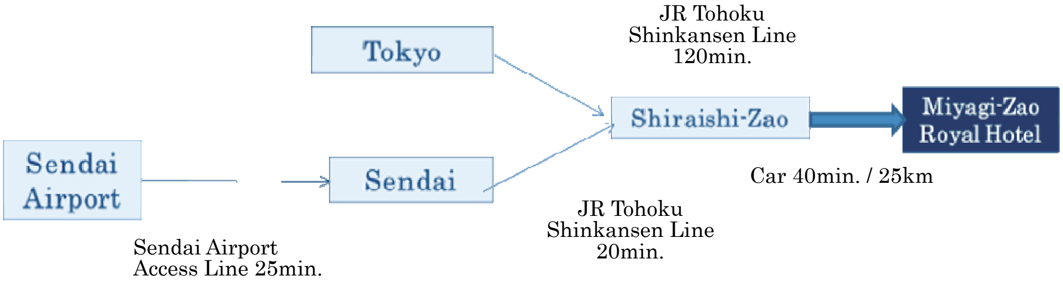
The format of the technical sessions is similar to many of summer Gordon Conferences: relaxed atmosphere in the morning and evening sessions and a plenty of free discussion time in midday. Only the exception is that we plan to publish proceedings in Springer “Advances in Materials Research” series.

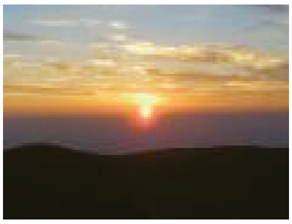
Since this will be the first one for our WPI, we are quite open to constructive suggestions and input before we finalize the format in detail (by the end of January 2009). Please feel free to give us your comments.

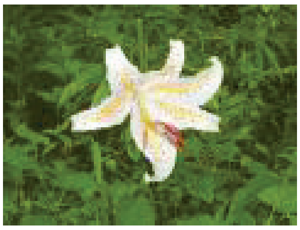
Followings are tentative list of invited speakers at this time:

Toyonobu Yoshida, Department of Materials Engineering, University of Tokyo
Subra Suresh, MIT, USA (pending)
Kunio Takayanagi, Tokyo Institute of Technology (pending)
Manfred Ruhle, Max Planck Institute for Metals Research, Germany
Steve Pennycook, Oak Ridge National Lab. USA
Ke Lu, Institute for Metal Research, China Academy of Sciences, P.R. China
Akihisa Inoue, Tohoku University
William L. Johnson, California Institute of Technology, USA (pending)
Lindsay Greer, University of Cambridge, UK
C. T. Liu, Oak Ridge National Lab. USA (upending)
Juergen Eckert, IFW Dresden, Germany (pending)
Hans-Joachim Freund, Department of Chemical Physics, Fritz-Haber-Institut, Germany
Hong Guo, Department of Physics, McGill University, Canada
H. Hilgenkamp, MESA Institute for Nanotechnology, University of Twente, The Netherlands
Yoshitaka Tateyama, WPI International Centre for Materials Nanoarchitectonics, NIMS
Qi-Kun Xue, WPI-AIMR & Department of Physics, Tsinghua University, P. R. China
Akira Ohtomo, IMR, Tohoku University (pending)
Max G. Lagally, WPI-AIMR, University of Wisconsin-Madison, USA
Yoshihiro Iwasa, IMR, Tohoku University (pending)
Shuji Hasegawa, University of Tokyo (pending)
Yukio Hasegawa, University of Tokyo (pending)
Taeghwan Hyeon, National Creative Research Initiative, Seoul National University, Korea
Takanori Fukushima, Functional Soft Matter Engineering Team, RIKEN
Hiroshi Jinnai, Kyoto Institute of Technology
Toshiharu Teranishi, Department of Chemistry, University of Tsukuba
Takashi Inoue, Department of Polymer Science and Engineering, Yamagata University
Kazushi Kinbara, IMRAM, Tohoku University, Japan
Tetsuro Higashi, Tokyo Electron Limited, Japan,
Ryutaro Maeda, AIST, Japan,
Youichi Sakakibara, AIST, Japan
Koji Ando, AIST, Japan

Access







More information will follow in the coming months…

Appl. Phys. Lett. in press.

M. Kawasaki, T. Makino, and K. Ueno

“A highly-efficient UV sensor using conducting polymer/ZnO Schottky junction”

A wide gap semiconductor zinc oxide (ZnO) is one of the promising compounds for transparent oxide electronics because its constituents are produced from abundantly deposited minerals. Elaborate techniques of process and property control for ZnO allow us to develop further electrical applications. The development of a solar-blind photo-sensor is the subject of tremendous investigation, in response to the industrial demands in the fields of electronics, environmental sciences, and bio-technologies. Zinc oxide, which is transparent to the visible light, is suitable for the purpose because the photon-electron conversion efficiency is very high for ultraviolet (UV) light of the electromagnetic spectrum (below 400 nm in wavelength). In ZnO, their photo-created electrons are stored in the form of “charge-neutral” states, so that an additional contacting layer (so-called a Schottky electrode) is indispensable to extract these as current from the surface of ZnO.

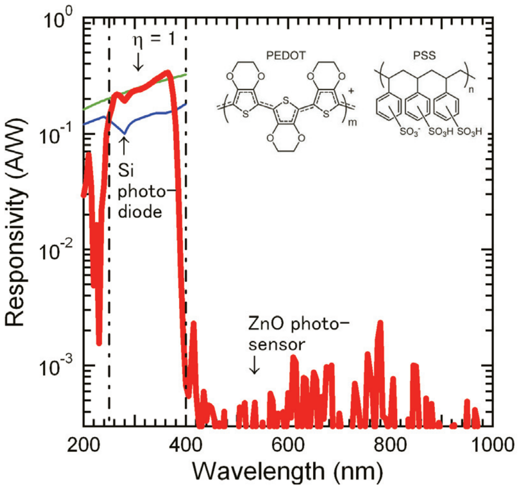


Fig. 1: Spectral response of the PEDOT:PSS/ZnO photo-sensor at V=0 with its molecular structure in the inset. Also shown for comparison are the spectrum for a Si photo-sensor and a “100%-efficiency-line”.

In this news-letter, we report the high-performance photo-sensor using a transparent conducting polymer, poly(3,4-ethylenedioxythiophene) poly(styrenesulfonate) (PEDOT:PSS) as a Schottky contact, which is compatible to simple spin-coating process[1]. The chemical 2structure of PEDOT:PSS is shown in Fig. 1. The use of the *transparent* organic contact is advantageous because the illuminated light is efficiently delivered to the active layer of the ZnO-based sensor without sizable loss at the contacting layer. Besides, our ZnO photo-sensor can very efficiently suppress the noise level, so that it can detect even very small flux at UV photons very sensitively, as were characterized by the external quantum efficiency (conversion efficiency from photon to electron) as high as 100% in the UV region and a visible rejection ratio of 1000. Because of the low cost and easy-to-make process, this device is promising for the application of UV light detection [2]. Work was conducted under the collaboration with M. Nakano, A. Tsukazaki, A. Ohtomo, and T. Fukumura at IMR, Tohoku Univ. and people in ROHM Corp.

References:
[1] M. Nakano, *et. al.*, Appl. Phys. Lett. **91**, 142113 (2007)
[2] M. Nakano, *et. al.*, Appl. Phys. Lett. in press.

Proceedings of the National Academy of Science 2008

D. Pan, A. Inoue, T. Sakurai and M. W. Chen

"Experimental Characterization of Shear Transformation Zones for Plastic Flow of Bulk Metallic Glasses"

The mechanical behavior of disorder solids, such as bulk metallic glasses (BMGs), has received increasingly intense scientific and technological interests. Nevertheless, the underlying physical processes of dynamics and rheology of these solids are still poorly known. Recently, a cooperative shearing model (CSM) of STZs by Johnson and Samwer (***Phys Rev Lett* 95**, 195501(2005)) has been shown to provide an effective interpretation of low temperature plasticity in metallic glasses. In the Johnson-Samwer model, the mechanical behavior of BMGs is intrinsically dependent on the actual volumes of STZs. Despite the intense theoretical and numerical efforts to identify STZ volumes of BMGs, an experimental quantitative measurement of the STZ volumes is missing. In this work, we developed an experimental method to characterize the STZs of BMGs based on the Johnson-Sawmer CSM. The accordance between measured STZ volumes and those predicted by theoretical analysis and MD simulations unambiguously demonstrates that the plastic deformation of metallic glasses occurs upon cooperative shearing of unstable clusters of atoms, instead of individual atom motion. The experiments presented herein pave a new way to gain a quantitative insight into the atomic-scale mechanisms of BMG mechanical behavior and the physical processes in the dynamics and rheology of a plentiful variety of noncrystalline solids.

From the Johnson-Samwer CSM, we derived the STZ volume, $\Omega = kT / C'mH$, where k is Boltzmann constant, T is temperature, C' is a constant, m is strain rate sensistivity, H is hardness. In this study, six BMGs ($Pd_{40}Ni_{40}P_{20}$, $Pt_{57.5}Cu_{14.7}Ni_{5.3}P_{22.5}$, $Cu_{60}Hf_{25}Ti_{15}$, $Zr_{55}Cu_{25}Ni_{10}Al_{10}$, $Ni_{53}Nb_{20}Ti_{10}Zr_{8}Co_{6}Cu_{3}$, and $Zr_{44}Cu_{44}Al_{6}Ag_{6}$) were selected as model systems to represent a wide variety of chemical compositions, mechanical and physical properties in the BMG family. As shown in **Figs. 1a** and **1b**, the mild rate dependence of hardness of BMGs was successfully measured by our rate-jump nanoindentation method. Hence, the rate sensitivity is extracted for calculation of STZ volume. The determined STZ sizes of the selected BMGs vary from 2.5 to 6.6 nm^3, or about 200-700 atoms. Strikingly, the measured STZ sizes in this study agree well with those predicted by theoretical analysis and MD simulations, which clearly demonstrates that the plastic yielding of metallic glasses occurs upon cooperative shearing of unstable clusters of atoms, viz. STZs, instead of individual atom motion under shear stresses. Moreover, our experiments demonstrated that the measured STZ volumes correlate well with Poisson's ratio (**Fig. 1c**), suggesting an intrinsic relationship between BMG ductility and their atomic structures. ((***PNAS***) as an Early Edition article)

Mingwei Chen (Email: mwchen@imr.tohoku.ac.jp)

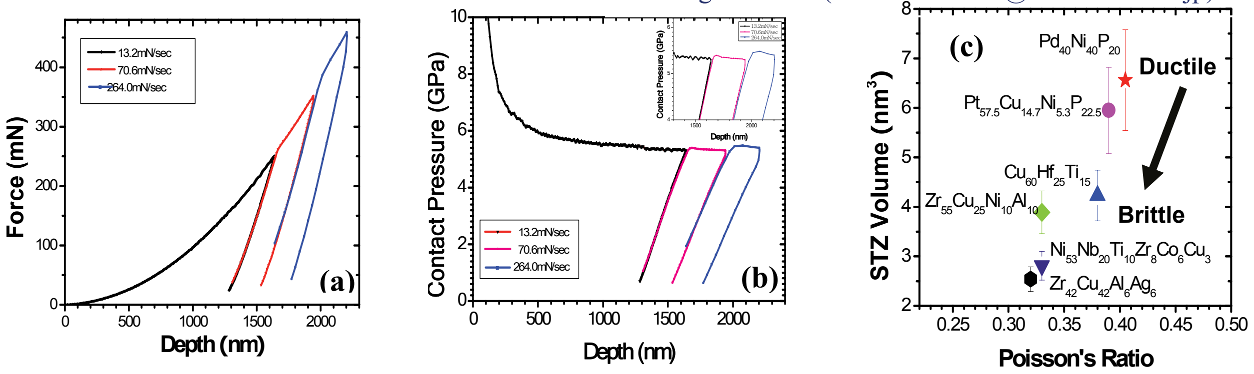
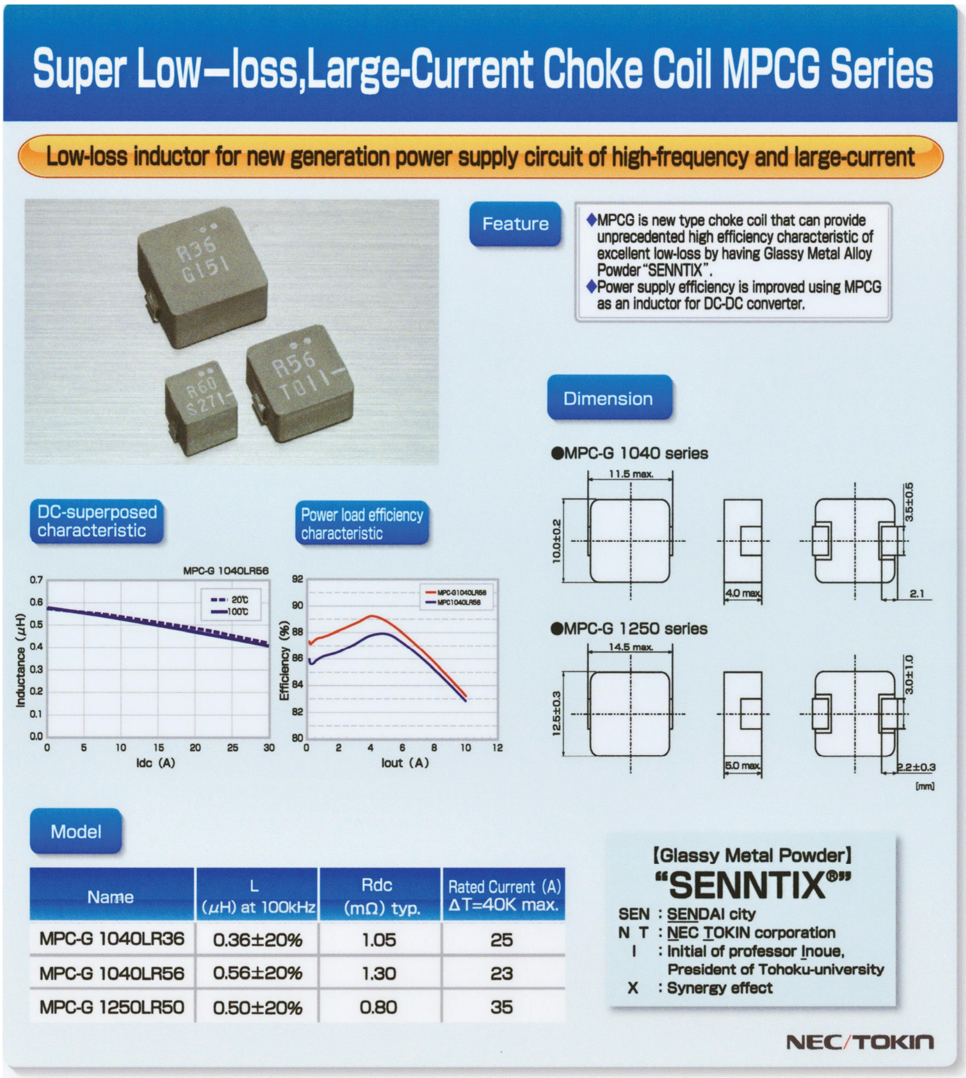


Figure 1 (a) P-h curves at various loading rates by nanoindentation; (b) Corresponding H-h distributions of (a); (c) STZ volume correlation with ductility.

Akihisa Inoue

Commercialization of Fe-based Soft Magnetic Bulk Glassy Alloys

Recently, *Inoue group* developed new type of soft magnetic powder cores based on Fe-Nb-B-Si and Fe-Nb-B-Si-P systems in collaboration with NEC TOKIN Corporation. The new magnetic powder cores have been named as “SENNTIX” and exhibit the lowest core losses among all kinds of magnetic powder cores developed up to date. “SENNTIX-II” powder cores in Fe-Nb-B-Si-P system has enabled us to reduce more than 50 % core loss from existing metal powder and save thermal issue at personal computer board, resulting in the significant extension of battery life time of Note Personal Computer. Therefore, the “SENNTIX” powder cores have been supported as “Next Generation 2009 Reference Design” by major power international corporation suppliers. As a result, the “SENNTIX” powder cores have been produced on a large scale of several million pieces per month at NEC TOKIN factories in Vietnam and China



Super Low–loss,Large-Current Choke Coil MPCG Series

Low-loss inductor for new generation power supply circuit of high-frequency and large-current

Feature

◆MPCG is new type choke coil that can provide unprecedented high efficiency characteristic of excellent low-loss by having Glassy Metal Alloy Powder“SENNTIX”.

◆Power supply efficiency is improved using MPCG as an inductor for DC-DC converter.

Dimension

●MPC-G 1040 series

●MPC-G 1250 series

DC-superposed characteristic

Power load efficiency characteristic

Model

Name	L (μH) at 100kHz	Rdc (mΩ) typ.	Rated Current (A) ΔT=40K max.
MPC-G 1040LR36	0.36±20%	1.05	25
MPC-G 1040LR56	0.56±20%	1.30	23
MPC-G 1250LR50	0.50±20%	0.80	35

【Glassy Metal Powder】

“SENNTIX®”

SEN : SENDAI city
N T : NEC TOKIN corporation
I : Initial of professor Inoue, President of Tohoku-university
X : Synergy effect

NEC/TOKIN

Pictures of the commercialized TOKIN products developed by Inoue group

Dr. Peter V. Shusko's University Research Fellowship (URF) of the Royal Society

The WPI-AIMR is pleased to announce that Dr. Peter V. Sushko, Associate Professor of WPI-AIMR（p.sushko@ucl.ac.uk）has been awarded a prestigious University Research Fellowship (URF) of the Royal Society, which is the UK National Academy of Sciences established in 1660 **(http://royalsociety.org)**.

The URF scheme "aims to provide outstanding scientists, who should have the potential to become leaders in their chosen field, with the opportunity to build an independent research career". The Fellowship offers salary and research funds for a Fellow initially for 5 years followed by an extension for 3 years and, in exceptional circumstances, a further extension for another 2 years.

The Royal Society URF is a highly competitive scheme of international standing. It is opened to all citizens of the European Economic Area and Switzerland as wells as to all those who obtained a PhD degree from the universities of these countries or worked there as a researcher for at least two years. Approximately 30 Fellowships are awarded each year in all fields of natural science including agriculture, computer science, mathematics, physics, chemistry, biology, materials science, technology, medical, and engineering sciences.

Dr. Sushko's research project was awarded 0.5 M British pounds (¥100 M, $0.92 M) over initial five years and it is one of 7 condensed matter physics and materials science proposals supported in the 2007 call. He will work on computational studies of the electron gas in quasi-two-dimensional systems including layered inorganic electrides and heterostructures of insulating oxides. The latter part correlates with and was inspired by the experimental work carried out in the laboratory of Professor Kawasaki, WPI member.

Dr. Sushko will maintain his ties with the WPI-AIMR as Adjunct Associate Professor and we would like to congratulate him and his advisor, Professor Alex Shluger, WPI-AIMR Principal Investigator, with the award and wish them productive research in collaboration with other WPI members in the years to come.

The results of the 2008 International Physics Olympiad

http://ipho2008.hnue.edu.vn/Competition/Results/

In the end of July, the 39th International Physics Olympiad was held in Hanoi, Vietnam, with 84 countries participated.
The results are tabulated below.
A few observations; 1) P. R. of China is usually number one for a number of years. 2) Among the western countries, USA and Russia are strong. 3) Quite a few students of USA, Canada, Australia teams are of Asian origin.

calculated by JSF

2008

Subject (Entry per country) Total		The # of medals	JPN	CHN	KOR	PRK	TWN	SGP	THA	AUS	VNM	IDN	IND	IRN	ISR	TUR	KAZ	USA	CAN	GBR	FRA	GER	ITA	RUS
Mathematics	Gold	43	2	5	4	2	2		2		2			1		3	1	4				1		6
(6)	Silver	84	3	1	2	4	4	1	3	5	2	1		5	1	1	2	2	2	4	1	2	3	
535	Bronze	111	1					3	1	1	2	1	6		2	2	3		4	2	4	3	3	
Chemistry	Gold	30		4	3		2	1	1		2	1		1								1		4
(4)	Silver	53					1	1	3	3		1	3	2	1	2	4	1	1	2	1		2	
257	Bronze	79	4		1			2		1	2	1	1	1	2	2		3	3	2	3	3	2	
Biology	Gold	23		2	3		4	2	3	2			1					4				1		
(4)	Silver	47	3	2	1			2	1	2		2	2	2		1			2	3	3	1		1
220	Bronze	68	1								3	2	1	2		2	1		2	1	1	2	2	3
Physics	Gold	46	1	5	4		5	1	3		4	2	4			1		4	1			1		3
(5)	Silver	47	1		1			3	2	1		2	1		1	1		1	2		4	1	2	1
370	Bronze	78	1					1		3	1	1		5	3	1	2		2	4	1	3		1
Information	Gold	24	1	3	1		2		2	1		1						2	1			1		2
(4)	Silver	47	1	1	3		1	1	1	1	2						2	2		3			1	2
283	Bronze	69	2				1	3	1	1	2	3	3			2			2		1	2	2	

2007

Subject (Entry per country) Total		The # of medals	JPN	CHN	KOR	PRK	TWN	SGP	THA	AUS	VNM	IDN	IND	IRN	ISR	TUR	KAZ	USA	CAN	GBR	FRA	GER	ITA	RUS
Mathematics	Gold	39	2	4	2		2		1		3			1				2		1	1	1	1	5
(6)	Silver	83	4	2	4		3		3		3	1	3	3				3	1			3	1	1
520	Bronze	131					1	5	2					2	3			1	3	3	2	1	3	
Chemistry	Gold	31		4	3		2		1		1		2	1					1		1	2		4
(4)	Silver	58			1		2	2	3		2	2	1	1	1			3		2		2	1	
256	Bronze	72	4					2				2	1	1	1			1	1	2	1		2	
Biology	Gold	20		4	4		2		2			1	1					4		2				
(4)	Silver	43	1					4	2		1	1	3	4					2	1		1		1
192	Bronze	54	3				2				1	1							2	1	3	2		1
Physics	Gold	37	2	4	2		1	2	1		2	1	2	2				2	2	1	1			3
(5)	Silver	46	2	1	3		2	1	2		2	3	2	2				3		1	3	5		1
327	Bronze	51	1				2	2	2			1		1					2	1	1		2	
Information	Gold	25	1	4			2		1					1				2				1		3
(4)	Silver	48	1		2		1	1	3		1		1	2	4			1					2	1
285	Bronze	72	1		2		1	2			3	2	2					1	2	2	3		2	

2006

Subject (Entry per country) Total		The # of medals	JPN	CHN	KOR	PRK	TWN	SGP	THA	AUS	VNM	IDN	IND	IRN	ISR	TUR	KAZ	USA	CAN	GBR	FRA	GER	ITA	RUS
Mathematics	Gold	42	2	6	4		1		1		2			3				2			1	3	2	3
(6)	Silver	89	3		2		5	2	2		2			3	3			4	5	4			2	3
498	Bronze	122	1					3	2		2		5		1				1		3	1		
Chemistry	Gold	28	1	4	3		3	1	1		2		1						1			1		3
(4)	Silver	56	3		1		1	2	2		2	1	2	2				3	2	1	2	2		1
255	Bronze	81						1	1			3	1	2	1			1	1	3	1	1	1	
Biology	Gold	20		4	3		3	2	3									2						
(4)	Silver	40			1		1	2	1			2	3	3				2	2	3		2		2
185	Bronze	61	3								4	2	1	1					2	1		2		2
Physics	Gold	37		5	4		3	1	1			4	2	1				4	2			2		2
(5)	Silver	49	1		1		2	1	3			1		4	2			1			2	2		3
398	Bronze	82	3					3			4				2				1	5	3	1	4	
Information	Gold	24	2	4	1									1				1						3
(4)	Silver	51			3		3				1		2	2				3	3		1			
284	Bronze	70	1				1	2	3		3		2		3				1	2	2	2	2	1

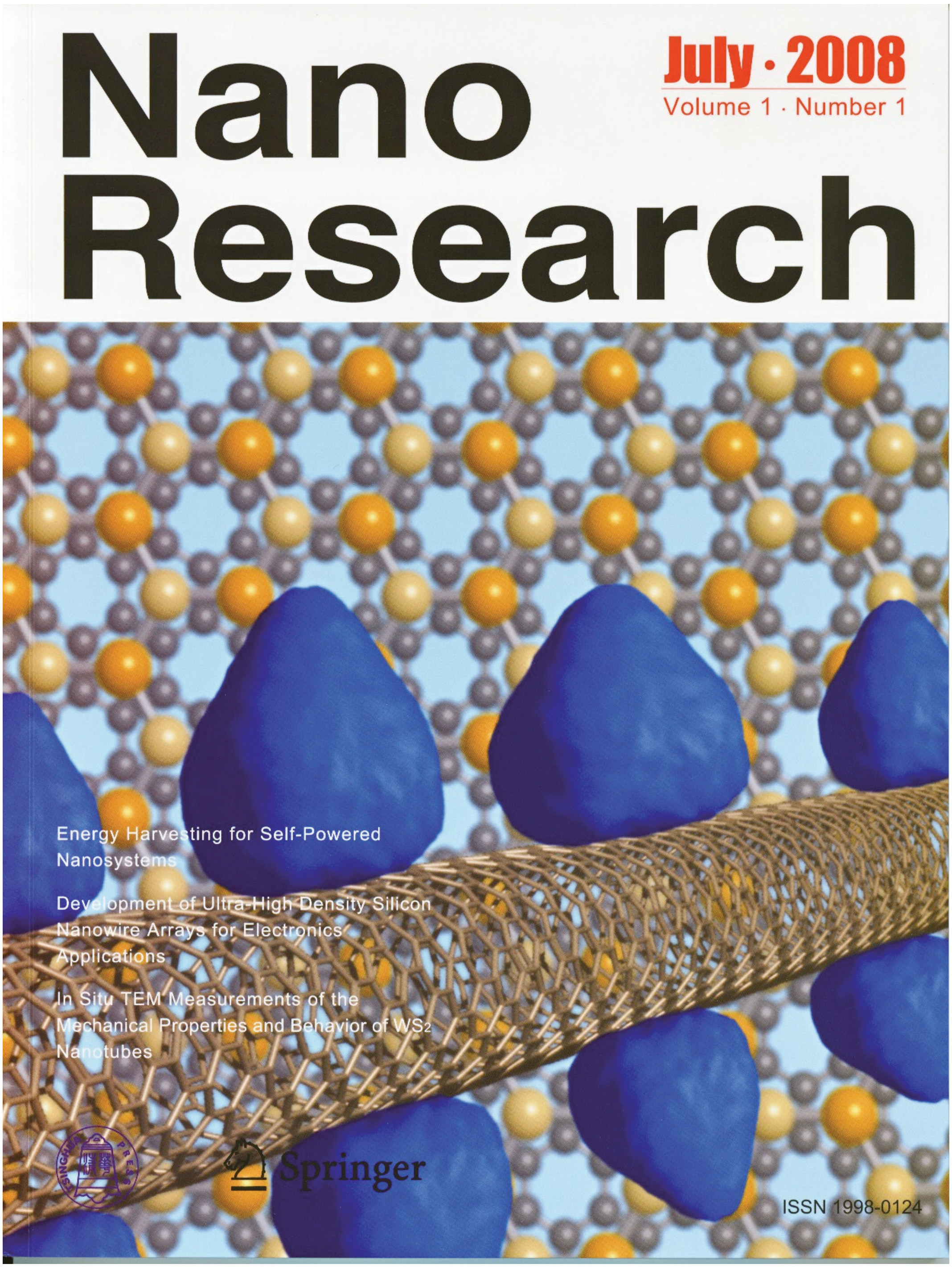
External Research Grant List of Research Staff (As of September 1, 2008)

(Unit: thousand yen)

The Name of Researchers	**Total**	**Grant-in-aid for Scientific Research; "KAKENHI"**						**Joint Research**	**Commissioned Research**	**Competitive research funds** in Commissioned Research (Excepted to KAKENHI)
		Specially Promoted Research	Scientific Research on Priority Areas	Scientific Research (S)	Scientific Research (A)	Young Scientists (A)	Others			
INOUE, Akihisa	**131,853**		3,000	89,310				39,543		
LOUZGUINE, Dmitri V.	**18,490**		16,800				1,690			
TAKAHASHI, Takashi	**68,500**						3,500		65,000	65,000
SOUMA, Seigo	**12,090**					12,090				
RICHARD, Pierre	**1,651**						1,651			
KAWASAKI, Masashi	**127,865**						900	12,230	114,735	114,735
ITAYA, Kingo	**48,682**				27,690				20,992	3,000
IKEDA, Susumu	**2,080**						2,080			
KUZUME, Akiyoshi	**390**						390			
YAMADA, Kazuyoshi	**22,531**	1,700	4,040	2,000			3,970		10,821	8,910
TANIGAKI, Katsumi	**47,900**		41,200		3,900		2,500	300		
NOUCHI, Ryo	**2,860**						2,860			
OHMI, Tadahiro	**132,707**	108,160						24,547		
ESASHI, Masayoshi	**89,281**			31,720				42,221	15,340	
AKIYAMA, Kotone	**4,250**		2,300				1,950			
YOSHIDA, Shinya	**1,729**						1,729			
NAKAZAWA, Masataka	**80,470**	80,470								
MIYAZAKI, Terunobu	**54,947**								54,947	
TOKUYAMA, Michio	**1,040**						1,040			
SHIMOMURA, Masatsugu	**26,790**		1,300		7,540		2,400	7,550	8,000	8,000
ISHII, Daisuke	**1,755**						1,755			
YAMAGUCHI, Masahiko	**15,840**			14,040			1,800			
YASUI, Yoshizumi	**2,210**						2,210			
ADSCHIRI, Tadafumi	**164,589**			45,370				77,099	42,120	42,120
MINAMI, Kimitaka	**8,000**								8,000	
CHEN, Mingwei	**1,100**						1,100			
FUJITA, Takeshi	**3,250**						3,250			
NISHI, Toshio	**1,690**							1,690		
NAKAJIMA, Ken	**8,970**					8,970				
TSUKADA, Masaru	**43,600**		35,000						8,600	8,600
HASHIZUME, Tomihiro	**75,100**							55,100	20,000	
HIITOSUGI, Taro	**19,600**								19,600	19,600
IKUHARA, Yuichi	**24,041**		18,200		5,300				541	
TSUKIMOTO, Susumu	**3,000**		3,000							
SAITO, Mitsuhiro	**1,716**						1,716			
SUSHKO, Peter V.	**3,916**						1,716	2,200		
	1,254,483	**190,330**	**124,840**	**182,440**	**44,430**	**21,060**	**40,207**	**262,480**	**388,696**	**269,965**

Inauguration of new journal “Nano Research”

Dr. Qikun Xue, WPI-AIMR Principal Investigator, Cheung Kong Professor of Tsinghua University, and academician of Chinese academy of Sciences, P.R. China, has founded a new journal “Nano Research” and will run it as Editor-in-Chief together with Professor Hongjie Dai, Stanford University. The monthly research journal is published by Springer. Good luck!!!



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Research Prospect

Surface Chemical Reactivities Modulated by Quantum Size Effect

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Abstract

We report on a direct observation of a quantum reactivity with respect to the amounts of O_2 adsorbed and the rates of surface oxidation as a function of film thickness on ultrathin (2~6 nm) Pb mesas by scanning tunneling microscopy. Simultaneous spectroscopic measurements on the electronic structures reveal a quantum oscillation that originates from quantum well states of the mesas, as a generalization of the Fabry-Pérot modes of confined electron waves. This quantum reactivity is further confirmed by thickness-directed adsorption and self-assembly of cobalt phthalocyanine (CoPc) molecules. The work provides a novel approach for nanostructure tuning of surface reactivities and rational design of heterogeneous catalysts.

1. Introduction

For a given solid, except for surface irregularities such as impurities and defects, surface reactivity is often solely determined by its crystallographic orientation. At a reduced size, however, particularly when the characteristic length scale enters the nanometer regime, the situation can change considerably from that of the bulk [1,2]. For example, in nature Au is the most stable metal, yet an Au nanoparticle becomes chemically reactive (when the size is ~3nm), and can catalyze the oxidation of CO [1]. Thin films are another such example where size-dependent surface chemical activities have been observed, when the thickness is in the nanometer scale [3,4]. Such properties of nanostructured materials are usually attributed to the quantum size effects (QSE). However, the materials used in most previous studies suffer from size fluctuation, resulting in not well-defined material properties, and hence the evidences for the QSE are at best qualitative [4]. In the case of thin films, a far more convincing proof of the QSE would be the direct observation of an oscillatory dependence of the chemical reactivities on the film thickness, which is reported here. Although bulk Pb is not a catalyst, it may function as a catalyst at the reduced size, just like the Au [1]. More importantly, a quantum modulation of the chemical reactivity is a general phenomenon, reflecting the quantum size effect in the electronic states, which should not depend on any particular material.

Our Pb mesa samples were prepared on clean Si(111)-7×7 surfaces by the molecular beam epitaxy (MBE) technique. Semiconductor silicon was chosen as the substrate to achieve the required electron confinement within the Pb mesas [5-8]. Figure 1a shows a typical scanning tunneling microscopy (STM) image of the mesas. All mesas have flattop geometry, presumably driven by surface energy minimization, but their bottom extends laterally over several (typically 5 to 10) atomic steps on the Si substrates. For the mesa shown in Fig. 1a, five consecutive thicknesses, 11 to 15 ML, are present. The high resolution STM images (Figs. 1c and 1d) clearly reveal that the top surface is exclusively (111) and of single domain, regardless of thickness variation. Such a unique geometry enables us simultaneously measure the electronic structure, oxygen adsorption, and oxidation of the Pb films of *different* thicknesses under identical experimental conditions.

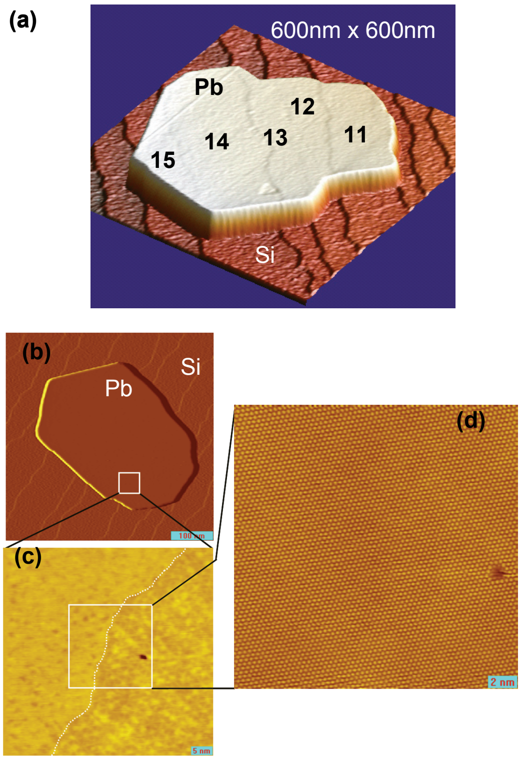

Figure 1. The Pb(111) mesa substrate used for this study. (a) STM image of a typical Pb mesa grown on the Si(111)-7×7 substrate, shown in a three-dimensional view. From right to left, the thickness varies from 10 to 16 ML. (b) Two dimensional view of the wedge shaped Pb island. (c) Zoom-in STM image from (b) showing the atomically flat nature of the Pb mesa surface. The dotted line indicates the step at the Pb/Si interface. (d) Atomic resolution STM image zoomed-in from (c) showing that the Pb surfaces are (111)-oriented with a lattice constant of 0.35 nm. This kind of images could be obtained at any part of the mesa in Fig. 1(a). All images were recorded at 80K with a tunneling current of 100pA.

Single crystal Pb is highly resistant to oxygen [9]: appreciable oxidation takes place only at relatively high temperature (≥370K) or at considerable oxygen coverage at room temperature, which turns out to have destroyed the geometry of the sample in Fig. 1a. To protect the wedge-shaped mesas from possible geometry damage by high-temperature annealing, we have developed a two-step approach: (i) low temperature (~100K) O_2 adsorption, followed by (ii) annealing at elevated temperatures to above 220K.

2. Results and Discussion

Figure 2 shows the STM image of a mesa surface (the mesa is on the same Si substrate and is nearby from the mesa shown in Fig. 1a) after 60L oxygen exposure at a substrate temperature of ~100K. The image contains four different layer thicknesses (9 to 12ML). The bright spots have a typical size of approximately 1.2 nm, and are identified as chemisorbed oxygen clusters based on the scanning tunneling spectroscopy (STS) where a strong binding of the adsorbed clusters and the surface is observed [10,11]. Because the clusters are irregular both in size and shape, their exact chemical nature is currently unknown. Despite that all the mesas are (111) oriented, here oxygen adsorption exhibits a clear thickness dependence; the areal density of the adsorbed spots on the even layers are always larger than that on the odd layers, while adsorption in the same layer is essentially homogeneous. Figure 2a shows the thickness dependence of the adsorbed oxygen (averaged over 10 samples). Except for an anomaly at 17ML, which will be discussed later, a well-defined up-down oscillation with a period of 2ML in the adsorbed oxygen coverage is immediately evident.

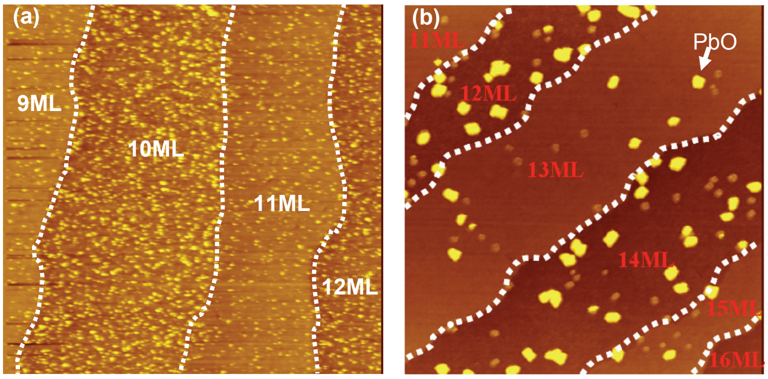

Figure 2. Thickness-dependent oscillatory adsorption of oxygen and oxidation. (a) STM image (339×339 nm^2) of an oxygen adsorbed surface after 60L oxygen exposure at 100K. (b) STM image (50×50 nm^2) of the oxidized surface showing the formation of PbO monoxides at six (from 11ML to 16ML) thicknesses. The sample was first exposed to 60L oxygen exposure at 100K and then warmed up to room temperature with additional oxygen exposure of 120L. All images were recorded at 80K with a tunneling current of 100pA.

Remarkably, an oscillatory behavior in surface oxidation (Fig. 2b) was observed, when the samples were warmed up to room temperature with an additional oxygen exposure of 120L to enhance the oxidation effect. Based on the anisotropic shape and linear chain structure in high resolution STM images (not shown), the yellowish rectangular islands in Fig. 2b are identified as massicot monoxides (PbO) [9]. Variable-temperature STM experiment reveals that the adsorbed oxygen clusters are stable up to 180K, above which the formation of the monoxide will take place. The monoxide always develops from the previously existing oxygen clusters, and grows by forming depressed holes of one monolayer deep around these clusters, suggesting that no significant diffusion of the adsorbed oxygen clusters had taken place, and that only Pb atoms around the oxygen clusters were involved in the initial monoxide formation. Surprisingly, if the same amount of oxygen was exposed to the surface at room temperature, neither adsorbed oxygen nor surface oxides were observed, and the Pb surface remains its intrinsic (111)-1×1 structure.

We have taken high-resolution STM images of the surfaces for all oxygen coverages at the adsorption temperature, and separately at the observation temperatures after annealing. The results indicate that localized electronic states associated with surface steps and defects (most of which are dislocations) do not play any significant role in either adsorption or oxidation. Strain is another factor to be considered, as epitaxial strain could lead to different layer spacings along the normal direction of the film. However, lattice relaxation usually takes place in the first a few layers near the Pb/Si interface, while near the top surface layer spacing within the mesa is nearly the same as that of bulk Pb [12,13]. Therefore, strain effect should not contribute significantly to the reactivity variation. Furthermore, if strain is indeed important, surface oxidation should exhibit a monotonic, rather than an oscillatory, behavior with thickness. Note that, on bulk Pb(111) surfaces, such an oscillatory oxidation behavior does not exist. It can thus be concluded that the film thickness is the deterministic factor for the variation of the surface reactivity observed here.

One may speculate that surface kinetic process such as thickness-dependent diffusion may play some important role in the oscillations. We measured the areal density of oxides as a function of thickness (the black squares in Fig. 3a), and found that the

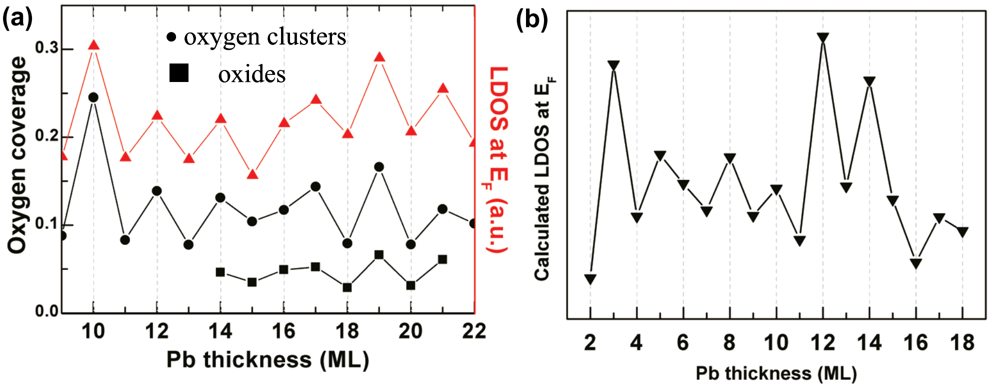

Figure 3. Correlation between the coverage of adsorbed oxygen and the LDOS. (a) The measured adsorbed oxygen coverage (black dots for clusters and black squares for oxides) and the LDOS at the Fermi energy (red triangles) as a function of the Pb film thickness at 100K. The oxygen coverage is defined as the areal density of adsorbed clusters (oxides) on the surface of Pb islands, measured as the integrated volume of these clusters (oxides) per surface unit area, assuming that the volume density of oxygen molecules are uniform and the same for different clusters. In the volume measurement by STM, a spherical shape of clusters was assumed. (b) The calculated LDOS at the Fermi energy as a function of the film thickness by first-principles method.

absolute ratio of the amounts of oxides is equal to that of the adsorbed oxygen clusters almost for any two-adjacent-thicknesses (except for 17ML). For oxidation, some clusters have to diffuse and coalesce to form oxides while some decompose and desorb from the surfaces. This observation suggests that the diffusion of oxygen species involved in oxidation should not play a significant role in the oscillating oxidation observed. We cannot rule out a possible column-crossing diffusion, but net flow of the diffusing species should be small according to this measurement. Because of different electronic structures (see Fig. 4a, to be discussed below), the boundary between the adjacent heights should behave like a “step”. If diffusion were important, either denuded zones or preferential adsorption/reaction along the boundaries separating the even and odd layers, like that with usual surface steps and domain boundaries where diffusion resulted structure decoration takes place as clearly observed on the single crystal Pb(111) surface, should have been seen.

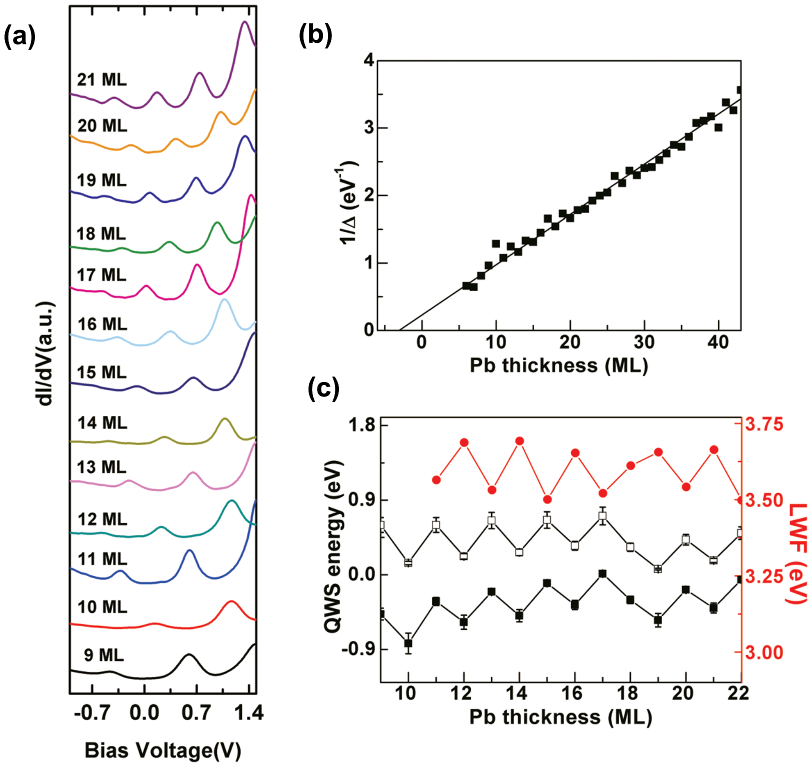

Figure 4. Measurements of the QWS and LWF. (a) A series of dI/dV curves showing the formation of QWS in the Pb mesas. The first QWS peak below and above the Fermi energy (located at zero bias) corresponds to the HOQWS and LUQWS, respectively. (b) Inverse of the energy gap between HOQWS and LUQWS as a function of the Pb film thickness (from 6ML to 43ML). (c) The measured QWS energy (with respect to the Fermi energy) and the LWF, as a function of the film thickness. Open circles and filled squares are the LUQWS and HOQWS, respectively, whereas the red dots are the LWF.

The observed oscillatory reactivity can be preliminarily attributed to the QSE [3,4]. When the thickness of a metal film is comparable to the wavelength (λ_F) of the electrons at the Fermi energy (E_F), the film can be treated as a Fabry-Pérot interferometer of the electron de Broglie waves [15]. For Pb, λ_F=1.06nm, which is nearly 4 times of the inter-planar distance d_0 along the crystallographic [111] direction. This coincidence ($\lambda_F \approx 4d_0$) suggests that, when 1ML of Pb is added or removed, electron interference will change from being constructive to destructive and *vice versa*, leading to a 2ML modulation of the electronic structure [16-20]. More accurate analysis indicates that the exact period should be 1.8ML. The small difference between 2ML and 1.8ML results in a 9ML-beating mode on top of the finer 2ML oscillations. This explains the anomaly observed at 17ML here and in previous studies [18,19]. The great resemblance between QSE in chemical reactivity and QSE in physical transport properties [21-24] is unprecedented, suggesting a unified mechanism possibly originated from the unique behavior of the electrons at or within a small thermal energy window near the E_F.

To further understand the oscillatory reactivity, we have measured the surface local density of states at the E_F [LDOS(E_F)]. The LDOS(E_F) as a function of the film thickness is shown by the red triangles in Fig. 2a, in which a 2ML oscillation, superimposed on a 9ML beating envelope, is clearly seen. The beating node appears at 17ML, and again at 26ML (not shown), in total agreement with that of the surface chemical reactivity (shown by the black dots in Fig. 3a).

Figure 3b shows the thickness-dependent LDOS(E_F) calculated by first-principles method. Qualitatively speaking, experiment and theory are consistent with each other: both indicate an even/odd oscillation and the existence of a 9ML-beating mode. The influence of the electronic structure on the chemical reactivity has been studied theoretically before [25-29]. According to the simplest Newns-Anderson adsorption model [26], as an oxygen molecule approaches the surface of the Pb (which can be treated as a free-electron-like metal), the anti-bonding Π^* state of the O_2 hybridizes with the sp-band of the surface such that the Π^* state broadens into a resonant state. Surface one-electron image potential will shift this resonant state down in energy to below the E_F. This downshift and subsequent filling of the Π^* state leads to the dissociative adsorption. A lower LDOS(E_F) implies that the Pb film has fewer electronic states to respond, whereas a higher LDOS(E_F) implies the film has more electronic states to respond, to the presence of the oxygen. Therefore, a higher LDOS(E_F) means a higher probability in the above hybridization process, causing the Π^* resonance to move to lower energies and to be occupied or, in other words, a higher surface reactivity.

Next, we discuss how the LDOS in a broader energy range would respond to the quantization of the electronic states. Figure 3a shows a series of dI/dV curves in the energy range from −0.9eV to +1.50eV for thicknesses between 9ML and 21ML. The results here reveal clearly the formation of well-defined quantum well states (QWS) in the LDOS, namely, the sharp peaks in Fig. 4a, at every layer thickness. This can be compared to our previous photoemission study [19,23], in which the QWS was only measured in the normal direction to the film surface. The distinctive sharp peaks here are characteristic of the QWS at different quantum numbers. In Fig. 4a, the zero bias corresponds to theE_F. Thus, peaks closest to zero at negative and positive biases correspond to the highest occupied QWS (HOQWS) and lowest unoccupied QWS (LUQWS), respectively. When the film thickness increases, the LUQWS peak moves down to cross E_F and becomes occupied for every two added layers, resulting in a 2ML oscillation. The 17ML film is an exception for which the QWS resides right at E_F. The same was found again at 26ML and 35ML with a 9ML separation, which is nothing but the long wavelength-beating mode discussed earlier. When fitting the inverse of the energy gap (Δ) between the HOQWS and LUQWS, a good linear relationship between 1/Δ and film thickness is obtained, as shown in Fig. 4b [5,7].

Figure 4a further shows that an l ML thickness change can induce an appreciable shift in the QWS energy, typically in the range of several hundreds of a meV, for example, 200 meV between 21ML and 22ML. Because of the large increase of the LDOS at the QWS peak positions, for a given total number of states, the resulting QSE modulation on the electronic structure and hence surface reactivity could be quite significant.

The work function, which is the minimum energy required to emit an electron from surface to vacuum, is thought to be one of the most fundamental properties for surface reactivity. Therefore, it was simultaneously measured here with the STM topographic image [30,31]. The formation of the QWS also leads to an oscillatory local work function (LWF), as shown by the red curve in Fig. 4c. The LWF varies in an energy range between 3.5eV and 3.7eV with the same oscillatory behavior as the HOQWS discussed above: the closer the HOQWS is to the Fermi energy, the smaller the value of the LWF is. This is reasonable because the LWF was measured at a negative sample bias, at which electrons tunneling from HOQWS to the tip usually dominate the current [17].

The above results suggest that an electronic state of the Pb mesa is very much confined to a region of the same thickness, such that the Fabry-Pérot interference of the electron wave can provide a characteristic fingerprint of that thickness [32].

As for the relationship between LWF and QWS, it comes mainly from the spatial distribution of the QWS electrons near the surface. Based on the density functional theory calculations, we find that the decay of the electronic state normal to the surface is much slower than others. For the latter, although they may be closer to E_F, their spatial distributions are much more localized. Because the magnitude of the electron density above the surface is decisive to the tunneling current and hence to the measurement of the LWF, the LWF is predominantly determined by states close to the Brillouin zone center with well-defined QWS.

To examine whether this oscillation behavior is limited only to oxygen, we carried out experiment using very different molecules of cobalt phthalocyanine (CoPc) [33]. The result is shown in Fig. 5. In this case, the thickness-dependent adsorption behavior is even much more obvious; all CoPc molecules diffuse long enough and could reach the energetically favorable regions (12, 14, 17 and 19ML) where stronger oxygen adsorption and oxidation were always observed, to form an ordered self-assembled monolayer, leaving other regions (11, 13, 15, 16 and 18ML) intact (Fig. 5b). With this experiment, the influence thickness-dependent diffusion can safely be ruled out. Moreover, here there is no difficulty in identifying the adsorbed species, the individual CoPc molecules are clearly resolved and identified in the high resolution STM image in Fig. 5c.

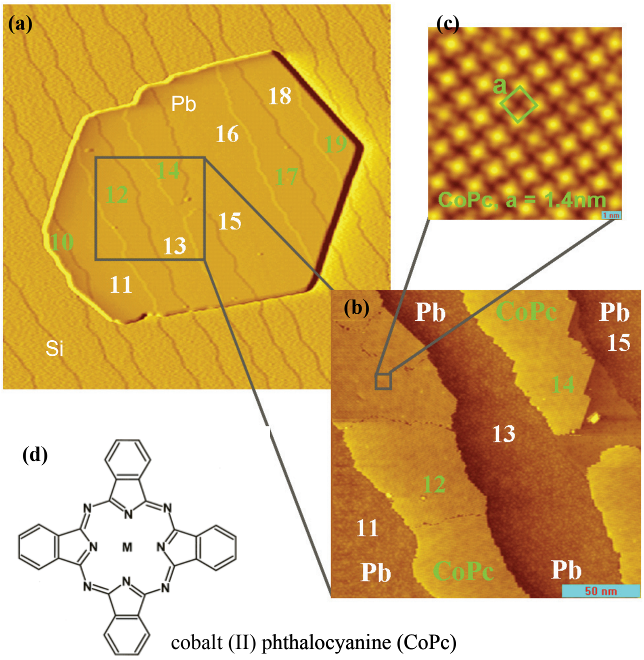

Figure 5. Thickness-dependent oscillating adsorption and self-assembly of CoPc molecules on Pb(111) mesa. (a) STM image (700×700 nm^2) after 0.45ML CoPc molecules were deposited on the Pb mesa surface. (b) STM image (0.5V and 100pA, 200×200 nm^2) zoomed from (a) showing the selective preferential adsorption of CoPc molecules at 12ML and 14ML. Note that molecules are completely missing at 11ML, 13ML and 15ML, where bare Pb surface is present. (c) STM image (-0.2V and 98pA, 11×11nm^2) showing the structure of CoPc molecules and the self-assembled monolayer formed on the Pb(111) surface. (d) The schematic illustration of the CoPc molecule.

3. Conclusion

By synthesizing flat-top Pb mesas on Si(111) substrate, the oscillatory surface reactivity due to quantum size effect is unambiguously demonstrated for the first time by using a two-step oxygen adsorption/annealing method. Our in-depth study further provides quantitative accounts of the correlations between the quantum surface reactivity, the QSE, the surface local density of states, and the local work function. We expect the quantum surface reactivity to be a general phenomenon beyond just Pb and hence has broad applications such as modifying the surface chemistry of metals and to serve as a guide to nano tailoring metal catalysts.

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Theory of Scanning Probe Microscopy and Electron Transport in Nano-Structures

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1. Introduction

Recent progress of nano-technology has been remarkable and much expectation has been arisen for further epoch making developments, but this would be only possible with strong cooperation of basic science and technology, cooperation among different disciplines, that between experiment and theory. Theory really plays an important role for predicting novel functions of nano-structures and make useful proposals of designing and fabricating such systems from the atomic scale.

Scanning Probe Microscopy (SPM) is a family of powerful experimental methods to observe the atomic scale structure and properties of nano-scale materials[1,2] and used as a tool of atom manipulation[3]. In spite of profound information that SPM can in principle provide, it is not quite easy to analyze experimental data without a support from theoretical simulation[4]. This is because the measured quantities by SPM are obtained by a rather strong or subtle atomic scale local interaction between the tip and the sample[5]. In the following sections, some topics will be introduced from results obtained by Project of "Development of Versatile Scanning Probe Simulator" supported by JST from October 2004 to March 2008 conducted by author's group.

We also discuss some topics of the quantum transport through molecules connected to metallic electrodes. Remarkable natures of coherent electron transport are predicted including the nature of the resonant tunneling via molecular levels and a large loop current induced by the source-drain current. With the coupling of the electron motion to the molecular vibrations or electro-magnetic environment, dissipative or hopping transport becomes prevailing. Transition from the coherent to dissipative regime is also discussed.

2 Models of the tip

We have developed a software which can generate large scale atomistic models of the tip as well as its coarse grained continuum model in a computer. Various structures of the tip limited by facets can be formed from the crystal atomic structure freely so as to minimize the surface energy of the tip using a convenient GUI (Graphycal User Interface). Reconstruction of the top most atoms can be made with evaluating the total surface energy of the tip.

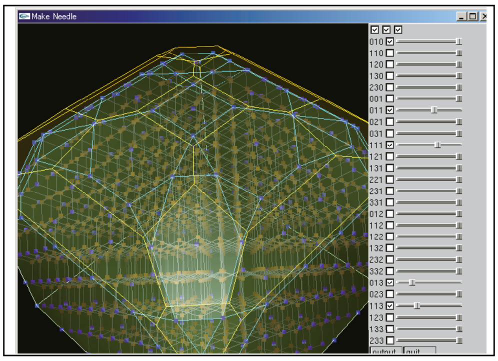

Figure 1. A GUI frame for designing the tip atomic structure by cutting facets manually by the right bars.

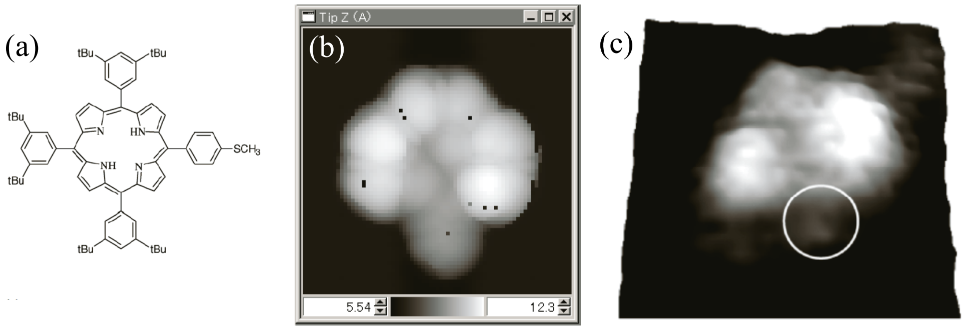

Figure 2. (a) Structure, (b) simulated and (c)experimental AFM image of MSTBPP.

3. Simulation of AFM images

With use of the hydrogen atom tip, the AFM image of methylthiophenyl-tris- t-buthyl phenyl-porphyrin (MSTBPP) is simulated. As seen in Fig.2, the theoretical image reproduces the experimental observation fairly well[6]. In this simulation, the molecular shape and position are fixed. However, if they are allowed to deform by a strong repulsive force by the tip, regular images are gradually lost, and we observe an interesting deformation behavior of the sample molecule.

Fig.3 (a) and (b) are the simulated frequency shift image and the dissipation image of the chemisorbed methyl group on a hydrogenated Si(100) dimmer surface, respectively[7]. The model of the tip used is Si_4H_9 cluster model. The angle of the bond connecting the methyl to the Si atom is easily bent by a repulsive force by the tip. Therefore the image is rather vague and hydrogen atom can be observed only as a dark crescent area. The dissipation image produces a rather sharp shape but the analysis is difficult without theoretical simulation.

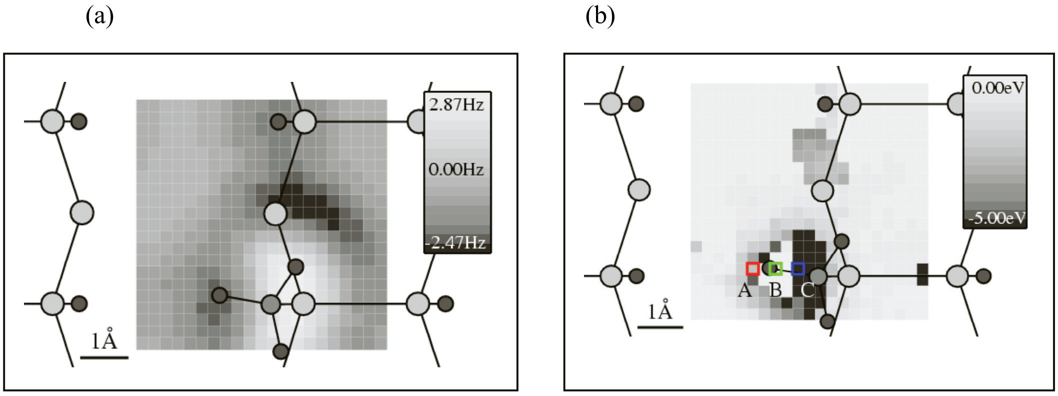

Figure 3. NcAFM image of methyl group chemisorbed on the dimer Si atom of hydrogenated Si(100) surface taken by the frequency shift (a) and the dissipated energy (b).

4. Theory of SPM in water

There are several difficult problems for the simulation of dynamic AFM in liquids. First, the cantilever bending oscillation as a flexible elastic body should be solved simultaneously with fluid dynamics as shown in Fig.4. Fig.5 shows a resonace curve of rectangular silicon slab cantilever in water. We can see that the resonant frequency is lowered by about 1/5, and the width of the resonance is enlarged by the order of 10^3. It is remarkable that the amplitude of the bending angle of the tip apex does not decay so much at the higher frequency side, which reproduces the experimental features.

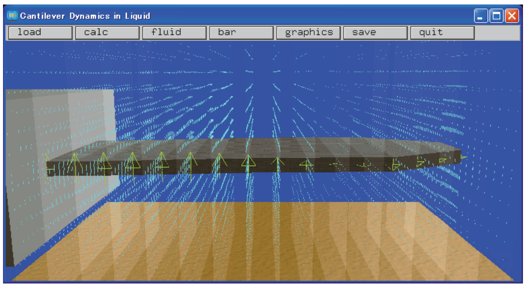

Figure 4. Oscillation of cantilever in water.

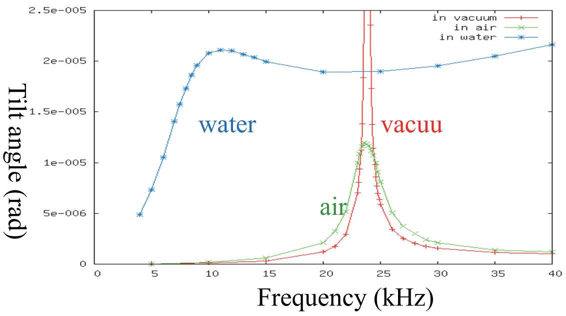

Figure 5. Resonant curves of the thin Si rectangular cantilever in water, air and in vacuum.

When a tip approaches to the sample, it feels the force mediated by water molecules. This effect to the cantilever motion determines the AFM image in liquids. Fig.6 shows the three-dimensional force map of the CNT(carbon nano-tube) tip over a mica surface in water. It can be seen that the oscillatory solvation force develops near the surface, but its phase sensitively depends on the lateral position of the tip. The oscillatory solvation force is caused by the layer-like distribution of water molecules near the sample and the tip surfaces as seen in Fig. 6(b).

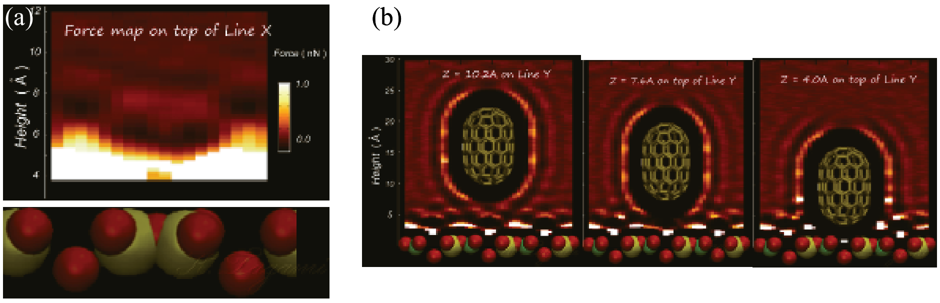

Figure 6. (a)The 3D force map of mica by CNT tip and (b) The layer structure of the distribution of water molecules near the tip and mica.

5. SPM simulation for protein molecules

Mechanical deformation and stress effect on various physical and chemical properties of proteins provide rich information on the functionality of protein molecules, which can be elucidated by the theoretical simulation [8]. Not only AFM images, but also the tip force-distance curve reveal important structural, mechanical, chemical properties of protein molecules, and the interpretation of these are major target of the simulation.

As an example, a constant force AFM image of a single fragment collagen molecule adsorbed on a graphite substrate is calculated both under ultra high vacuum and in a wet condition[9]. As the tip model for this simulation, a narrow capped carbon nano-tube is adopted as shown in Fig.7. The effect of the water molecules on the tip-sample interaction force immersing the collagen has been also investigated.

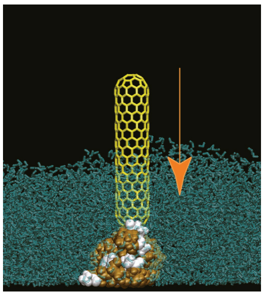

Figure 7. The simulation model of CNT tip and the callagen sample immersed in water.

The image of Fig. 8 shows a nodal structure, which reflects the triple helix structure of the collagen. In the case of the system immersed in water the amplitude and phase of the oscillatory solvation force is different between on top of the collagen molecule and on top of the graphite surface, which requires careful analyses of the image [8].

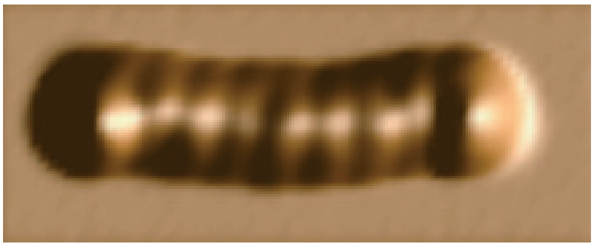

Figure 8. The simulated constant force mode AFM of a short collagen model.

Green fluorescent protein (GFP) emits green fluorescent light when illuminated with blue light. It has been found that the fluorescent activity of the chromophore, which is located at the hydrophobic cavity inside the β-barrel structure, is remarkably suppressed on the compression by the tip. We performed the simulation of the compression process of the GFP by the all-atom molecular mechanics with a hybrid ONIOM9 (QM/QM) calculation [9]. Upon compression the hydrogen bond network around the chromophore is broken, and the potential barrier for the conformation change disappears opening a non-radiative reaction pathway, which causes the quenching of the fluorescence.

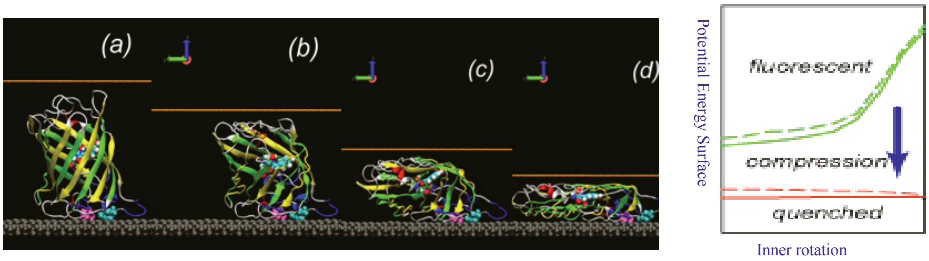

Figure 9. Cpmpression of GFP and associated change of the potential energy surface of excited (dashed line) and ground state (full line).

6. Coherent transport through molecular bridges

The transport through molecular bridges is strongly influenced by the connecting part to the electrodes. An example has been found in the tape-porphyrin molecules[10]. Tape porphyrin is a sort of the oligomer of the porphyrin, which shows the vanishing of the HOMO-LUMO gap for a very long chain length. We investigated four different linkage structures of the tape-porphyrin to the gold electrodes as shown in Fig.10. For all the cases, the numbers of the porphyrin molecules in the chain is assumed to be eight (n=6). The calculated results of the transmission spectra are shown in Fig.11. It is remarkable that only a small difference of the linkage part dramatically influences the conductance of the molecular bridge. Namely among the four bridges from A through D shown in Fig.10, the case B shows the largest conductance, because there is prominent transmission peak very close to the Au electrode Fermi level.

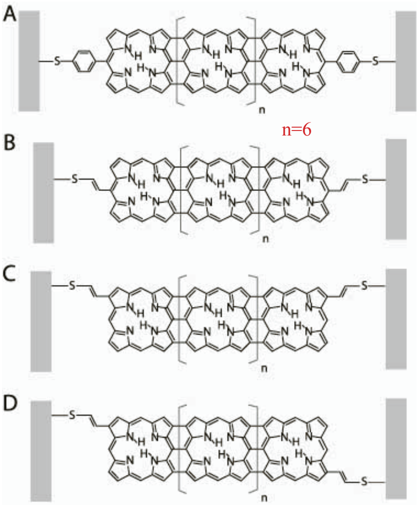

Figure 10. Four different likage structures of the tape porphyrin to the gold electrode.

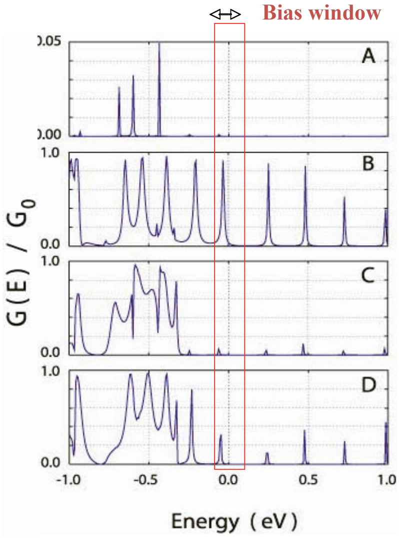

Figure 11. Electron transmission spectra for the four different linkage structure of Fig.10 to the Au electrodes.

The internal current distribution within the molecule, which is induced by the source-drain current, also shows remarkable quantum nature. Namely, when the electron incident energy is close to a degenerate molecular level, a large loop current is often generated inside the molecule[11].

Figure 12(a) illustrates internal current in a triangular nano-graphene sheet bound with zigzag edges. The connection to the source-drain electrode is made by the vinyl group to the atoms at the same zigzag edge[12]. The electron incident energy is set as $E = -0.165t$. Noticeably, a large current loop appears circulating a large area of the graphene molecule. Figure 12(b) schematically illustrates the orientation of the current flow, which is reversed by changing the bias polarity. The strength of the current is by more than ten times larger than the source-drain current. Interestingly enough, the same carrent distribution appears for the the isolated molecule under a static magnetic field. One might speculate a close relationship between the source-drain induced loop current and the molecular diamagnetic current and nano-scopic persistent current induced by magnetific field.

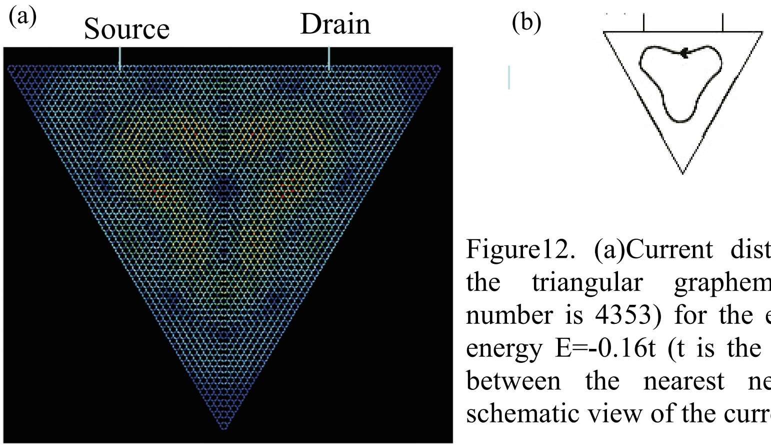

Figure12. (a)Current distribution in side the triangular grapheme (total atom number is 4353) for the electron with the energy E=-0.16t (t is the hopping integral between the nearest neighbor). (b) A schematic view of the current distribution.

7. Effect of coupling to the outer environment

Since the electron number in a molecule and the phase of the electron wave-function are mutually conjugate physical quantities, there is an uncertainty relation between the two. If the bottleneck at the connection part between the molecule and the electrodes is weak, the phase tends to be a good quantum number, and a coherent quantum transport throughout the whole system described above is expected. However, if the bottleneck is strong, the electron number in the molecule tends to be a more defined quantum quantity. In this case the electron transfer is associated with the energy dissipation to the outer environment as molecular vibration or the electro-magnetic field. Then the dissipative electron(hole) hopping transition becomes dominant and the Coulomb blockade or "Polaron blockade" phenomena emerges as will be seen in the I-V characteristics as shown schematically in Fig.13. In Fig.13 E_C is the order of the blockade energy determined by the effective capacitance C

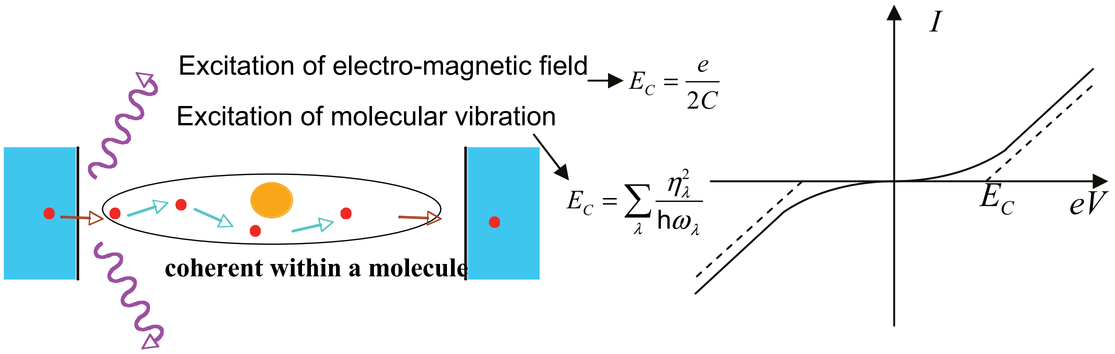

Figure 13. Dissipation processes of the electron transition between the electrode and the molecule (right), and associated Coulome or Polaron blockade effect on the I-V curve.

($E_C = \frac{e^2}{2C}$) or the coupling energy to the molecular vibration ($E_C = \sum_\lambda \frac{\eta_\lambda^2}{\hbar\omega_\lambda}$) where $\eta_\lambda, \omega_\lambda$ are electron-vibration coupling energy and the eigen frequency of the mode λ, respectively.

With the decrease of the transfer integral inside the molecular region, the electronic state changes from the extended state to a polaron like localized state. By considering the transition over the polaron-like states, the carrier transfer in the molecular chain bridge can be properly analyzed. The model we analyzed (Fig.14) consists of a chain of thiophene molecules and two outer electrodes.

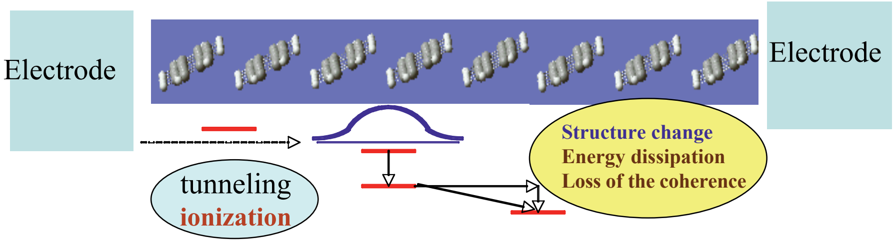

Figure 14. A schematic view of the molecular chain bridge

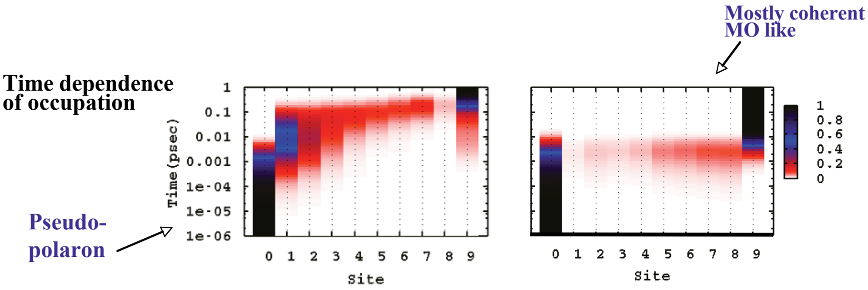

Figure 15. Time dependence of the electron occupation at each site after injection Hopping integral for left 0.2eV, for right o.5eV.

Figures 15(left) and (right) show the time-dependent occupation of each site after injection. The 0th and 9th site mean the left and the right electrode, respectively[13]. After a short passage time, the occupation at the left electrode rapidly decreases and the right electrode increases. If the bare hopping integral V is relatively weak(0.2eV, the left case of Fig.15), the eigen-states relevant to the transition are more or less composed by a dressed states and the electron mobility is considerably slowed down compared with the case of the stronger bare hopping integral(0.5eV, the right case of Fig.15). For bulk organic materials, time-of-flight (TOF) experiments are frequently used to estimate the carrier mobility. The result of the mobility in Fig.15 roughly reproduces the behavior observed by TOF.

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Nanostructured Assembly at Solid Surfaces and Nanomaterials in Energy and Environment Application

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1. Introduction

Nanostructured self-assembly with organic molecules is increasingly realized as a feasible bottom-up route for the fabrication of molecule-based devices in the future [1]. So far, various sophisticated architectures have been achieved in ambient or UHV environments by using the non-covalent interactions, including van der Waals interactions, H-bonds, and π-π interactions [2,3]. From a fundamental point of view, the investigation on the organic molecules adsorption at the solid/liquid interface will be helpful in understanding the intermolecular interaction and molecule surface molecule surface interaction and how they determine the formation of self-assembled ordered structures. The information is of great value to guide the construction of self-assembly structures on the surface. The adsorption of organic adsorbates is closely related to the electrocatalysis, electrochemical reaction, photovoltaic applications, and many others. On the other hand, nanostructure materials are attracted interests in energy and environment application. In this paper, we briefly report our recent progress in both surface assembly fabrication and nanomaterial preparation.

2. Metallamacrocyclic Supramolecular Assemblies

Among various building blocks, the metallamacrocyclic supramolecular assemblies represent a class of interesting materials not only bearing a beautiful topological structure but also possessing magnetic, photophysical, electronic, and redox properties that may not be accessible from purely organic systems [4,5]. Fabricating desirable and stable devices from these assemblies on solid surfaces and understanding the rules governing their self-organization on solid supports are significant fundamental steps toward realizing useful nanodevices and nanostructures.

The rectangle [(1,8-bis(trans-Pt(PEt_3)2)-anthracene)(4,4’-bpy)]2$(PF_6)_4$ is found to form a highly ordered molecular adlayer, as shown in Figure 1a. The adlayer has a rectangular unit cell of $(7\times3\sqrt{3})$ structure. As revealed by high-resolution STM images (Figure 1b), each molecule consists of a set of four bright spots, which correspond to the aromatic rings of the supramolecular rectangle, with dimensions of 2.0 nm × 1.2 nm, consistent with the size of the rectangle determined from single-crystal X-ray crystallography [6]. The supramolecular rectangle adopts a flat-lying configuration on the Au(111) surface, and a dark depression is seen in the center of each rectangle. Similar to the supramolecular rectangle, two other supramolecular assemblies with square and cage shapes are found to form an ordered adlayer on Au(111) as well [7].

However, these supramolecular assemblies cannot form an ordered stable adlayer on the HOPG surface, which is mainly due to the weak interaction between molecules and the HOPG surface. When mixing the rectangle and cage supramolecules together, they tend to separate to form individual domains on the surface.

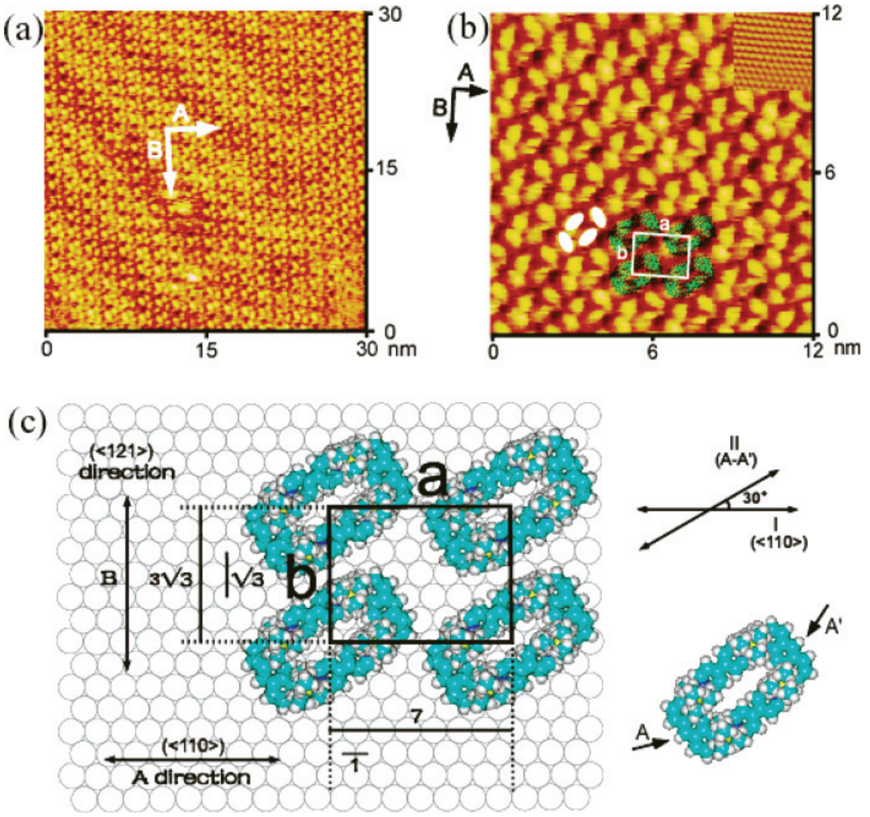

Figure 1. (a) Large-scale and (b) high-resolution STM images of the self-assembled supramolecular rectangles adsorbed on a Au(111) surface. Underlying Au(111)-(1 × 1) lattice is shown inset. (c) Proposed structural model for the adlayer.

3. Ordered Calixarene/fullerene Array

Fullerene self-organization is receiving increased attention due to the possibility to integrate molecules with different functions and to fabricate novel nanostructures. Moreover, to construct an ordered array of fullerene is very important for device fabrication based on fullerene, owning to its unique physical and chemical properties and myriad potential applications [8,9]. By taking advantage of the host-guest interaction between calixarene and fullerene, an ordered fullerene array is obtained on Au(111) [10].

Figure 2a is a typical STM image of the adlayer of a calix[8]arene derivative (OBOCMC8) on the Au(111) surface in 0.1 M $HClO_4$. The molecular adlayer consists of regular rows of round shaped calix-like features with dark depressions in the center.

The distance between the centers of the dark depressions is 1.2 ± 0.1 nm along the A direction and 1.7 ± 0.1 nm along the B direction. The molecular rows in the A and B directions cross each other at an angle of 95 ± 2°. The dimension of round protrusion matches well with the size of the OBOCMC8 molecule and, therefore, each calix-like feature appearing in the STM image can be assigned as an individual OBOCMC8 molecule. In the structural model, each molecule is adsorbed on the surface in an upright configuration through the carboxyl-gold interaction. The surrounding protrusions and the dark depressions of calices in the STM images are attributed to the phenyl groups and the molecular cavity, respectively.

A typical STM image of the adlayer of a C_{60}/OBOCMC8 complex on the Au(111) surface is shown in Figure 3a. An interesting feature of the C_{60}/OBOCMC8 adlayer is the well-ordered bright spots, which appear to fill the dark depressions that were observed in the OBOCMC8 adlayer, presumably due to the inclusion of C_{60} molecules.

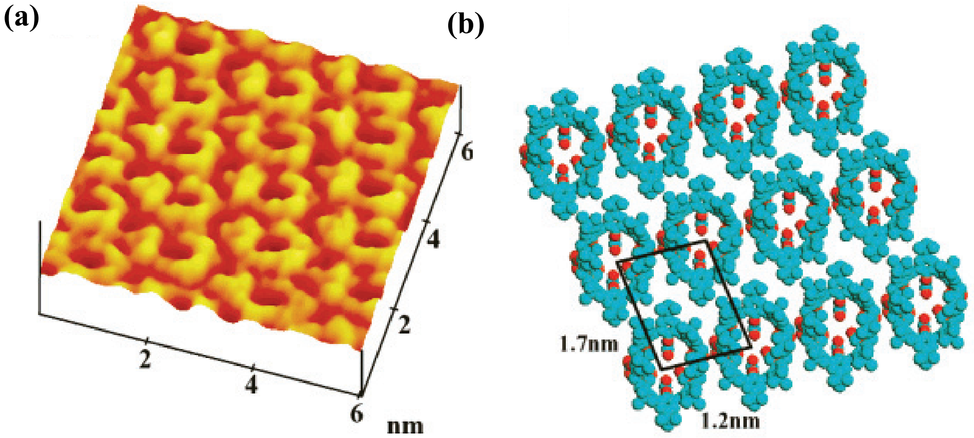

Figure 2. (a) Height-shaded surface plot of a high-resolution STM image of the OBOCMC8 adlayer on Au(111). (b) Proposed structural model. The biased voltage and tunneling current were -213 mV and 670 pA, respectively.

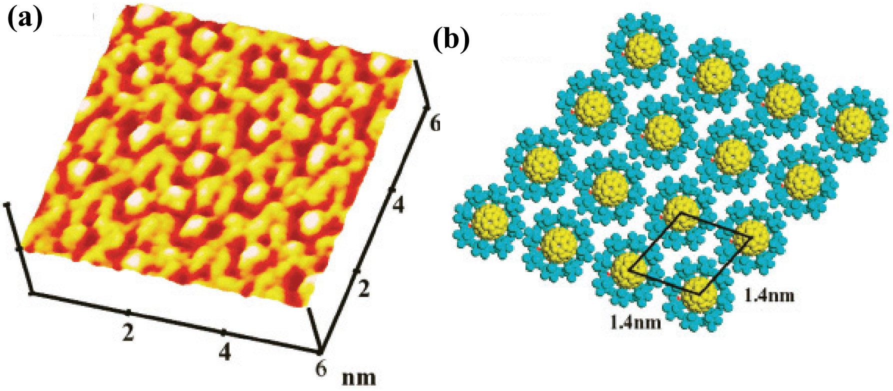

Figure 3. (a) Height-shaded surface plot of a high-resolution STM image of the C_{60}/OBOCMC8 adlayer on Au(111). (b) Proposed structural model. The biased voltage and tunneling current were -140 mV and 1.0 nA, respectively.

The inter-distance of bright spots along the molecular rows is measured to be 1.4 ± 0.1 nm, which is approximately the size of the C_{60}/OBOCMC8 complex. The individual bright spots are surrounded by circular protrusions. As shown previously, the C_{60}/OBOCMC8 complex tends to be in the upright configuration on the Au(111) surface bonded through the carboxyl groups. Therefore, the bright spot and circular protrusion can be assigned as C_{60} and phenyl units, respectively, with each OBOCMC8 cavity filled with a C_{60} molecule.

The same strategy could be used to assemble other fullerene derivatives, clusters, and organic molecules. The so-obtained architecture with stable configuration and well-defined array should be interested in nanodevice and sensor applications.

4. Nanostructured materials and their applications

4.1 Pt hollow nanospheres.

Considerable attention has been paid to alternative energy sources such as hydrogen and fuel cells as energy sources in an attempt to relieve the pollution and energy crisis. Among various candidates, Pt has stimulated considerable research into its use [11]. However, a critical problem with Pt-based catalysts is their prohibitive cost. Hollow metallic nanospheres exhibit catalytic activities different from their solid counterparts with the advantages of low density, saving of material, and reduction of costs.

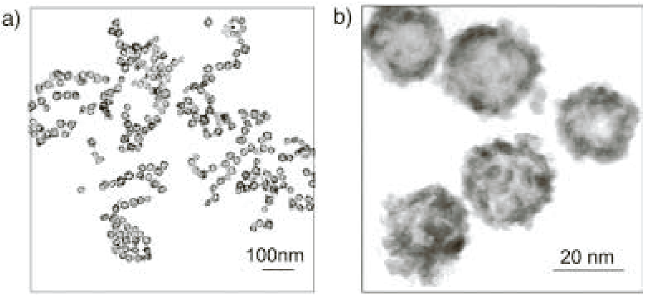

Figure 4. (a) and (b) TEM images of Pt hollow nanospheres.

The Pt hollow nanospheres is synthesized via the replacement reaction between Co nanoparticles and H_2PtCl_6 [12]. As this replacement reaction occurs rapidly, the Pt atoms nucleate and grow into very small particles, eventually evolving into a thin shell around the cobalt nanoparticles. Figure 4a is a typical large-scale TEM image. It was found that the centers of the spheres are brighter than the edges. The individual Pt spheres (Figure 4b) are composed of an empty core with a shell, that is, a hollow structure. The thickness of the shell is ~2 nm. The diameter of the nanospheres was statistically calculated to be 24 ± 2 nm. The shells of the Pt hollow nanospheres seem to be rough and consist of Pt nanoparticles with a size of ~2 nm. Another feature is that the shell is incomplete and porous, not solid. This feature endows the Pt hollow nanospheres with a high surface area.

The electrocatalytic activity of the Pt hollow nanospheres for the oxidation of methanol is demonstrated and compared with that of solid Pt nanoclusters by using a well-used electrochemical reaction in H_2SO_4 [13]. From the CVs in Figure 5, both the Pt hollow nanospheres and nanoclusters show catalytic behavior for the electro-oxidation of methanol by the appearance of an oxidation current in the positive potential region. The onset potentials are around 0.3 V vs. SCE. The peak potentials for the oxidation of methanol are approximately 0.65 V vs. SCE, in good agreement with the literature values. The remarkably high oxidation current for the hollow-sphere catalysts is directly related to the high surface area. Since the Pt hollow nanospheres are coreless, a larger number of Pt nanospheres were obtained relative to that found with the same loading of solid Pt nanoclusters. The incomplete shell of hollow nanospheres may also provide the interior surface for the catalytic reaction. Assuming that the inner and outer surfaces of a hollow nanosphere can participate in the catalytic reaction, the surface area of the single hollow nanosphere is ~ 1.16 times as that of a single solid nanocluster. The higher surface area of Pt nanospheres results in a higher catalytic activity.

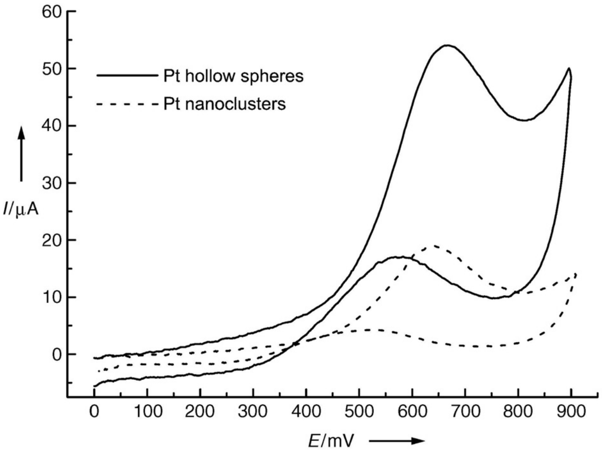

Figure 5. CVs of Pt solid nanoclusters (dashed line) and hollow nanospheres (solid line) on a glass carbon disk electrode in H_2SO_4 (0.5 M) and methanol (0.6 M). The same loading of nanospheres and solid nanoclusters was applied to the electrodes (0.0175 mgcm^{-2}). Scan rate=50 mVs^{-1}.

4.2 ZnS nanoporous nanoparticles (NPNPs)

Environmental problems associated with organic pollutants and toxic water pollutants provide the impetus for sustained fundamental and applied research in the environmental remediation. Semiconductor photocatalysis offers the potential for complete elimination of toxic chemicals through its efficiency and potentially broad applicability [14]. An important application of ZnS is as a photocatalyst in environmental protection through the removal of organic pollutants and toxic water pollutants. However, the development of cost-effective methods suitable for the large-scale synthesis of ZnS nanoporous nanostructures with high catalytic activity and easy separation represents a critical challenge to their practical applications.

ZnS NPNPs were prepared by a facile solution-phase thermal decomposition route in the presence of poly(N-vinyl-2-pyrrolidone) (PVP) [15]. Figure 6a shows a typical TEM image of a ZnS sample, revealing a large number of well-dispersed spherical nanoparticles with uniform size and shape. The average size of these particles is about 60 nm. The high-magnification TEM image in Figure 6c shows many spots with a clear contrast difference in each individual nanoparticle, indicating that the NPNPs consist of smaller nanoclusters (NCs) with a size of 3–5 nm which are assembled in a nanoporous structural configuration. A selected-area electron diffraction (ED) pattern of ZnS NPNPs is presented in the inset of Figure 6c. The ED pattern shows a set of concentric rings instead of sharp spots as a result of the small crystallites. A representative high-resolution TEM (HRTEM) image of ZnS NPNPs in Figure 1d, with an inset image taken on the outside of the particles, shows the lattice fringes of nanocrystals in nanoparticles with a spacing of 0.31 nm, which corresponds to an interplanar distance of the (002) plane of hexagonal ZnS.

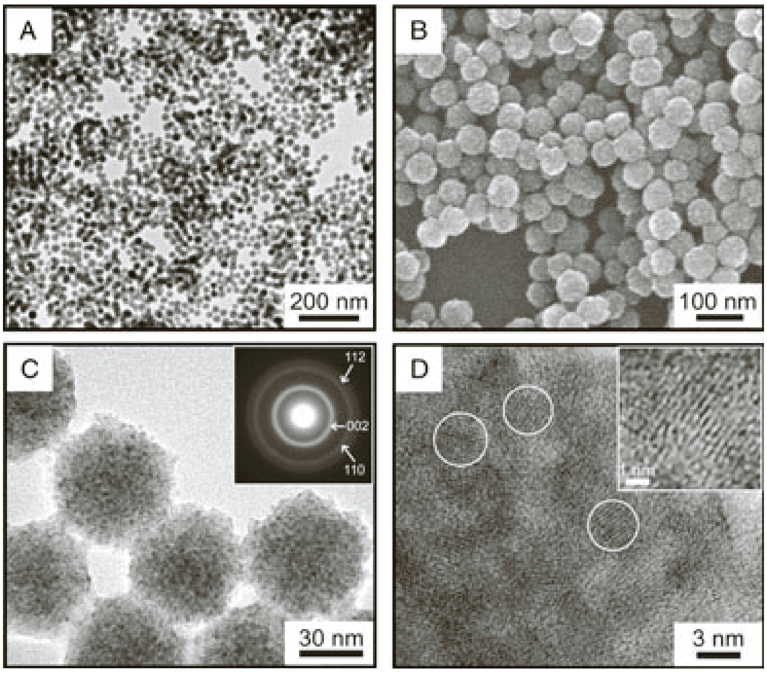

Figure 6. (a) Low-magnification TEM image, (b) SEM image, (c) high magnification TEM image, and (d) HRTEM image of ZnS NPNPs. The inset in (c) is the electron diffraction pattern. The inset in (d) shows the enlarged lattice fringes.

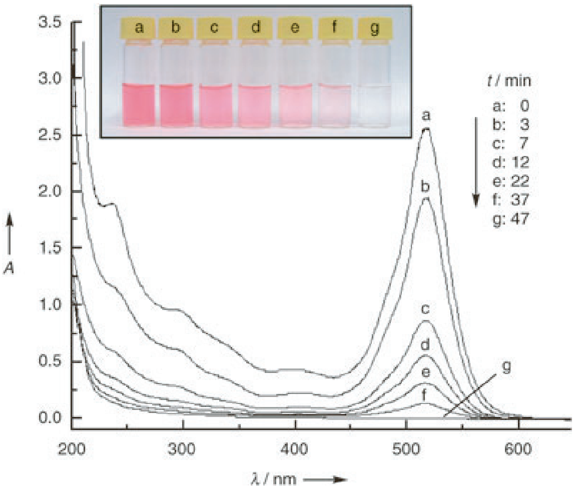

Figure 7. Absorption spectrum of a solution of eosin B (5.0 ×10—5 M, 30 mL) in the presence of ZnS NPNPs (10 mg) under exposure to UV light.

The photocatalytic activity of the ZnS NPNPs was investigated in comparison with those of ZnS NCs prepared by a literature method and of a commercial photocatalyst (Degussa P25 titania), with the photocatalytic degradation of eosin B as a test reaction. The characteristic absorption of eosin B at 517 nm was chosen as the monitored parameter for the photocatalytic degradation process. Figure 7 shows the absorption spectrum of an aqueous solution of eosin B (initial concentration: 5.0 × 10^{-5} M, 30 mL) in the presence of ZnS NPNPs (10 mg) under exposure to

UV light for various durations. The absorption peaks corresponding to the eosin B molecule, such as the sharp peak at 517 nm, diminish gradually as the exposure time increases and completely disappear after about 40 minutes. No new absorption bands appear in either the visible or ultraviolet regions, which indicate the complete photodegradation of eosin B. The color-change sequence in the sample during this process is shown in the inset of Figure 7, from which it is clear that the intense pink color of the starting solution gradually disappears with increasingly longer exposure times.

5. Summary

Innovative assemblies with designable structures have been achieved on the surface either by tuning intermolecular interactions, such as H-bonding, van der Waals interactions, π-π interactions, or electrode/molecule interactions. The active role of potential at the electrochemical solid/liquid interface adds another dimension of control over the orientation of molecules or the organization of the surface assembly on the surface. This perplexing but also fascinating feature of electrochemical adlayer may open new horizons for the development of new functional elements in future sensor and device design. In addition, tailored surface structures on the surface afford the highly efficient, controllable reactions on the surface. It is reasonable to believe that new heights for the building of complex architectures with specific structures and functions will be achieved in future.

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Supercritical Hydrothermal Synthesis of Organic-Inorganic Hybrid Nanoparticles

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1. Introduction

Nanoparticles of gold are known to mankind since Roman times. In nature nanomaterials exist ever since the earth came into existence. The term nanotechnology was first used by the Japanese researcher Taniguchi in 1974 when he referred to the ability to engineer materials at the nanometer scale [1]. The main idea behind the usage of this terminology was the miniaturization in the electronics industry.

Today this term nanotechnology is popularly used to define technology where dimensions and tolerances are in the range 1 – 100 nm, larger than size of atom until about wavelength of light. What is certainly new is the availability of an extraordinarily wide range of nano-sized materials, many of which have unique properties and exciting applications [2]. The nanomaterials are known for their unique mechanical, chemical, physical, thermal, electrical, optical, electronic, magnetic and specific surface area properties, which in turn define them as nanostructures, nanoelectronics, nanophotonics, nanobiotechnology, nanoanalytics, etc. During 1980s, the concept of size quantization was formulated for semiconductors and accordingly nanoparticles possess unique optical and electronic properties not observed for corresponding bulk samples [3,4].

In the last few years, a trend has been set in the processing of a new class of nanomaterials including coordination polymers, in which isolated metal ions or clusters are linked into arrays by organic ligands, and extended inorganic hybrids, such as hybrid metal oxides in which there is M-O-M connectivity in 1-, 2-, or 3-dimensions. Such hybrid frameworks represent an enormous class of new materials that can harness the advantages and versatility of both organics and inorganics with a scope that is vastly greater than the combined fields of coordination chemistry and organometallics. These new class of organic-inorganic hybrid materials have a tremendous application potential as sensors, biological tags, catalysts, bioelectronics, solar energy conversion, mechanics, membranes, protective coatings, transparent pigments, electro-magnets, cosmetics, etc [5,6]. The concept of "hybrid inorganic-organic" materials exploded only very recently with the birth of soft inorganic chemical routes, where mild synthetic conditions allow access to chemically designed hybrid inorganic-organic materials [7,8]. The small size and high surface to volume ratio of the individual nanoparticles imparts distinct size tunable physical and electronic properties that have prompted some to refer to them as "artificial atoms". As the number of nanoparticle systems under strict synthetic control has expanded, the parallel to the development of a “new periodic table” is also under consideration [9].

A highly controlled self-assembly of these hybrid nanoparticles when dispersed in organic solvents into two-dimensional and/ or three-dimensional ordered structures or super-lattice structures remains a relatively unexplored area. In recent years, there are lots of publications on such self-assembled nanoparticle structures in the literature. It is to be noted that a major challenge in the nanomaterial fabrication whether organic, or inorganic or composite nanoparticles, is the preparation of highly dispersible unagglomerated nanoparticles with an accurate control over the size and shape, which in turn is directly linked with the nanomaterial processing method. Owing to the higher surface energy of the particles in nanoscale, there is a greater tendency for nanoparticles agglomeration and aggregation. At the same time, it is difficult to break down the aggregation of nanoparticles into individual particles size. Therefore, a new strategy for an effective solution to this problem has to be worked out. In this context, the hydrothermal technique can be very effective to combat these issues in nanomaterials fabrication. On the whole, the hydrothermal technique is gaining popularity in recent years for processing a wide range of materials in the polyscale i.e. from bulk to nanosize [10-12].

2. Supercritical Hydrothermal Technique

2.1 What is Supercritical Hydrothermal Technique?

The term hydrothermal can be defined as any homogeneous or heterogeneous chemical reaction in the presence of a solvent (whether aqueous or non-aqueous) above the room temperature and at pressure greater than 1 atm in a closed system [10]. There are several other related terms commonly used in hydrothermal like solvothermal, supercritical hydrothermal, glycothermal, alcothermal, ammonothermal, carbonothermal, lyothermal, and so on. These different terms are basically used depending upon the type of solvents employed in the reactions. Each one of these techniques has some specific advantages and suitable for processing of a particular type of materials. The conventional hydrothermal refers to the reactions in the presence of an aqueous solvents, and solvothermal refers to the non-aqueous solvents. The ammonothermal refers to the ammonium based solvents, which are probably the best for the processing of nitrides including GaN. Similarly, the supercritical hydrothermal refers to the reactions near or above critical temperature.

The supercritical hydrothermal technique has a lot of other advantages as it accelerates interactions between solid and fluid species, phase pure and homogeneous materials can be achieved, reaction kinetics can be enhanced, the hydrothermal fluids offer higher diffusivity, low viscosity, facilitate mass transport and higher dissolving power. Most important is that the chemical environment can be suitably tailored. A great variety of materials have been obtained using the supercritical hydrothermal method.

The basic principle used in the hydrothermal synthesis of nanoparticles is that the solute raw material or the precursor material along with the appropriate solvent are taken in an autoclave which is maintained at a high temperature either below or above the critical temperature of the solvent over a period of time, which allows the solute to dissolve and recrystallize to the desired product. The solvent becomes highly corrosive under elevated temperature and pressure conditions and majority of the substances show higher solubility under hydrothermal conditions.

A fluid is supercritical when its temperature and pressure are higher than their critical point values (Tc, Pc), as shown in Fig.1. Most of the interesting applications of supercritical fluids occur at 1< T/Tc <1.1 and 1<P/Pc< 2 [13], since the properties change greatly around the critical point (Figs.1 and 2). Under these conditions the fluid exists as a single phase for light gas-water or organic molecules-water (Figs.3 and 4). Further, supercritical hydrothermal is also known for making new materials under mild conditions, since they increase the chemical reactions, improve the mass transfer, and greatly assist in the stability of selected or desired products [14-16].

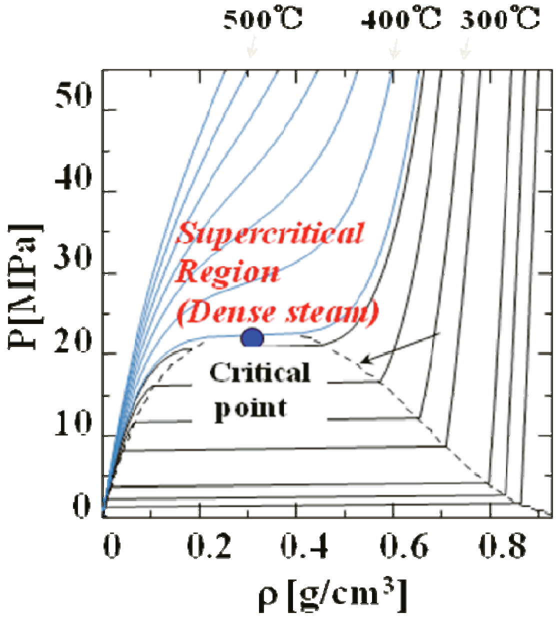

Figure 1. Density-pressure-temperature curve for water.

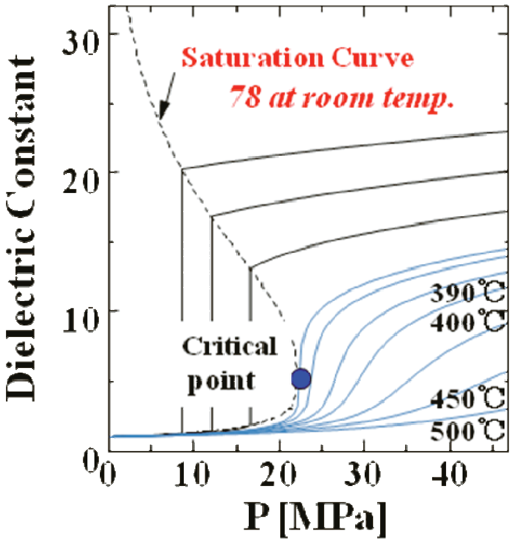

Figure 2. Dielectric constant of water.

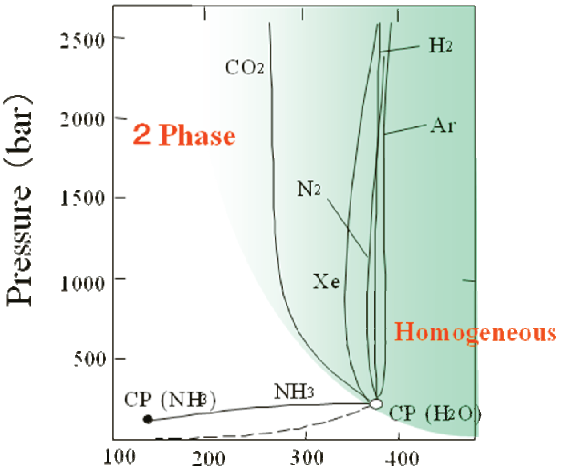

Figure 3. Critical loci for light gas-water systems.

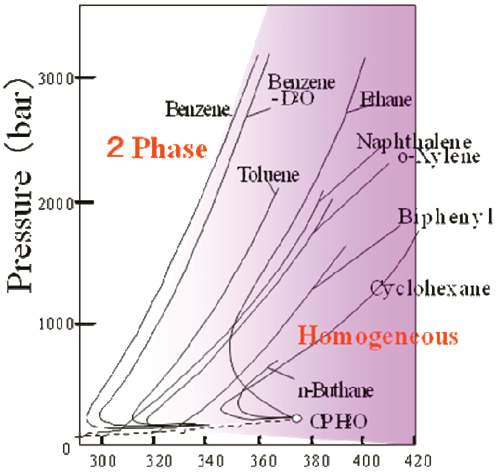

Figure 4. Critical loci for water-organic compounds systems.

2.2 Apparatus for nanoparitcle synthesis in supercritical fluid

There is a wide range of apparatus used in the supercritical hydrothermal research to suit the specific conditions and the product. However, the most commonly used apparatus are batch reactors and flow reactors.

The batch reactors are the cone-cold sealed type autoclaves usually made of hastalloy or stainless steel (SS316) with an ease to handle because of simple reactor design. A typical inner volume of these batch reactors is usually 5 mL. Sometimes the platinum lining or platinum capsules are provided to these reactors to prevent the corrosion. Depending upon the pressure and temperature of the reaction and density of water in those conditions, a required amount of precursors are loaded into the reactor. These reactors can be stirred or shaken during the experiments. A series of such batch reactors can be mounted on a single frame and experiments can be run conveniently by varying several experimental parameters.The experimental duration is normally varied from 5 minutes to several hours. Figure 5 shows the schematic diagram and a typical batch reactor. The product recovery process from the batch reactors is very important while dealing with nanoparticles fabrication.

Figure 5. Batch reactor.

Figure 6 shows the typical experimental set up used in the flow type of hydrothermal reactor. An aqueous metal salt solution is first prepared and fed into the apparatus in one stream. In another stream, distilled water is pressurized and then heated to a temperature above the desired reaction temperature. The pressurized metal salt solution stream and the pure *sc*H_2O stream are then combined at a mixing point, which leads to rapid heating and subsequent reactions in the reactor. After the solution leaves the reactor, it is rapidly quenched. In-line filters are used to remove larger particles. Pressure is controlled with a back-pressure regulator. Fine particles are collected in the effluent. By this rapid heating method, the effect of the heating period on the hydrothermal synthesis is eliminated; thus specific features of supercritical hydrothermal synthesis can be elucidated. There are several advantages in supercritical hydrothermal flow reactors, which provide nanoparticles with desired shape, size and composition in a shortest possible residence time. Hence, this technique has an edge over the conventional methods.

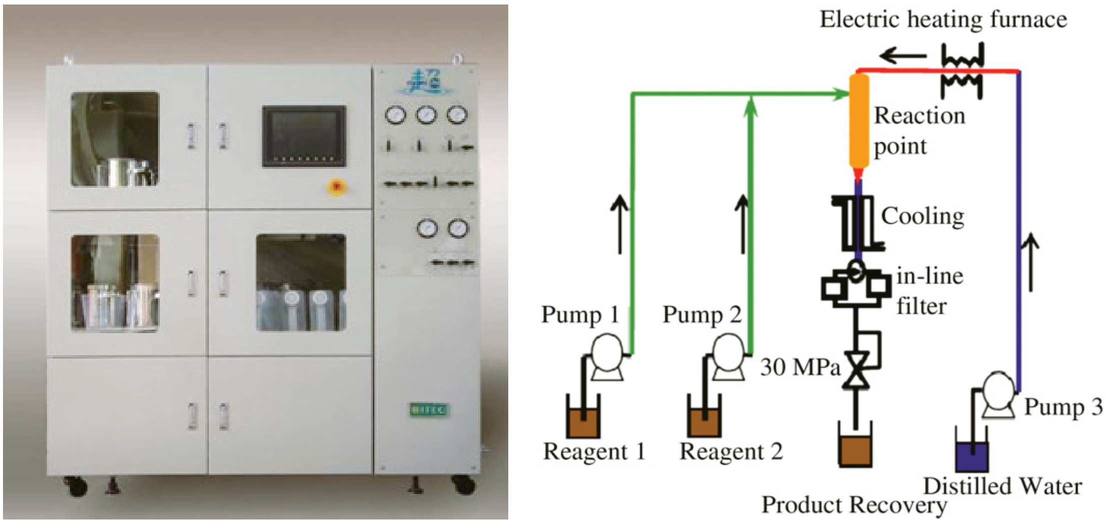

Figure 6. Schematic of a typical flow reactor.

3. Supercritical hydrothermal synthesis of hybrid organic-inorganic nanoparticles

3.1 Supercritical hydrothermal synthesis of metal oxides

A wide range of metal oxide nanoparticles have been obtained under supercritical hydrothermal conditions for applications not only in ceramics, coatings, catalysts, sensors, semiconductors, magnetic data storage, solar energy devices, ferrofluids, but also in medicalfield such as hyperthermia, bioimaging, cell labeling, special drug delivery systems, and so on. However, their application potential is dictated by their surface nature, particle size, and also shape. Although the synthesis of metal oxides is not new, their applications were limited. With the discovery of size quantization effect in these materials during 1980s, there is a seminal progress in the synthesis of these metal oxides with desired properties for several new applications. Researchers like Adschiri, Arai, Johnston, Lester and Poliakoff, etc. have contributed extensively on the synthesis of metal oxides and proposed a systematic mechanism [15-17]. Metal oxides as Al_2O_3, Ga_2O_3, In_2O_3, SiO_2, GeO_2, ZnO_2, V_2O_5, TiO_2, CeO_2, ZrO_2, CoO, α-Fe_2O_3, γ-Fe_2O_3, NiO, Co_3O_4, Mn_3O_4, γ-MnO_2, Cu_2O, $CoFe_2O_4$, $ZnFe_2O_4$, $ZnAl_2O_4$, Fe_2CoO_4, $BaZrO_3$, $BaTiO_3$, $BaFe_{12}O_{19}$, $LiMn_2O_4$, $LiCoO_2$, La_2O_3, etc., have been prepared by the above method. Usually the particles obtained in the subcritical water conditions are larger than those in the *sc*H_2O, because, there is a particle growth with an increase in the residence time, whereas under supercritical conditions such a phenomenon has not been observed. The hydrothermal reaction rate in *sc*H_2O is higher, and the solubility of the metal oxides is much lower than that in subcritical water. This leads to the generation of higher degree of supersaturation. The nucleation rate is expected by the function of degree of supersaturation and the surface energy according to the nucleation theory. Thus, extremely high nucleation rate can be expected at supercritical conditions, which leads to the formation of nano-size particles. Figure 7 shows the mechanism for the fine CeO_2 particles formation in *sc*H_2O. More or less a complete list of the materials obtained under supercritical hydrothermal conditions is available in the works of Reverchon and Adami (2006) and Byrappa and Adschiri (2007) [11,18]. Basically hydrothermal synthesis method is available for the metal oxides by conventional hydrothermal synthesis method. The point to be noted here is that under supercritical hydrothermal conditions, nanometer size metal oxides could be synthesized and crystallinity of the nanoparticles would be much higher when compared to the metal oxides obtained under conventional hydrothermal conditions, wherein bulk single crystals are formed. This sometimes leads to the specific characteristics of the products. Phosphor nanoparticles show high luminescence without heat treatment which is usually necessary for the products obtained by low-temperature wet method [19,20].

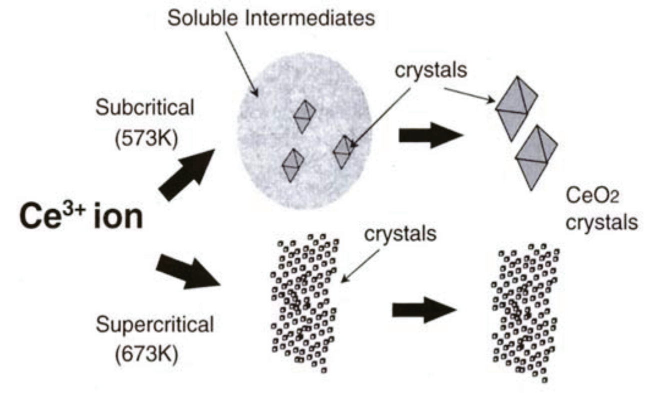

Figure 7. Mechanism of CeO2 nanoparticles formation under supercritical hydrothermal conditions.

3.2 Supercritical hydrothermal synthesis of organic-inorganic hybrid nanoparticles

In order to resolve the problem of particle aggregation, to achieve the perfect control over the size and morphology of the particles, and to obtain a desired surface property to the nanoparticles, a new processing strategy has been proposed by Adschiri and group utilizing the supercritical hydrothermal technology [12,21-25]. Figure 8 shows a schematic representation of highly effective strategy for the synthesis of metal oxide nanocrystals in the organic-ligand assisted supercritical hydrothermal technology [21]. The method yields perfect hybrid organicinorganic nanocrystals with very high dispersibility, and a precise control over the size and shape of the nanoparticles, as shown in Figure 9. The organic components are introduced into the system during the hydrothermal synthesis and *in situ* surface modification is obtained with a ultra-thin layer of organics surrounding the inorganic unlike the case of silane coupling on the metal oxides. The organic ligands and supercritical water form a homogeneous phase (Fig.4) and it is known that under these conditions water molecules themselves work as acid or base catalyst for various organic reactions. Depending upon the applications of nanoparticles, one can select suitable functional groups to introduce hydrophobicity or hydrophilicity property to the surface of the modified nanoparticles.

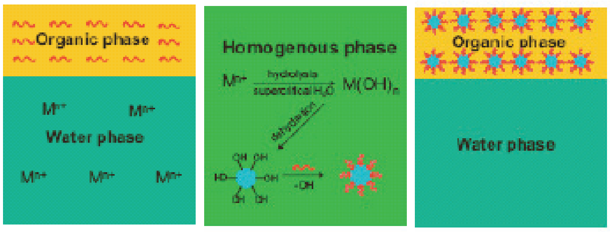

Figure 8. The strategy for the synthesis of metal oxide nanocrystals in the organic-ligand assisted supercritical hydrothermal technique [21].

Understanding on the mechanism of formation of organic-inorganic hybrid nanoparticles is very important and it deals with the interaction of the organic ligand molecules with the inorganic metal oxide surfaces. Adschiri and his group have worked out in detail the theory and mechanism of the hybrid organic-inorganic nanoparticle formation under supercritical hydrothermal conditions. In order to understand the mechanism of this hybrid nanoparticles formation, it is necessary to investigate the charge distribution on the surface of the metal oxide particles, which in turn reveal the chemical interaction between the modifier and the surface of the metal oxide nanoparticle. In aqueous systems, metaloxide particles are hydrated and M-OH groups cover completely their surface and

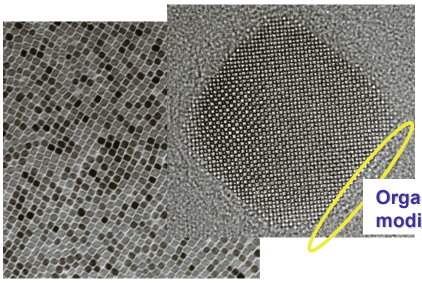

Figure 9. Organic-inorganic hybrid nanocrystals synthesized in supercritical water.

the surface is neutral. The M-OH sites on the surface of particles can react with H^+ or OH^- ions from dissolved acids or bases, and positive ($M\text{-}OH^{2+}$) or negative ($M\text{-}O^-$) charges develop on the surface, and type of the reaction depends on *pH* of the solution. In the absence of specific adsorption of ions, amphoteric metal oxides have a characteristic pH, the *pH* of the point of zero charge (PZC), where the net surface charge is zero, i.e. the positive and negative sites are in equal amount (isoelectric point, *iep*). At *pH* lower than *iep*, the pure metal oxide surface is positively charged, while it has negative charge above it [26-28]. Normally the modifiers attach onto the surface of the nanoparticles either by physisorption or chemisorptions through strong hydrogen bond. If we consider R-COOH as modifier reagents in a highly acidic *pH* of the reaction medium, the dissociation of modifier does not occur and the conjugation is due to the strong hydrogen bonding between hydroxylic groups on the surface of nanoparticles and functional groups of modifier [29]. If the *pH* of the reaction medium is in the range of modifier dissociation, another type of interaction between the modifier and the metal oxide surfaces is expected [30]. Similar chemical bonding is expected even for amines or alcohol or aldehyde as the organic ligands in the system. The addition of surface modifiers also helps to inhibit the crystal growth that facilitates the smaller particles size with a narrow particle size distribution. Figure 10 shows nanoparticles of Fe_2O_3, Co_3O_4, CeO_2, and $CoAl_2O_4$ obtained under supercritical hydrothermal conditions without and with organic modifiers. As is clearly seen from Figure 5, those nanoparticles without modifier are aggregated and they do not

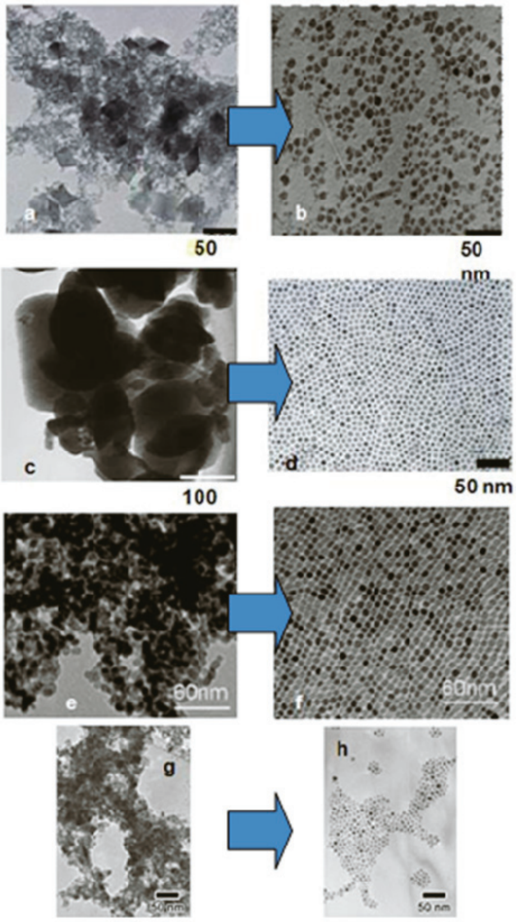

Figure 10. TEM images of hybrid nanoparticles synthesized under supercritical hydrothermal conditions: a) Fe_2O_3 (without modifier); b) Fe2O3 (with modifier); c) Co_3O_4 (without modifier); d) Co_3O_4 (with modifier); e) CeO_2 (without modifier); f) CeO2 (with modifier); g) TiO_2 (without modifier); h) TiO_2 (with modifier) (from the works of Adschiri).

disperse in the aqueous solvents. Also the particle size is larger compared to the modified particles. When the *pH* of the reaction medium is highly acidic or highly basic, very small particles along with the large particles are formed leading to a broader size distribution. It seems that because of redissolving of nanoparticles at very high and low *pH*, Ostwald repining occurs. Therefore, in surface modification, *pH* of the medium, isolectric point (*iep*) and another important parameter, viz. dissociation constant (*pKa*) of the modifiers are very important. At *pH* below *pKa*, the modifier does not dissociate. Moreover, below *iep*, the surface of metal oxide nanoparticles is surrounded by positive charges (major) and hydroxylic groups (minor). Under these conditions there is no chemical reaction occurring between the modifier and the metal oxide nanoparticle surface, but it is only through a strong hydrogen bonding the modifier can attach to the nanoparticles surface. In contrary, at higher *pH* than *pKa*, dissociation of modifier takes place and results in chemical reaction between dissociated part of modifier and OH_2^+ from particles surface. Thus, by dehydration reaction modifier attaches to the surface of the particles. The possible different types of conjugation between the surface modifier and the surface of the nanoparticles are schematically represented in Figure 11. By considering the chemical reactions, mass balances, charge balance in the actual system, *pH* and the modifier can be fixed for most of the systems. From the literature data, the values of *pKa* for several surfactants are available.

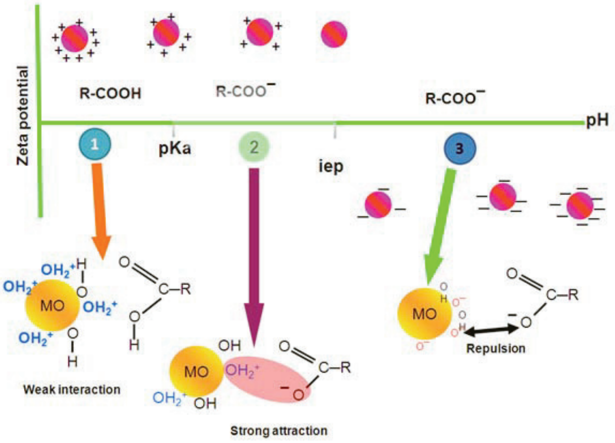

Figure 11. Schematic representation of the reaction mechanism of *in-situ* surface modification of metal oxide nanoparticles with R-COOH as a modifier (from Adschiri's work).

3.3 Study of the supercritical hydrothermal synthesis of organic-inorganic hybrid nanoparticles with size and shape control

The experimental studies on the preparation of some selected organic-inorganic hybrid nanoparticles under supercritical hydrothermal conditions are discussed here based on the discussion in the previous section. Figure 12 shows the schematic diagram of the shape control of ceria nanoparticles under supercritical hydrothermal conditions in the presence of organic ligand molecules [21]. The ceria nanocrystals unmodified were truncated octahedral, which corresponds to the results of the earlier workers [31]. However, when decanoic acid was introduced into the system under supercritical hydrothermal conditions, the organic ligand molecules become miscible with water, they contribute to the change in morphology of ceria nanocrystals from truncated octahedral to cube, which is mainly because of the suppression of the crystal growth on the (001) face. When decanoic acid (molar ratio to ceria precursor 6:1) was added to the reaction system, the resulting nanocrystals were nanocubes with an average size of 6 nm. As the CeO_2 (001) surface is less stable than the (111) surface, the organic ligand molecules were likely to interact preferentially with the (001) surface thereby reducing the crystal growth along the [001] direction. If the amount of decanoic acid was further increased (molar ratio to ceria precursor, 24:1), the ceria nanocrystal size decreased to about 5 nm, and the shape of the nanocrystals also changed drastically, because of the growth inhibition not only along the [001] direction, but also along the [111] direction.

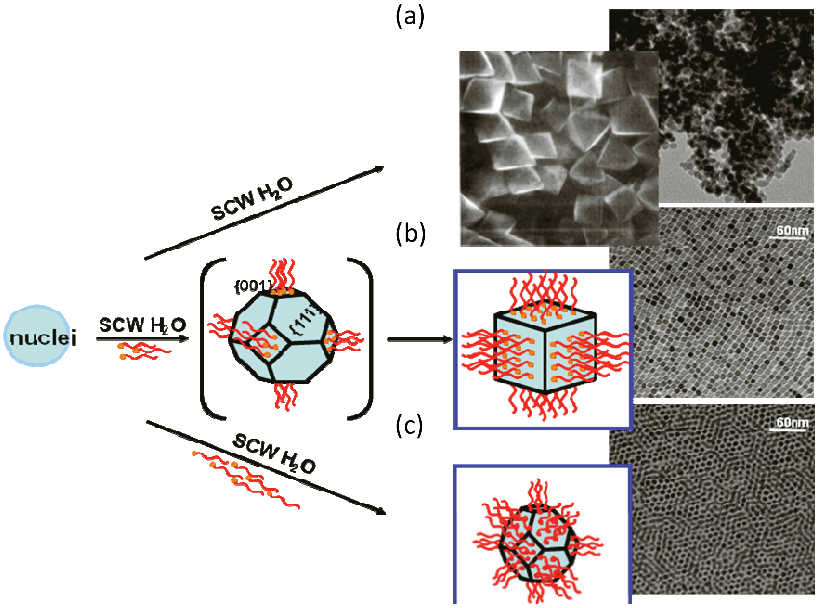

Figure 12. The shape control of ceria nanoparticles: a) truncated octahedron in the case when no organic ligand molecules are used; b) at a low decanoic acid to ceria precursor ratio, the preferential interaction of the ligand molecules with the ceria (001) planes slows growth of (001) faces relative to (111) faces, which leads to the formation of nanocubes; c) at a high deconoic acid to ceria precursor ratio, organic ligand molecules block growth on both (001) and (111) faces, which leads to the formation of truncated octahedral and smaller crystals.

3.4 Dispersibility of organic-inorganic hybrid nanoparticles

It is to be noted that the surface modified organic-inorganic hybrid nanoparticles synthesized under supercritical hydrothermal conditions can be easily recovered by extraction with organic solvent from the water suspension phase, and well dispersed in organic solvents. Normally transparent solutions are obtained for the well crystallized and very small hybrid nanoparticles when dispersed. Through the dynamic light scattering (DLS) studies also, it can be confirmed that the particles are not aggregated, but suspended as individual nanoparticles. Figure 13 shows the perfect dispersion of CeO_2 nanoparticles in the organic solvents.

Figure 13. Perfect dispersion of $CoAl_2O_4$ nanoparticles (b) in water (a) and CeO_2 nanoparticles in the organic solvent (c). Tyndall effect was clearly observed (c).

4 Recent topics

Finally, the recent topics regarding supercritical hydrothermal synthesis technique are introduced briefly here. There are mainly three topics under extensive research in our group now. These three topics are all based on the unique properties of organic-inorganic hybrid nanoparticles synthesized in supercritical fluid as mentioned in the previous sections(Fig.14).

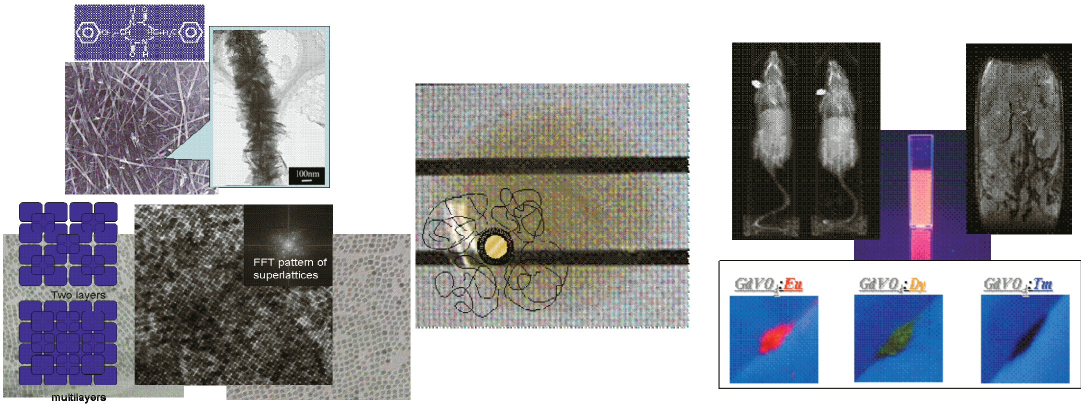

Figure 14. Evolution of organic-inorganic hybrid nanoparticles: Self-assembly of organic modified nanoparticles, hybrid polymer molecules, and bio-imaging probes.

4.2 Self-assembly of organic-inorganic hybrid nanoparticles

Self-assembly is a generic term used to describe a process leading to the ordered arrangement of molecules and small components such as small particles like nanoparticles occurring spontaneously under the influence of certain forces such as chemical reactions, capillary forces and electrostatic attraction, etc. Self-assembly and more generally self-organization of particles in a solvent is considered to be a powerful process for building patterns up to nanoscopic level through multiple interactions among the components of the system under consideration. Ordered assemblies of nanometer size particles represent an interesting class of nanomaterials that provide exceptional potentials for a wide variety of applications. These structures would be useful for various applications like displays, sensors, data storage, photonic band gap materials, etc owing to their exceptional physical, chemical and electronic properties [32-35]. Common approaches to noncovalent assembly strategies employ van der Waals/ packing interactions, hydrogen bonding, ion pairing, and host-guest inclusion chemistry [36-39]. These self-assembly methods provide direct access to extended structures from appropriately designed nanoparticle building blocks. Although the assembly of nanoparticles from solution into close-packed monlayers and super-lattice structures on solid surfaces has met with a fair degree of success [40-42], and in contrary, the controlled assembly of nanoparticles in the organic solvent has not been understood precisely. In order to meet the major challenge in nanotechnology in realizing many of the desired technological goals, the self-assembly provides a possible convenient route, but controlling size, size distribution, shape, and surface chemistries of the nanohybrid particles is critical in achieving desired structures. Initial syntheses have yielded nearly spherical shapes due to the thermodynamic driving force of minimizing surface area, and self-assembly has been limited to the close-packing of spheres [43,44]. The several reviews are published on this aspect [45,46]. However, it is to be noted that the self-assembly of hybrid organic-inorganic nanoparticles synthesized through supercritical hydrothermal routes are seldom found in the literature.

4.3 Super hybrid nanoparticles with Polymers

After successful production of surface modified nanopartilces, we have been trying to manufacture polymer-surface modified nanoparticle hybrid materials. In principle, inorganic material and organic compounds have tradeoff functions e.g. hard and soft, electro conductivity and insulation and highly thermal conductivity and adiathermic and so on, so that inorganic and polymer hybrid blends must show these tradeoff functions at the same time. According to the background, we're in charge with the New Energy and Industrial Technology Development Organization (NEDO) granted program: Development of Super-Hybrid materials. Among the series of high performance functional hybrid materials the target materials are focused on high refractive index materials and high thermal conductive materials in the project. For high refractive index materials, the single nano-sized high refractive index fillers have to be dispersed the polymer matrix without aggregation at high volume concentration, furthermore the material should keep the plasticity for further fabrications and of course the transparency against to visible light has to be achieved. For high thermal conductivity materials, the linkage between the inorganic fillers and total design of the hybrid materials are important. These tradeoff functions have to be accomplished for the new hybrid materials.

4.4 Bioimaging and Super drug delivery using water soluble nanoparticles synthesized in supercritical fluid

Recently, the cancer diagnosis and treatment using nanoparticles is extensively investigated. To image the tissues, comparably heavy metals are generally used such as Gd for Magnetic Resonance Imaging. These heavy metal ions are toxic and such kind of nanoparticles should be stable in the body. We take particular note of chemical stability of metal oxide nanoparticles synthesized in supercritical fluid. Modification of the surface of nanoparticles is also important to fit those particles to the living body as well as suppression of agglomeration of the particles. We can use the same technique as synthesis of organic-inorganic hybrid nanoparticles as mentioned above. Only difference is that nanoparticles should be dispersed not in organic solvent but in water. We are now trying synthesis nanoparticles soluble to water now. Agglomeration free nanoparticles without surfactant that may lead to biological toxin are strongly needed to realize bioimaging with high accuracy and safety.

5 Summary

Supercritical hydrothermal synthesis of advanced nanomaterials like organic-inorganic hybrid nanoparticles has been reviewed in detail starting from the basic principles to the specific features of the methodology. The supercritical fluids are very active in such extreme PT conditions and are highly suitable to synthesize even complex structures, because of the drastic change in the fluid properties like density and dielectric constant, which in turn lower the solubility of the materials. Although supercritical hydrothermal technique gives highly crystalline nanoparticles with homogeneous composition, still there is a problem of larger size, coagulation and poor dispersibility of nanoparticles in aqueous solutions. Hence, there is a trend to use organic ligands, capping agents, surfactants, etc., which generate a new class of nanomaterials, viz. organic-inorganic hybrid nanomaterials. This strategy is based on the miscibility of the organic ligand molecules with supercritical water due to the lower dielectric constant of the water; and the nanocrystal shape control by selective reaction of organic ligand molecules to the specific inorganic crystal surface. A great variety of organic ligand molecules including

DNA, proteins, peptides, amino acids, decanoic acid, oleic acid, etc. have been used for this purpose to obtain high quality organic-inorganic nanoparticles, which can be used as sensors, phosphors, data storage, photonic band gap, displays, biomedical, etc. These hybrid nanoparticles can be obtained with such a precise size and shape control. They show excellent dispersibility in the organic solvents and also self-assemble to form super-lattice structures. By choosing different types of modifiers with varying carbon chain length, the super-lattice of the self-assembled nanoparticles can be monitored precisely. Hence the supercritical hydrothermal synthesis method holds a strategy for the future advanced nanomaterials processing.

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WPI-AIMR Newly Appointed Research Staff

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ACADEMIC:

1984-1991	Undergraduate Student, Moscow State Institute of Steel and Alloys, Moscow, Russia
1995-1998	Dr. Eng. Course, Tohoku University, Japan

ACADEMIC DEGREE: Doctor of Engineering, 1998, Tohoku University, Japan

PROFESSIONAL EXPERIENCE:

1991-1994	Researcher, Moscow State Institute of Steel and Alloys, Moscow, Russia
1998-2005	Research Associate, Institute for Materials Research, Tohoku University, Japan
2005-2007	Associate Professor, Institute for Materials Research, Tohoku University, Japan
2007-present	Professor, WPI Advanced Institute for Materials Research, Tohoku University, Japan

SCIENTIFIC PUBLICATIONS:

- **162** research and review papers in world-leading peer-reviewed Journals (about 90% of which are ISI indexed) including Acta Materialia (4 papers), Applied Physics Letters (12), Materials Science and Engineering (8), Journal of Materials Research (6), Philosophical Magazine (3) and many others.
- **5** chapters in books.
- **10** Invited Talks at International Conferences.

RECOGNITION:

- Monbusho scholarship awarded to complete Dr. Eng. Course, Japan (1994)
- Young participating scientist award at 9th International Symposium on Metastable, Mechanically Alloyed and Nanocrystalline Materials (ISMANAM 2002) Sept. 8-12, Seoul (2002)
- MRS 2007 Fall Meeting Best Poster Award: T. Wada, D. V. Louzgine-Luzgin and A. Inoue MRS 2007 fall meeting, Boston, USA

CURRENT RESEARCH:

Investigation of thermal stability, structure, formation mechanisms, phase transformations, deformation behaviour, mechanical and physical properties of bulk metallic glasses, metallic glasses, nanostructured crystalline/quasicrystalline materials, composite materials having a mixed structure containing nanoparticles embedded in the glassy matrix and high-strength crystalline alloys. I have a long-term experience in various types of structural analysis techniques. In particular, Transmission Electron Microscopy (TEM) of nanostructured and glassy materials including nanobeam diffraction and high-resolution TEM imaging. Extraction of radial distribution functions from Synchrotron-radiation XRD data. I also apply computer-simulation to materials science (phase transformations, crystallography).

Kazuto AKAGI

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ACADEMIC:

1994	B.S. in Physics, The University of Tokyo, Japan
1996	B.S. in Physics, The University of Tokyo, Japan
1999	Dr. in Physics, The University of Tokyo, Japan

PROFESSIONAL EXPERIENCE:

1999	JSPS Fellow (PD), Institute for Solis State Physics, The University of Tokyo, Japan
1999-2002	Research Associate, Institute for Solis State Physics, The University of Tokyo, Japan
2002-2008	Research Associate, Department of Physics, Graduate School of Science, The University of Tokyo
2008-present	Associate Professor, WPI Advance Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

Investigation of chemical reaction process at various surfaces and solid/liquid interfaces based on first-principles molecular dynamics calculation. Development of computational simulation method for scanning probe microscopy.

Taro HITOSUGI

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ACADEMIC:

1994	B.S. in Engineering, The University of Tokyo, Japan
1996	M.S. in Engineering, The University of Tokyo, Japan
1999	Dr. Eng., The University of Tokyo, Japan

PROFESSIONAL EXPERIENCE:

1999-2003	Researcher, Sony Corporation, Japan
2003-2007	Assistant Professor, Department of Chemistry, The University of Tokyo, Japan
2003-present	Researcher, Kanagawa Academy of Science and Technology (KAST), Japan
2007-present	Associate Professor, Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

✦Solid State Chemistry, Solid State Physics, Surface Science
✦Studies on inorganic/organic thin films and nano-scale oxide materials.

Ken NAKAJIMA

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ACADEMIC:

1992	B.E. in Applied Physics, The University of Tokyo, Japan
1994	M.E. in Applied Physics, The University of Tokyo, Japan
1997	Dr. Eng. in Applied Physics, The University of Tokyo, Japan

PROFESSIONAL EXPERIENCE:

1997-1999	Special Postdoctoral Researcher, Frontier Research System, RIKEN, Japan
1999-2003	Frontier Researcher, Frontier Research System, RIKEN, Japan
2003-2008	Assistant Professor, Tokyo Institute of Technology, Japan
2008-present	Associate Professor, Tohoku University

CURRENT RESEARCH:

Single molecular detection by scanning probe microscopy, polymer physics, nanorheology and nanotribology of polymeric surfaces and single polymer chains, basic studies on rubbery elasticity

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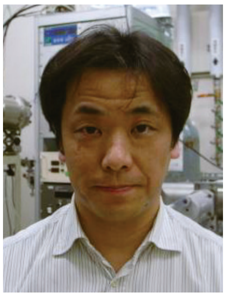
Koji S. NAKAYAMA



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ACADEMIC:

1990	B.S. in Applied Physics, Tokai University, Japan
1992	M.S. in Engineering, Yokohama National University, Japan
1995	Dr. Eng. in Engineering, Yokohama National University, Japan

PROFESSIONAL EXPERIENCE:

1995-1996	Research Scientist, Department of Engineering, Yokohama National University, Japan
1996-1999	Postdoctoral fellow, Department of Chemical Engineering and Materials Science, University of Minnesota, USA
1999	Postdoctoral fellow, Department of Chemistry, The University of Tokyo, Japan
1999-2001	Lecturer, Institute for Materials Research, Tohoku University
2001-2005	Visiting Research Assistant Professor, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, USA
2005-2008	Associate Professor, Institute for Materials Research, Tohoku University
2008-present	Associate Professor, WPI-Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

- ✦Growth and characterization of nanowires of metallic glassy alloys
- ✦Mapping of the electronic density of states using scanning tunneling spectroscopy

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ACADEMIC:

1994 B.S. in Physics, St. Petersburg State University, Russia
1996 M.S. in Quantum Theory of the Solid State, St.Petersburg State University, Russia
2000 Dr. Physics, The Royal Institution of Great Britain and University College London, UK

PROFESSIONAL EXPERIENCE:

2000	Visiting Researcher, Environmental Molecular Sciences Laboratory (EMSL), Pacific Northwest National Laboratory (PNNL), Richland WA, USA
2000-2001	Research Assistant, Department of Physics & Astronomy, UCL, UK
2001-2004	Research Fellow, Department of Physics & Astronomy, UCL, UK
2005-2007	Senior Research Fellow, Department of Physics & Astronomy, UCL, UK
2007-2008	Senior Research Fellow, London Centre for Nanotechnology, UCL, UK
2008-present	Associate Professor, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

- Theoretical/computational modelling of defect processes in the bulk and at surfaces of ionic materials.
- Photo-induced excited states, charge trapping, and mechanisms of defect formation in oxide nanostructures.
- Photo-chemistry of oxide surfaces.
- Mechanisms of photo-induced desorption.
- Modelling of defects and mechanisms of defect processes in high-K materials and at their interfaces with Si.
- Electronic properties of confined semiconductors and confined electron gas.
- Novel computational techniques.

Akira TAKEUCHI

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ACADEMIC:

1988 B.S. in Metallurgy, Nagoya Institute of Technology, Japan
1990 M.S. in Materials Science and Engineering, Nagoya Institute of Technology, Japan
1993 Dr. in Materials Science and Engineering, Nagoya Institute of Technology, Japan

PROFESSIONAL EXPERIENCE:

1993-2003	Research Associate, Institute for Materials Research, Tohoku University
2003-2008	Associate Professor, Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

Materials Science, Non-Equilibrium Materials, Computer Science, Metallic Glasses, Glass Transition, Thermodynamics

Takayuki MAKINO

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ACADEMIC:

1993	B.S. in Engineering Science, Kyoto University, Japan
1995	M.S. in Human and Environmental Studies, Kyoto University, Japan
1998	Dr. in Human and Environmental Studies, Kyoto University, Japan

PROFESSIONAL EXPERIENCE:

1998-2001	Special Postdoctoral Researcher, The Institute of Physical and Chemical Research (RIKEN), Japan
2001	Frontier Researcher, The Institute of Physical and Chemical Research (RIKEN), Japan
2001-2002	Foreign Postdoctoral Researcher at the CNRS, Laboratory of Physical Spectrometry, University of Grenoble I, France
2002-2003	Frontier Researcher, The Institute of Physical and Chemical Research (RIKEN), Japan
2003-2005	Researcher, The Institute of Physical and Chemical Research (RIKEN), Japan
2005-2007	Research Associate, Graduate School of Material Science, University of Hyogo, Japan
2008-present	Lecturer, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

The study of solid state photo-physics for optoelectronic applications based on oxide materials

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ACADEMIC:

1995	B.S. in Materials Engineering, Nagoya University, Japan
1997	M.S. in Quantum Engineering, Nagoya University, Japan
2000	Dr. Eng. in Quantum Engineering, Nagoya University, Japan

PROFESSIONAL EXPERIENCE:

2000	Postdoctoral Fellow, Venture Business Laboratory, Nagoya University, Japan
2000-2002	Postdoctoral Fellow, Max-Planck-Institute for Metals Research, Germany
2002-2007	Research Associate, Department of Materials Science and Engineering, Kyoto University
2007-2008	Assistant Professor, Department of Materials Science and Engineering, Kyoto University
2008-present	Lecturer, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

✦ Cu-alloy thin films (interconnects) with self-formed barrier layers for LSI devices.
✦ Low resistance electrodes for wide-gap compound semiconductors.
✦ Functional ceramics and metals controlled the interface (and defect) structures.

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ACADEMIC:

1996 B.S. in Physics, Tohoku University
1998 M.S. in Physics, Tohoku University
2006 Ph.D. in Physics, Tohoku University

PROFESSIONAL EXPERIENCE:

2004-2006	Technical staff, Institute for Solid State Physics, The University of Tokyo, Japan
2006-2007	COE Post Doc., Institute for Materials Research, Tohoku University
2007-2008	Assistant Professor, Institute for Materials Research, Tohoku University
2008-present	Assistant Professor, WPI Advanced Institute for Materials, Tohoku University

CURRENT RESEARCH:

Scanning probe microscopy aiming for data storage/Conductance measurement of nano-materials based on high-resolution AFM lithography

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ACADEMIC:

1993 B.S. in Physics, Jahangirnagar University, Bangladesh
1995 M.S. in Physics, Jahangirnagar University, Bangladesh
2002 M.Phil. in Physics, Jahangirnagar University, Bangladesh
2007 Ph.D. (Science) in Physics, Tohoku University

PROFESSIONAL EXPERIENCE:

1995-2001	Lecturer, Department of Physics, Chittagong University of Engineering and Technology (Former BIT, Chittagong), Bangladesh
2001-2007	Assistant Professor, Department of Physics, Chittagong University of Engineering and Technology, Bangladesh
2007-2008	Assistant Professor, Institute for Materials Research, Tohoku University
2008-present	Assistant Professor, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

- ✦LEEM/PEEM and SPM study of growth and organization of nano-structured device materials, dynamical phenomena on surfaces and growth of thin films
- ✦Organic devices

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ACADEMIC:

1998 B.S. in Material Science and Engineering, Kyushu University, Japan
2000 M.S. in Material Science and Engineering, Kyushu University, Japan
2003 Dr. in Material Science and Engineering, Kyushu University, Japan

PROFESSIONAL EXPERIENCE:

2003-2003	Assistant Professor, Department of Engineering, Kyushu University, Japan
2003-2005	Visiting scientist (JSPS fellow), Center for Solid State Science, Arizona State University, USA
2005-present	Assistant Professor, Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

Transmission electron microscopy such as energy-dispersive X-ray spectrometer (EDS), electron energy-loss spectroscopy (EELS), high resolution electron microscopy (HVEM), electron holography, and electron tomography for advanced materials.

Daisuke HOJO

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ACADEMIC:

1996 B.S. in Natural Sciences, University of Tsukuba, Japan
1998 M.S. in Science and Engineering, University of Tsukuba, Japan
2003 Dr. Eng. in Engineering, University of Tsukuba, Japan

PROFESSIONAL EXPERIENCE:

1999-2000	Part time Research assistant, Texas Instruments Japan, Japan
2000-2003	Doctoral Research, Department of applied physics, University of Tsukuba, Japan
2003-2005	AIST Research Fellow, Advanced Semiconductor Research Center, National Institute of Advanced Industrial Science and Technology (AIST), Japan
2005-2007	Post-doc., Institute of Multidisciplinary Research for Advanced Materials, Tohoku University
2008-present	Assistant Professor, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

✦Thin film deposition with exotic methods as supercritical field
✦Constructing novel nano-structure by impregnating functionalized nanoparticles into porous materials
✦Replicating template structure for optical and catalytic application
✦Nanotechnology-based device development

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ACADEMIC:

1990	B.S. in Earth and Planetary Materials Science, Tohoku University
1997	M.S. in Geology (Earth and Planetary Materials Science), The University of Tokyo, Japan
2000	Dr. Sci. in Geology (Earth and Planetary Materials Science), The University of Tokyo, Japan

PROFESSIONAL EXPERIENCE:

2000-2002	JSPS Postdoctoral Fellow, Department of Complexity Science and Engineering, The University of Tokyo, Japan
2003	21st COE Program Postdoctoral Researcher, Department of Chemistry, The University of Tokyo, Japan
2004	Postdoctoral Researcher, Department of Complexity Science and Engineering, The University of Tokyo, Japan
2005-2006	Research Associate, Department of Complexity Science and Engineering, The University of Tokyo, Japan
2007	Assistant Professor, Department of Complexity Science and Engineering, The University of Tokyo, Japan
2008-present	Assistant Professor, WPI Advanced Institute foe Materials Research, Tohoku University

CURRENT RESEARCH:

✦ Growth of high quality single crystals of organic semiconductor from solution
✦ Electronic devices using single crystals of organic semiconductor
✦ Oriented film growth of organic materials by graphoepitaxy

Daisuke ISHII

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ACADEMIC:

2001	B.A. in Engineering, Tokyo Institute of Technology, Japan
2003	M.S. in Engineering, Tokyo Institute of Technology, Japan
2006	Dr. Eng. in Engineering, Tokyo Institute of Technology, Japan

PROFESSIONAL EXPERIENCE:

2006-2007	Special Postdoctoral Researcher, Frontier Research System, RIKEN, Japan
2007-2008	Special Postdoctoral Researcher, Center for Intellectual Property Strategies, RIKEN
2008-present	Assistant Professor, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

✦ Dissimilar interface and functional surface.
✦ Self-assembly and self-organization.
✦ Organic-inorganic composite material.
✦ Responsible material. (photo chemical, electro chemical, etc）

Jing JU

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ACADEMIC:

1996	B.S. in Chemistry, Jilin University, P.R.China
1999	M.S. in Chemistry, Jilin University, P.R.China
2006	Ph.D. in Chemistry, Peking University, P.R.China

PROFESSIONAL EXPERIENCE:

2003-2007	COE Fellow, Low Dimension, P.R.China
2007-present	Assistant Professor, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

✦ The study of advanced space-charge transport materials based on transition metal borates.

Akiyoshi KUZUME

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ACADEMIC:

1999	B.S. in Chemistry, The University of Tokyo, Japan
2001	M.S. in Chemistry, The University of Tokyo, Japan
2004	Ph.D. in Chemistry, University of Liverpool, UK

PROFESSIONAL EXPERIENCE:

2004	Post-doctoral research fellow, University of Liverpool, UK
2004-2006	Post-doctoral research fellow, Institute of Electrochemistry, Alicante University, Spain
2006-2008	Research Associate, Keio University, Japan
2008-present	Assistant Professor, WPI Advanced Institute for Materials research, Tohoku University

CURRENT RESEARCH:

✦ Electrochemical studies (atomic-scale etching processes) on solid/liquid interfaces using single crystal metal and semiconductor surfaces.

Hongwen LIU

Assistant Professor
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ACADEMIC:

1993	B.S. in Applied Physics, Dalian University of Technology, P.R.China
2001	Ph.D. in Electronic Physics, Peking University, P.R.China

PROFESSIONAL EXPERIENCE:

1993-1996	Assistant Engineer, Shanghai Automation Instrumentation Co., Ltd., P.R.China
2001-2003	Assistant Professor, Institute of Physics, Chinese Academy of Sciences, P.R.China
2003-2005	Postdoctoral Fellowship, The Institute of Scientific and Industrial Research, Osaka University, Japan
2005-2008	Specially Appointed Assistant Professor, The Institute of Scientific and Industrial Research, Osaka University, Japan
2008-present	Assistant Professor, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

✦ Scanning probe microscopy (SPM)-related surface science
✦ STM-induced molecular fluorescence
✦ Plasmonic photonics

Kimitaka MINAMI

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ACADEMIC:

2000	B.S. in Biochemical Engineering, Tohoku University
2002	M.S. in Chemical Engineering, Tohoku University
2005	Dr. in Chemical Engineering, Tohoku University

PROFESSIONAL EXPERIENCE:

2005-2006	Research Fellow, Research Center for Compact Chemical Process, National Institute of Advanced Industrial Science and Technology, Japan
2006-2007	Post-doc., Institute of Multidisciplinary Research for Advanced Materials, Tohoku University
2007-present	Assistant Professor, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

The studies about the synthesis of organic surface-modified inorganic nanoparticles, and the decomposition and solubilization of biomass, by using solvent effects of supercritical water and organic solvents mixtures

Sigemi MIZUKAMI

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1996	B.S. in Applied Physics, Tohoku University
1998	M.S. in Applied Physics, Tohoku University
2001	Dr. Eng. in Applied Physics, Tohoku University

PROFESSIONAL EXPERIENCE:

2001-2005	Research Associate, College of Engineering, Nihon University, Japan
2005-2008	Lecturer, College of Engineering, Nihon University, Japan
2008-present	Assistant Professor, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

✦ The search for new and highly functionalized magnetic materials
✦ Spin dynamics for magnetic multilayer and novel magnetic materials
✦ Basic research of RF spintronics devices using spin momentum transfer

Masanori MUROYAMA

Assistant Professor
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ACADEMIC:

2000	B.E. in Electrical Engineering and Computer Science, Kyushu University, Japan
2002	M.E. in Computer Science and Communication Engineering, Kyushu University, Japan
2008	Ph.D. in Computer Science and Communication Engineering, Kyushu University, Japan

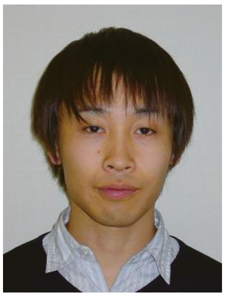
PROFESSIONAL EXPERIENCE:

2005-2008	Assistant Professor, System LSI Research Center, Kyushu University, Japan
2008-present	Assistant Professor, Tohoku University

CURRENT RESEARCH:

✦ The study of integration of LSI and MEMS using low-power and high-reliability design techniques for innovative applications

Ryo NOUCHI



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ACADEMIC:

2000	B.S. in Electronics, Doshisha University, Japan
2002	M.S. in Nuclear Engineering, Kyoto University, Japan
2005	Ph.D. in Nuclear Engineering, Kyoto University, Japan

PROFESSIONAL EXPERIENCE:

2005-2007	Research Fellow, Core Research for Evolutional Science and Technology, Japan Science and Technology Agency (c/o Department of Chemistry, Okayama University), Japan
2007-2008	Specially-Appointed Assistant Professor, Graduate School of Engineering Science, Osaka University, Japan
2008-present	Assistant Professor, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

Molecular electronics using charge transport measurements by means of field-effect transistors and/or adsorbate-solid interactions

Chunling QIN

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ACADEMIC:

1985	B.S. in Chemistry, Zhengzhou University, Zhengzhou, P.R.China
1988	M.S in Chemistry, Zhengzhou University, Zhengzhou, P.R.China
2003	Dr. Eng. in Materials Science and Engineering, Tohoku University

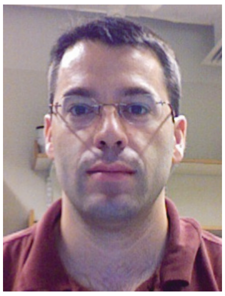
PROFESSIONAL EXPERIENCE:

1988-1991	Research Associate, Department of Chemistry, Huanghe University, P.R.China
1991-1996	Lecturer, Department of Chemistry, Zhengzhou University, P.R.China
1996-2000	Lecturer, Department of Chemistry, Hebei Normal University, P.R.China
2003-2004	Postdoctoral fellow, Institute for Materials Research, Tohoku University
2004-2007	Researcher, Japan Science and Technology Agency (JST), Japan
2007-present	Assistant Professor, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

✦ The study of advanced nonequilibrium metallic materials with amorphous/glassy or glassy composites etc. exhibiting useful physical and chemical properties

Pierre RICHARD



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ACADEMIC:

1998	B.S. in Physics, Université de Sherbrooke, Canada
2000	M.S. in Physics, Université de Sherbrooke, Canada
2004	Ph.D. in Physics, Université de Sherbrooke, Canada

PROFESSIONAL EXPERIENCE:

2005-2008	Postdoctoral Fellow, Department of Physics, Boston College, USA
2008-present	Assistant Professor, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

✦ Photoemission study of the electronic band structure of transition metal oxides and other complex materials (cuprates, cobaltates, ruthenates etc …)

Mitsuhiro SAITO

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ACADEMIC:

1999	B.S. in Physics, Gakushuin University, Japan
2001	M.S. in Materials Science, The University of Tokyo, Japan
2004	Ph.D. in Materials Science, Universität Stuttgart, Germany

PROFESSIONAL EXPERIENCE:

2001-2005	Ph.D./Scientific Co-worker, Max-Planck-Institute for Metals Research, Germany
2005-2006	Postdoctoral Fellow, Max-Planck-Institute for Metals Research, Germany
2006-2008	Postdoctoral Fellow, Advanced Electron Microscopy Group, National Institute for Materials Science, Japan
2008-present	Assistant Professor, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

Quantitative analysis of a local atomic structure of a crystal interface, a grain boundary, and a strongly correlated electron material by an annular dark field (ADF) image in a scanning transmission electron microscopy (STEM) and by a high resolution transmission electron microscopic (HRTEM) image.

Seigo SOUMA

Assistant Professor
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ACADEMIC:

1999	B.S. in Physics, Tohoku University
2002	M.S. in Physics, Tohoku University
2005	Dr. Sci., in Solid-State Physics, Tohoku University

PROFESSIONAL EXPERIENCE:

2005-2006	Postdoctoral Fellowship for Research Abroad, JSPS, Japan
2006-2007	Assistant Professor, Department of Physics, Tohoku University
2007-present	Assistant Professor, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

- ✦Development of spin-resolved ultrahigh-resolution angle-resolved photoemission spectrometer
- ✦Development of high-brilliance plasma discharge lamp for ultra-high resolution photoemission s pectroscopy
- ✦Electronic structure of ordinal or newly discovered exotic superconductors
- ✦Electronic structure of heavy Fermion rare-earth compounds

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Kazunori UENO

Assistant Professor
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ACADEMIC:

1999	B.S. in Engineering, The University of Tokyo, Japan
2001	M.S. in Science, The University of Tokyo, Japan
2004	Ph.D. in Advanced Materials Science, The University of Tokyo, Japan

PROFESSIONAL EXPERIENCE:

2001-2004	Visiting Scientist, National Institute for Advanced Industrial Science and Technology (AIST), Correlated Electron Research Center (CERC), Japan
2002-2003	Graduate student researcher, New Energy and Industrial Technology Development Organization (NEDO), Japan
2004-2008	Researcher, Institute for Materials Research, Tohoku University
2008-present	Assistant Professor, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

Thin film fabrications and device applications of oxide materials for utilizing their various physical properties.

Luyang CHEN

Research Associate
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ACADEMIC:

2001 B.S. in Material Chemistry, Nanjing University of Science and Technology, P.R.China
2006 Dr. Sci. in Inorganic Chemistry, University of Science and Technology of China, P.R.China

PROFESSIONAL EXPERIENCE:

2006-2007	BK21 Postdoctoral Fellow, Korea University, Korea
2007-present	Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

Nanoporous metals materials fabrication, surface enhanced Raman scattering (SERS) properties, and their applications in electrocatalysis.

So FUJINAMI

Research Associate
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ACADEMIC:

2002 B.S. in Applied Physics, The University of Tokyo, Japan
2004 M.S. in Applied Physics, The University of Tokyo, Japan
2007 Ph.D. in Organic and Polymeric Materials, Tokyo Institute of Technology, Japan

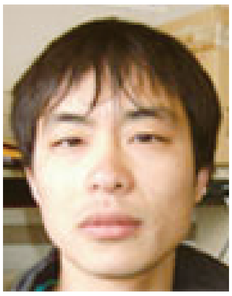
PROFESSIONAL EXPERIENCE:

2007-2008	Postdoctoral Fellow, Institute of Materials Structure Science, High Energy Accelerator Research Organization, Japan
2008-present	Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

Measurement and analyses of nanomechanical properties of polymeric and organic materials, especially using atomic force microscopy.

Nobuyuki FUKUI



Research Associate
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ACADEMIC:

2003	B.S. in Chemistry, Nagoya University, Japan
2005	M.S. in Chemistry, Nagoya University, Japan
2008	Ph.D. in Chemistry, Nagoya University, Japan

PROFESSIONAL EXPERIENCE:

2005 - 2007	Research Assistance (COE), Nagoya University, Japan
2006 - 2007	Grant for young Scientist in COE, Nagoya University, Japan
2007 - 2008	Research Assistance (G-COE), Nagoya University, Japan
2008-present	Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

✦The study of organic/inorganic interfaces by scanning tunneling microscopy (STM)
✦The study of structure of nano-carbon materials by STM

Pengfei GUAN

Research Associate
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ACADEMIC:

2000	B.S. in Solid State Physics, Jilin University, P.R.China.
2003	M.S. in Condensed Matter Physics, Jilin University, P.R.China
2008	Dr. Materials Science, Central Iron & Steel Res. Inst. (CISRI), P.R.China.

PROFESSIONAL EXPERIENCE:

2003-2004	Visiting Student, Institute of Physics, Chinese Academy of Science, P.R.China
2008-present	Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

✦Microcosmic mechanisms of physical and chemical properties in advanced materials

Hiroki HIRAGA

Research Associate
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ACADEMIC:

2003 B.S. in Chemistry, Kanagawa University, Japan
2005 M.S. in Chemistry, Kanagawa University, Japan
2008 Dr. Sci., in Materials Science and Engineering, Tohoku University

PROFESSIONAL EXPERIENCE:

2008- present Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

✦The study of coordination chemistry on functionalized oxide thin film

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Kazumasa HORIGANE

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ACADEMIC:

2002 B.S. in Physics, Aoyama-Gakuin University, Japan
2004 M.S. in Physics and Mathematics, Aoyama-Gakuin University, Japan
2008 Dr. Sci., in Physics and Mathematics, Aoyama-Gakuin University, Japan

PROFESSIONAL EXPERIENCE:

2004-2007 Research Supporter for COE Program, Department of Physics and Mathematics, Aoyama Gakuin University, Japan
2008-present Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

The Development of new materials in superconductor and the study of unusual cobalt oxides magnetism by means of neutron diffraction experiments.

Satoshi IIKUBO

Research Associate
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ACADEMIC:

- 2000 B.S. in Physics, Nagoya University, Japan
- 2002 M.S. in Physics, Nagoya University, Japan
- 2005 Dr. Sci. in Physics, Nagoya University, Japan

PROFESSIONAL EXPERIENCE:

2002-2005	JSPS Research Fellowship (DC), Japan
2005-2008	Post-doc., Quantum Beam Science Directorate, Japan Atomic Energy Agency, Japan
2008-present	Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

Anomalous Hall effect, High-Tc Cu oxides, Superconductor, Magnetic excitation, Non-trivial magnetic structure, Nano-materials, PDF analysis, Negative thermal expansion

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Zhaofei LI

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ACADEMIC:

- 2000 B.S. in Chemistry & Molecular Engineering, Peking University, P.R.China
- 2005 Ph.D. in Chemistry & Molecular Engineering, Peking University, P.R.China

PROFESSIONAL EXPERIENCE:

2005-2007	Postdoctoral Researcher, Institute of Geology, Mineralogy & Geophysics, Ruhr-University-Bochum, Germany
2007-2008	Postdoctoral Researcher, Department of Physics, Tohoku University
2008-present	Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

The study of solid state nano-materials with chemical species confined in nano-sapces. And the study of inorganic materials with exotic physical and chemical properties, especially superconductivity.

Shantanu MADGE

Research Associate
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ACADEMIC:

1995 B.E. in Metallurgy, University of Pune, India
1999 M.E. in Metallurgy, Indian Institute of Science, India
2003 Ph.D in Materials Science & Metallurgy, University of Cambridge, UK

PROFESSIONAL EXPERIENCE:

1995-1997	Graduate Engineer, Tata Motors, India
2003-2005	Guest Scientist, Forschungszentrum Karlsruhe, Germany
2005-2006	Post-Doctoral Research Associate, Arizona State University, USA
2006-2008	Scientist D, ARC International, India
2008-present	Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

Development of newer bulk metallic glasses, fundamental studies of crystallisation in glasses, their deformation and the optimisation of their mechanical properties.

Akira MASAGO

Research Associate
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ACADEMIC:

1995 B.S. in Science, Kochi University, Japan
1997 M.S. in Science, Kochi University, Japan
2001 Dr. Engineering in Science, Osaka University, Japan

PROFESSIONAL EXPERIENCE:

2001-2005	PD, ISIR-SANKEN, Osaka University, Japan
2005-2008	PD, Engineering, The University of Tokyo, Japan
2008-present	Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

The theoretical study of physical phenomena in the scanning probe microscopy

Keisuke TOMIYASU

Research Associate
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ACADEMIC:

- 1997 B.S. Waseda University, Japan
- 1999 M.S. Waseda University, Japan
- 2002 Dr. Sci., Waseda University, Japan

PROFESSIONAL EXPERIENCE:

2002-2005	Research Assistant, School of Science and Engineering, Waseda University, Japan
2005-2006	Postdoctoral Researcher, Neutron Science Laboratory, High Energy Accelerator Research Organization, Japan
2006-2007	Postdoctoral Researcher, Institute for Materials Research, Tohoku University
2007-present	Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

- ✦ Neutron scattering studies of magnetism, strongly correlated electrons, and methodology

Dong WANG

Research Associate
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ACADEMIC:

- 2001 B.S. in Chemistry, Hebei University, P.R.China
- 2004 M.S. in Polymer Chemistry and Physics, Hebei University, P.R.China
- 2008 Ph.D. in Materials Science and Engineering, Tsinghua University, P.R.China

PROFESSIONAL EXPERIENCE:

2008	Research Scientist in Honeywell Specialty Materials Asia Technology Center, P.R.China
2008-present	Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

- ✦ Nano-mechanical properties mapping of polymer nano-composites by atomic force microscopy
- ✦ 3D-visularization of polymer processing by 3D transmission electron microscopy

Zhongchang WANG

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ACADEMIC:

2001 B.S. in Materials Science, Anhui University of Technology, P.R.China
2004 M.S. in Materials Science, Chongqing University, P.R.China
2008 Ph.D. in Materials Engineering, The University of Tokyo, Japan

PROFESSIONAL EXPERIENCE:

2004-2008 Ph.D./Scientific Co-worker, The University of Tokyo, Japan
2008-Present Research Associate, WPI Advanced Institute for Materials Science, Tohoku University

CURRENT RESEARCH:

Quantitative analysis of a local atomic and electronic structure of a crystal interface and a grain boundary through combination of a scanning transmission electron microscopy (STEM) or a high resolution transmission electron microscopy (HRTEM) image with first principle simulation.

Daisuke WATANABE

Research Associate
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ACADEMIC:

2003 B.S. in Applied Physics, Tohoku University
2005 M.S. in Applied Physics, Graduate School of Engineering, Tohoku University
2008 Dr. Eng. in Applied Physics, Graduate School of Engineering, Tohoku University

PROFESSIONAL EXPERIENCE:

2005-2008 JSPS Fellow, Graduate School of Engineering, Tohoku University
2008-present Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

- ✦ Spin transfer phenomenon in nanoscale magnetic materials.
- ✦ Microfabrication process for magnetic tunnel junctions and development of magnetoresistive random access memory (MRAM)

Rui WEN

Research Associate
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ACADEMIC:

2000 B.S. in Physics, Hubei Normal University, P.R.China.
2005 M.S. Beijing Key Laboratory for Nano-Photonics and Nano-Structure, Capital Normal University, P. R.China.
2008 Ph.D. in Chemistry, Chinese Academy of Sciences, P. R.China.

PROFESSIONAL EXPERIENCE:

2008-present Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

- ✦ Atomic-scale Etching Processes of Semiconductor Electrodes
- ✦ Molecular Self-assembly on Electrode Surfaces

Feng WU

Research Associate
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ACADEMIC:

2003 B.S. in Metallurgy Science and Engineering, Central South University, P.R.China
2005 M.S. in Materials Physics and Chemistry, Chinese Academy of Science, P.R.China
2008 Dr. Materials Physics and Chemistry, Chinese Academy of Science, P.R.China

PROFESSIONAL EXPERIENCE:

2008-present Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

Half-metallic ferromagnetic and ferrimagnetic thin films with superior physical properties used in spintronic devices (MRAM)

Shinya YOSHIDA

Research Associate
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ACADEMIC:

2003 B.E. in Engineering, Tohoku University
2005 M.E. in Engineering, Tohoku University
2008 Ph.D. in Engineering, Tohoku University

PROFESSIONAL EXPERIENCE:

2008-present Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

The study of scanning multiprobe data storage systems using conductive polymer as recording media.

Xuefeng ZHANG

Research Associate
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ACADEMIC:

2004 B.S. in Material Science and Engineering, Dalian University of Technology, P.R.China
2008 Ph.D. in Materials Physics and Chemistry, Dalian University of Technology

PROFESSIONAL EXPERIENCE:

2008-present Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

- ✦ Nanocrystalline metals and aloys
- ✦ Synthesis and characterization of the nanomaterials
- ✦ Microwave absorption and electromagnetic response characteristics of magnetic nanoparticles

Takayuki NARUMI

Research Assistant
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ACADEMIC:

2005 B.S. in Physics, Keio University, Japan
2007 M.E. in Nanomechanics, Tohoku University
present Ph. D candidate in Nanomechanics, Tohoku University

CURRENT RESEARCH:

We study the mechanisms of the glass transition theoretically. Although liquids regularly crystallize at the melting point, under rapid quench they can become super-cooled liquids below the melting point, followed by glasses at the glass transition temperature. In these days, the bulk metallic glasses (BMGs) gather engineering attention as well as scientific one. The understanding of the mechanisms of the glass transition leads us to put super-cooled liquids to practical use, to produce more stable BMGs, and so on.

In order to reveal the mechanisms, we focUSAttention on the dynamical heterogeneity appeared in super-cooled liquids slightly above the glass transition temperature. We simulate super-cooled liquids for a simple model by means of molecular dynamics methods and put the results in perspective of statistical physics.

Varu RANI

Research Assistant
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ACADEMIC:

2002 B.S. in Chemistry, Ch. Charan Singh University, India
2004 M.S. in Chemistry, Ch. Charan Singh University, India
2007 M.Tech. in Advanced Chemical Analysis, Indian Institute of Technology, India
2008-present Ph. D candidate in Chemical Engineering, Institute of Multidisciplinary Research in Advanced Materials (IMRAM), Japan

CURRENT RESEARCH:

This is related to the synthesis of the nanoparticles using super critical fluid technology towards biomedical applications. Organic inorganic hybrid nano materials can be synthesized by using the super critical conditions and the particles can be designed so as to be perfectly dissolved into water, solvents or polymers. These hybrid nano materials shows unique properties which can be used in biomedical applications like multi imaging probe and super Drug Delivery System (DDS).

Ryota SHIMIZU

Research Assistant
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ACADEMIC:

2006 B.S. in Science, The University of Tokyo, Japan
2008 M.S. in Science, The University of Tokyo, Japan
2008-present Ph. D candidate in Chemistry, The University of Tokyo, Japan

CURRENT RESEARCH:

✦ Oxide surface
✦ Scanning tunnelling microscopy / spectroscopy

Jungwoo YOO

Research Assistant
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ACADEMIC:

2006 B.S. in Material Science and Engineering, Pohang University of Science and Technology, Korea
2008 M.S. in Material Processing, Tohoku University,
2008-present Ph.D candidate in Chemical Engineering, Tohoku University

CURRENT RESEARCH:

✦ Bio-imaging with quantum dots
✦ Synthesis of organic-inorganic hybrid nanoparticle
✦ Thermodynamical behavior of nanoparticles

In order to stable dispersion of nanoparticles, our laboratory suggested organic-inorganic hybrid nanoparticle, i.e., surface modification of inorganic core by organic surface modifier. We have established the in-situ supercritical hydrothermal synthesis of organic surface modified CeO_2 nanoparticles. These hybrid CeO_2 nanoparticles show high solubility for organic solvents, e.g., THF, $CHCl_3$ and cyclohexane. The solution doesn't show any aggregation even at the high concentration of hybrid nanoparticles. Furthermore, the particles show 'reversible solve and precipitate behavior' by cyclic cooling, heating, diluting and concentrating of the solution. These results suggest that the behavior of our hybrid nanoparticles in good solvents is more similar with that of nonpolar molecules than that of solid core particles and powders. In other words, it is quite similar to phase behavior of a solute-solvent binary system.

In the present study, we investigate the dispersion behavior of the hybrid CeO_2 nanoparticles in organic solvents and suggest a new thermodynamic system as the hybrid nanoparticle-solvent binary system.

Adjunct Professors

Hans-Jörg FECHT

PRIMARY AFFILIATION:

Chaired Professor and Director
Institute of Micro and Nanomaterials,
Ulm University
Albert-Einstein-Allee 47
D-89081 Ulm, Germany
E-mail: hans.fecht@uni-ulm.de

ACADEMIC:

1981	B.S. in Materials Science, Univ. Saarbrücken, Germany
1984	Ph.D. in Materials Science, Univ. Saarbrücken, Germany

PROFESSIONAL EXPERIENCE:

1984-1987	Post-Doctoral Research Associate, Department of Materials Science and Engineering, University of Wisconsin-Madison, USA
1987-1990	Senior Research Associate, Department of Materials Science, California Institute of Technology, USA
1990-1993	Professor of Metalphysics (C-3), University of Augsburg, Germany
1993-1997	Chaired Professor of Materials Science, Technical University Berlin, Germany
1997-present	Chaired Professor of Materials Science and Engineering Director Kompetenzzentrum “Nano- and MicroMaterials” University of Ulm, Germany
2001-present	Senior Scientist / Group leader INT-FZK, Karlsruhe

RECOGNITION:

- Fellow of Max-Kade-Gesellschaft (New York) (1984)
- G.W. Leibniz-Award (Deutsche Forschungsgemeinschaft, DFG) (1998)
- Pioneer of Nanotechnology (Deutsche Bank AG) (2003)
- Innovation Award of German Engineering Foundation VDI (2004)
- Head of Nanomaterials activity of DGM (2005)
- Member of Board ESF European Space Science Council (2006)
- Overseas Professor, Anna University Chennai, India (2007)
- Panel Chair Materials Science of ESSC at European Science Foundation (2008)
- Chairman of Board, High Tech Alliance under the auspices of BMBF (2008)

Chain. T. LIU

PRIMARY AFFILIATION:

Professor and Distinguished Research Professor
Department of Materials Science and Engineering,
The University of Tennessee
Knoxville, TN 37996-2200, USA
Email: liuct@ornl.gov
URL: http://www.ms.ornl.gov/index.shtml

ACADEMIC:

1960	B.S. in Mechanical Engineering, National Taiwan University, Taiwan
1964	M.S. in Materials Science, Brown University, USA
1967	Ph. D. in Materials Science, Brown University, USA

PROFESSIONAL EXPERIENCE:

1967-1982	Research Staff Member, Oak Ridge National Laboratory (ORNL), USA
1983-2005	Group Leader, Oak Ridge National Laboratory (ORNL), USA
1985-1997	Corporate Fellow & Senior Corporate Fellow, Oak Ridge National Laboratory (ORNL), USA
2005-present	Professor & Distinguished Research Professor, University of Tennessee, USA

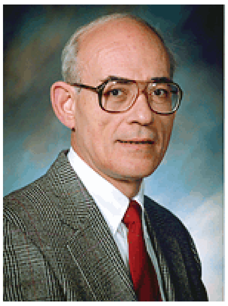
CURRENT RESEARCH:

Fundamental and applied research on plastic deformation and fracture of a variety of advanced materials (refractory alloys, precious metal alloys, superalloys, bulk amorphous alloys, ordered intermetallic alloys, and shape-memory alloys); glass forming ability and alloy design of bulk metallic glasses, thermodynamics and phase relationship; alloying behavior; alloy design of high-temperature structural materials; microstructure and property correlation; materials processing and characterization.

RECOGNITION:

- ✦American Society for Metals, Fellow (1984)
- ✦U.S. Department of Energy, E. O. Lawrence Award (US president Award) (1988)
- ✦Editor, Journal of Intermetallics (1992)
- ✦The Minerals, Metals and Materials Society (TMS), Fellow (1994)
- ✦Brown Engineering Alumni Medal Award, Brown University (1998)
- ✦Acta Metallurgic Inc., Acta Metallurgica Gold Medal (2001)
- ✦Information Sciences Institute, one of 1000 Most Cited Physicists (2001)
- ✦Information Sciences Institute (ISI), Highly Cited Researcher in Materials Science (2003)
- ✦National Academy of Engineering (NAE), Member (2004)
- ✦The Word Technology Network, Fellow (2003)
- ✦Governor of the Acta Materials Board, ASM (2005)
- ✦Chinese Academy of Engineering (CAE), Foreign Member (2006)
- ✦Honorary Member of Japan Institute for Metals (JIM) (2006)

John H. PEREPEZKO



PRIMARY AFFILIATION:

Professor
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ACADEMIC:

1967	B.S. in Polytechnic Institute of New York Brooklyn, USA
1968	M.S. in Polytechnic Institute of New York Brooklyn, USA
1973	Ph.D. Carnegie-Mellon University Pittsburgh, USA

PROFESSIONAL EXPERIENCE:

1968-1970	Assistant Scientist, Fundamental Research Laboratory, U.S. Steel Corporation, USA
1973-1974	Post-doctoral Research Fellow, Carnegie-Mellon University, USA
1975-1978	Assistant Professor, Department of Metallurgical and Mineral Engineering, University of Wisconsin-Madison, USA
1978-1981	Associate Professor, Department of Metallurgical and Mineral Engineering, University of Wisconsin-Madison, USA
1981-2000	Professor, Department of Materials Science and Engineering, University of Wisconsin-Madison, USA
2000-Present	IBM-Bascom Professor, Department of Materials Science and Engineering, University of Wisconsin-Madison, USA

CURRENT RESEARCH:

Study of the mechanism, kinetics and thermodynamics of phase transformations, nucleation during solidification, amorphous metals, rapid solidification processing, metastable phases, intermetallic alloys, high temperature alloys, composite materials and the structure and characteristics of interfaces.

RECOGNITION:

- Exceptional Creativity Award NSF (1982-83)
- University of Wisconsin Polygon Outstanding Professor Award (1983, 1985, 1989)
- American Society for Metals-Milwaukee Chapter Outstanding Service Award (1988)
- Crystal Growth Society - Pittsburgh Chapter Outstanding Research Award (1989)
- Senior Research Prize Award - Alexander von Humboldt Stiftung (Germany) (1996)
- Bruce Chalmers Award - TMS - (1997)
- Editor for Scripta Materialia (2001-2006)
- Senior Research Award – ISMANAM Conference-(2004)
- Fellow Award-TMS-(2004)
- National Academy of Engineering- (2004)
- Visiting Researcher Award – Japan Society for the Promotion of Science – (2005)

Curriculum Vitae of Adjunct Professor

Simon P. RINGER

PRIMARY AFFILIATION:

Professor and Director
Electron Microscope Unit (EMU),
The University of Sydney
NSW 2006, Australia
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ACADEMIC:

1985	B.S. in Metallurgy, The University of South Australia, Australia
1991	Ph.D. in Materials Science and Engineering , The University of New South Wales, Australia

PROFESSIONAL EXPERIENCE:

1991-1993	Research Fellow, Department of Materials Engineering, Monash University, Australia
1994-1995	Research Associate, Institute for Materials Research, Tohoku University
1995-1996	Japan Society for the Promotion of Science Postdoctoral Fellow, Institute for Materials Research, Tohoku University
1997	Acting College Head, Richardson Hall, Monash University, Australia
1996-1997	Deputy College Head, Richardson Hall, Monash University, Australia
1996-1998	Lecturer, Department of Materials Engineering, Monash University, Australia
1998-2001	Senior Lecturer, Department of Materials Engineering, Monash University, Australia
2001-2004	Associate Professor and Director, Electron Microscope Unit (EMU), The University of Sydney, Australia
2001-present	Executive Director and CEO of NANO
2004-present	Director, NANO Analytical Pty Ltd (ABN 112 219 799)

CURRENT RESEARCH:

Phase Transformations, Nanomaterials, Engineering Alloys, Structure/Property Relationships, Materials Characterisation, Al-Alloys, Magnetic Materials, Nuclear Materials, HSLA Steels, Welding, Transmission Electron Microscopy, Energy Dispersive X-ray Analysis, Electron Energy Loss Spectroscopy, Three Dimensional Atom Probe Field Ion Microscopy, Calorimetry, Mechanical Testing, Programming and Software Applications and Development in the UNIX, Mac/PC Environments.

RECOGNITION:

✦Awarded ARC Linkage Industry Research Fellowship (2003)
✦Elected as Fellow of the Institution of Engineers Australasia (2001)
✦City of Monash Business Awards Nominee; Waverley City Council, Victoria (2000)
✦Top 10 reviewer award for review services to the journal Acta Materialia (Elsevier)(1999)
✦42nd International Field Emission Symposium, Madison, WI, USA, Most Outstanding Poster Award (1995)
✦Awarded Japan Society for the Promotion of Science Research Fellowship (1993)
✦Alcan Bicentennial Scholarship, The University of New South Wales, Australia (1990)
✦Doktorand Stipendium', Luleå University of Technology, Sweden (1988)
✦Australian Welding Research Association, Sir William Hudson Memorial Award Winner (1987)

Akira SAKAI

PRIMARY AFFILIATION:

Professor
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ACADEMIC:

1974	B.S. in Physics, The University of Tokyo, Japan
1976	M.S. in Physics, The University of Tokyo, Japan
1981	Ph.D. Physics, The University of Tokyo, Japan

PROFESSIONAL EXPERIENCE:

1981-1987	Research Associate, Institute for Solid State Physics, The University of Tokyo, Japan
1983-1984	Resident Visitor, AT&T Bell Laboratories, Murray Hill, USA
1987-1989	Research Scientist, ULSI Research Center, TOSHIBA Corporation, Japan
1989-1994	Chief Scientist, ULSI Research Center, TOSHIBA Corporation, Japan
1992-2002	Professor, Mesoscopic Materials Research Center, Faculty of Engineering, Kyoto University, Japan
2002-2007	Professor, International Innovation Center, Kyoto University, Japan
2007	Professor, Innovative Collaboration Center, Kyoto University, Japan
2007- 2008	Professor, Graduate School of Engineering, Kyoto University, Japan
2008-present	Professor, Department of Materials Science and Engineering, Kyoto University, Japan

CURRENT RESEARCH:

✦Atomic and molecular contacts

✦Nano-structured materials

✦Surface physics

Koji KAJIMURA

PRIMARY AFFILIATION:

Vice President
Japan Society for the Promotion of Machine Industry
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ACADEMIC:

1965	B.E. in Electric Engineering, Osaka University, Japan
1967	M.E. in Physics, Osaka University, Japan
1972	Dr.Sci., The University of Tokyo, Japan

PROFESSIONAL EXPERIENCE:

1968-1998	Ministry of Economy, Trade and Industry, Electrochemical Laboratory, Japan
1988-1998	Chairperson of Superconductivity Promotion committee, National Institute of Advanced Industrial Science and Technology, Ministry of Economy, Trade and Industry, Japan
1998-1999	Director of National Institute of Advanced Industrial Science and Technology, Japan
1992-1999	Professor, Tsukuba University, Japan
1999-2001	Director of Agency of Industrial Science and Technology, Ministry of International Trade and Industry, Japan
2001-2008	Research Supervisor in Basic Research Programs, Japan Science and Technology Agency
2006-Present	Member of executive board in Science Council of Japan

Masahiro IRIE

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ACADEMIC:

1966	B.E., Kyoto University, Japan
1968	M.E., Kyoto University, Japan
1974	Ph.D., Osaka University, Japan

PROFESSIONAL EXPERIENCE:

1974-1978	Lecturer, the Institute of Scientific and Industrial Research, Osaka University, Japan
1978-1988	Associate Professor, the Institute of Scientific and Industrial Research, Osaka University, Japan
1988-1996	Professor, Institute of Advanced Material Study, Kyushu University, Japan
1996-2007	Professor, Graduate School of Engineering, Kyushu University, Japan
2007-Present	Professor, Rikkyo University, Japan

RECOGNITION:

- ✦Award of the Society of Polymer Science, Japan (1988)
- ✦Award of the Japanese Photochemistry Association (1993)
- ✦Vinci d’excellence “Science pour l’art” (LVMH) (1995)
- ✦Docteur Honoris Causa of University of Bordeaux 1 (2003)
- ✦Chemical Society of Japan Award (2004)
- ✦Mukai Award (Tokyo Ohka Foundation for Promotion of Science and Technology) (2007)
- ✦The Purple Ribbon Medal (2007)

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ACADEMIC:

1969	B.E. in Applied Chemistry, Osaka University, Japan
1971	M.E. in Applied Chemistry, Osaka University, Japan
1976	Ph.D. in Physical Sciences, The Flinders Univ. of South Australia, Australia

PROFESSIONAL EXPERIENCE:

1978-1980	Research Officer, Inorganic Chemistry Laboratory, Oxford University
1980-1981	Assistant Professor, Department of Chemistry, Hokkaido University, Japan
1981-1990	Associate Professor, Department of Chemistry, Hokkaido University, Japan
1990-1995	Professor , Department of Chemistry, Faculty of Science, Hokkaido University, Japan
1995- Present	Professor, Division of Chemistry, Graduate School of Science, Hokkaido University, Japan
1999-2000	Advisor to President, Hokkaido University, Japan
2000-2002	Director, Catalysis Research Center, Hokkaido University, Japan
2000- 2002	Senate, Hokkaido University, Japan
2005-2006	Chairman, Division of Chemistry, Hokkaido University
2007-Present	Concurrent Professor, College of Chemistry and Chemical Engineering, Nanjing University, P.R. China
2007-Present	Director, Collaborative Research Center for Molecular and System Life Sciences, Hokkaido University

RECOGNITION:

- ✦Science Award, The Electrochemical Society of Japan (1993)
- ✦Best Paper Award, The Electrochemical Society of Japan (2000)
- ✦Fellow, IUPAC(2002)
- ✦Fellow, The Royal Society of Chemistry, UK (2005)
- ✦Distinguished Alumni Award, The Flinders University of South Australia, (2006)

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ACADEMIC:

1992	B.S. in Science, Tohoku University
1994	M.S. in Science, Tohoku University
1999	Ph.D in Science, Tohoku University

PROFESSIONAL EXPERIENCE:

1995-1996	Research Fellowship for Young Scientist, Japan Society for the Promotion of Science, Japan
1996-2001	Research Assistant, Graduate School of Science, Tohoku University
2001-2003	Researcher, ERATO Nanospace Project, Japan Science and Technology Corporation (JST), Japan
2004-2007	Group Leader, ERATO Nanospace Project, Japan Science and Technology Agency (JST), Japan
2007-present	Laboratory Head, Advanced Science Institute, RIKEN, Japan
2006-present	Associate Professor, School of Engineering, The University of Tokyo, Japan

RECOGNITION:

- ✦The Society of Polymer Science Japan: Wiley Award (2005)
- ✦The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology, Japan: The Young Scientists' Prize (2008)

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ACADEMIC:

1983	B.S. in Chemistry, Nagoya University, Japan
1985	M.S. in Chemistry, Nagoya University, Japan
1989	Ph.D., Nagoya University, Japan

PROFESSIONAL EXPERIENCE:

1989-1990	Post-doctoral fellowship, Harvard University, USA
1990	Research Associate, Institute for Molecular Science, Japan
1993	Assistant Professor, Osaka University, Japan
2003	Lecturer, Osaka University, Japan
2004-present	Associate Professor, Osaka University, Japan
2002-2006	Researcher, "Synthesis and Control" project in Precursory Research for Embryonic Science and Technology (PRESTO), JST, Japan

WPI-IFCAM

WPI-IFCAM

International Frontier Center for Advanced Materials (IFCAM) was inaugurated in Institute for Materials Research (IMR), Tohoku University, in October 2001 to function, simply stated, as the world-first “materials science think-tank.” With wise steering by past directors, IFCAM has been performing well in its mission until now by 1) bringing in many world-renown researchers to IMR in the greater field of materials science/engineering, 2) enlightening / encouraging young scientists, post-doctoral fellows and graduate students by organizing and supporting workshops/summer schools, and 3) establishing and coordinating IFCAM branch offices around the world, including those in Cambridge University, Harvard University, Stanford University, and Institute of Physics, P.R. China.

We were also so fortunate to have had a government initial-equipment fund in 2002 to acquire several advanced tools, such as 3-dimention atom-probe tomography (3-D AP) and low energy electron microscope (LEEM). With untiring effort of able faculty members and their staff / graduate students, the LEEM program of IFCAM, for instance, has quickly become one of the most active and successful research centers in the world.

Realizing that IFCAM and newly established WPI-AIMR have essentially the same mission: namely, further promote international collaboration and cooperation in innovative research on advanced materials on a global bases, IFCAM was transferred from IMR to WPI-AIMR, effective of April 2008.

Briefly stated, WPI-IFCAM has following function and service.

□. Visiting Professorship
□. Workshops / summer schools

□. Visiting Professorship

Qualified researchers who may be interested in IFCAM visiting professorship should first contact the WPI principal investigator(s) of the related research fields. Your contact PIs will initiate the further process to materialize the joint research.

(1) Tenure: For a period of minimum one month to a maximum of 3 months.

(2) Financial: The salary varies, depending on the qualifications, based on the Tohoku University regulations. Roughly speaking, “full professor” receives Y600,000 per month and “Associate Professor” receives Y500,000 per month.

□. Workshops / summer schools

WPI-IFCAM will financially support the workshops and summer schools, if the scientific aims are along the WPI-AIMR missions. For more information, please contact WPI Administrative Office.

2008-2009 WPI-IFCAM VISITING SCHOLARS

	Candidate	Host	Position	Term							Term	Affiliation	Position	Graduated from	Diploma	Nationality	Age	Research Proposal
				From			~	Through										
1	**Tai-Gang NIEH**	M. Chen	Visiting Professor	H20	7	10	~	H20	8	16	1m17d	The University of Tennessee	Professor	Stanford University	Ph.D	USA	57	Shear Band formation of bulk metallic glasses
2	**Hongwei SHENG**	M. Chen	Visiting Associate Professor	H20	7	1	~	H20	8	25	1m26d	George Mason University	Assistant Professor	Institute of Metal Research, Chinese Academy of Sciences	Ph.D	P.R.China	37	Structural origin of the high forming ability of bulk metallic glass Zr-Cu-Ag
3	**Dong-Lai FENG**	M. Chen	Visiting Professor	H20	7	2	~	H20	8	30	1m29d	Fudan University	Professor	Stanford University	Ph.D	P.R.China	35	Electronic structure of strongly correlated systems
4	**Despo LOUCA**	K. Yamada	Visiting Associate Professor	H20	7	13	~	H20	9	11	1m30d	University of Virginia	Associate Professor	University of Pennsylvania	Ph. D	Cyprus	40	Spin Trasitions and PhaseCompetition in Perovskite Oxides
5	**Chong-Yu WANG**	M. Chen	Visiting Professor	H20	8	2	~	H20	10	30	2m29d	Tsinghua University	Professor; Academician of CAS	University of science and technology Beijing	Ph. D	P.R.China	75	Multiscale Modeling of Bulk Metallic Glasses
6	**Sishen XIE**	M. Chen	Visiting Professor	H20	9	16	~	H20	11	30	2m15d	Institute of Physics, Chinese Academy of Sciences	Professor; Academician of CAS	Institute of Physics, CAS	Ph. D	P.R.China	66	High-Pressure Physics of Single-walled Carbon Nanotubes Nonwoven
7	**Styabrata RAJ**	T. Takahashi	Visiting Associate Professor	H21	1	5	~	H21	3	25	2m20d	Indian Institute of Science Education and Research	Assistant Professor	Utkal University	Ph.D	India	33	Ultrahigh-resolution photoemission study of strongly correlated transition metal oxides

2008-2009 WPI VISITING SCHOLARS

	Candidate	Host	Position	Term							Term	Affiliation	Position	Graduated from	Diploma	Nationality	Age	Research Proposal
				From			~	Through										
1	**Lu-Chang QIN**	M. Chen	Visiting Associate Professor	H20	4	14	~	H20	6	13	2m	University of North Carolina at Chapel Hill	Associate Professor	Massachusetts Institute of Technology	Ph.D	P.R.China	44	Electron Holography and Tomography of Carbon Nanotubes

WPI Activity Report of Prof. Lu-Chang Qin
April 14 – June 13, 2008
Host: Professor Mingwei Chen

My research activities during my two month stay (14 April – 13 June 2008) at the Advanced Institute for Materials Research (WPI) on the Katahira Campus of Tohoku University, hosted by Professor Mingwei Chen, involved two areas: (1) Mechanical properties of Fe-Cu alloys studied by in situ synchrotron x-ray diffraction under hydrostatic pressure and (2) Structural analysis of carbon nanotubes by electron microscopy techniques.

In situ High Pressure X-Ray Diffraction of Fe-Cu Alloys:

In this study, we studied the mechanical and structural properties of two Fe-Cu alloys produced by ball milling. The endothermic process with a positive heat of mixing of the immiscible bcc-Fe and fcc-Cu crystals in the formation of an alloy by ball milling is of fundamental interest in materials science. The purpose of this study is to examine the changes of bulk modulus and the structural characteristics of the bcc-Fe when a small amount of fcc-Cu is added to form an alloy by ball milling. Using materials provided by collaborators, we have prepared three samples (Fe, $Fe_{0.9}Cu_{0.1}$ and $Fe_{0.8}Cu_{0.2}$) for in situ investigations to measure the bulk moduli of the Fe-Cu alloys using the dedicated synchrotron high pressure beam line at the Photon Factory in Tsukuba, Ibaraki. During the course of this study, we examined the changes of the lattice constants of each composition of the Fe-Cu alloys produced by ball milling and have collected powder x-ray diffraction data at various values of hydrostatic pressure up to 10 GPa. Preliminary examinations of the experimental data indicate that there is a noticeable change of the bulk modulus when the concentration of Cu elements is increased, even by 10%. More detailed analysis of the experimental data is underway and a manuscript summarizing the results for publication is in preparation.

Electron Microscopy Study of Carbon Nanotubes:

In the study of carbon nanotubes, it is of vital importance to know the exact atomic structure of the nanotube under examination when the relationship between structure and properties is sought for both fundamental understanding and eventual industrial applications as envisaged in the nanoelectronics devices. While it is now an established method to determine the chirality via chiral indices (n,m) of carbon nanotubes using electron diffraction, the information on the handedness is usually lost

in the electron diffraction intensities. The objective of this project is to utilize the electron holographic and electron tomographic techniques to obtain structural information on the chirality including the absolute handedness of carbon nanotubes using the state-of-the-art 300 kV Cs-corrected high-resolution transmission electron microscope (FEI-Titan). Unfortunately, due to unavailability of this microscope, we have not been able to collect usable experimental data as originally planned during my stay at WPI. In collaboration with Professor Chen and Dr. Takeshi Fujita, we will look for future opportunities to resume this experiment to tackle this problem when the high-performance TEM becomes operational and available.

During my stay at Tohoku University, I also had the opportunity to visit Professor Katsumi Tanigaki's laboratory (Laboratory of Solid State Nanonetwork Materials) in the Department and Physics on the Aobayama Campus and presented a seminar on "Determination of the Chirality of Carbon Nanotubes by Electron Diffraction". Potential and future collaborations with Professor Tanigaki and his group on the studies of the iron-based layered $La(O_{1-x}F_x)$ FeAs superconductors and nanowires were also discussed during my visit.

Last but not the least, I wish to thank Professor Mingwei Chen and WPI for offering me the opportunity to visit WPI and Tohoku University. The excellent support provided by the administrative staff of WPI, and in particular, Ms. Mariko Onodera (Administrate Assistant of the Chen Laboratory), has made my brief stay in Sendai a rewarding experience.

WPI Activity Report of Prof. T.G. Nieh
July 10 – August 17, 2008
Host: Professor Mingwei Chen

The purpose of my stay at WPI as a visiting professor was to study the mechanical properties of nanoporous (*np*) metals using nanoindentation, in particular using the newly-purchased high-temperature nanoindenter at WPI. Nanoporous metals are anticipated to be used for novel MEMS devices. These *np*-devices, sometimes, experience temperature spike which may cause significant softening and even spontaneous failure. Several room temperature nanoindentation experiments have been carried out on *np*-Au, however, high-temperature mechanical response of *np*-Au has not yet been investigated. This is primarily attributed to the fact that samples are generally small for conventional tension or compression experiments. Furthermore, a high temperature testing platform is unavailable. Therefore, my study includes both room temperature and elevated temperatures.

In the course of our study, we encountered several technical challenges associated with using the equipment. With the high accuracy and resolution (< nm), a tight and sustaining temperature control is always necessary in order to minimize the thermal drift of the nanoindentation instrument, especially during a long-time experiment, even at room temperature. The conventional high-temperature adhesive often used for mounting macroscopic specimen (~mm) is inappropriate for our miniature *np*-Au specimens. The texture of high-temperature adhesive is simply too coarse to hold firmly the *np*-samples. A mechanical/magnetic fixture is being designed to overcome this problem. We also modified the sample mount device because the vendor's design blocks the moving of indenter tip toward the testing sample and this can cause major damage of the indenter head.

Despite the above difficulties, a number of experiments have been or are being conducted and they are briefly described as follows.

1. Professor Chen's group has fabricated nanoporous Au (*np*-Au) with the smallest pore size. Thus, nanoindentation of *np*-Au with different ligament (or pore) sizes was conducted at room temperature, to look for a possible breakdown of the length scale.
2. Nanoindentation creep of *np*-Au (and in parallel, the microcompression of *np*-Au pillars fabricated by focus ion beam method) at non-ambient temperatures are being carried out to investigate the thermomechanical properties at elevated temperatures.
3. Nanoindentation of nanoporous noble metals, including *np*-Au, Pt, and Pd, are to be conducted. Professor Chen's group is the only group who can fabricate these samples from bulk metallic glasses. This study is to summarize the general behavior of fcc np-metals and to extend/modify the scaling law of Gibson-Ashby equations.
4. There are two practical ways to measure the strain rate sensitivity of a material using the nanoindentation method. One is to apply different indentation strain rates, and the other is to employ the load change technique during nanoindentation creep.

With the assistance of Dr. Dan, we have completed the nanoindentation creep of *np*-Au at room temperature and are currently analyzing the data. Considering the nanometer-scale ligament and grain sizes, thus a short diffusion distance, we believe the creep mechanism is diffusional, with surface diffusion as the rate controlling mechanism. I anticipated to publishing at least three journal articles using the experimental results obtained. This will place Tohoku U. in the leading position in the understanding of the mechanical behavior of *np*-metals.

Finally, I would like to express my sincere appreciation to Professor Mingwei Chen and every member in his group for their help, especially Dr. Deng Pan's technical support and Ms. Mariko Onodera's administrative assistance.

WPI Activity Report of Prof. Hongwei Sheng
July 1– August 25, 2008
Host: Professor Mingwei Chen

During Prof. H.W. Sheng's visit to WPI from July 1, 2008 trough Aug. 26, 2008, he has been working on topics related to the current research at WPI, in particular, the investigation of atomic-level structure of Zr-Cu-Ag bulk metallic glass (BMG) and the deformation mechanism of BMGs. More specifically, by using computer simulation, he has committed himself to the following topics:

1. Development of high-fidelity interatomic potentials for three multi-component BMG forming alloy systems: Zr-Cu-Ag, Zr-Cu-Al-Ag, and Pd-Ni-P. The development of high-accuracy and high-transferability semi-empirical potentials for multi-component systems has been known notoriously difficult, evidenced from the fact that there exist few interatomic potentials, if not none, in literature to study the many-body effect of complex metallic systems. Following an energy-landscape fitting scheme, he first produced large sets of reference states by performing extensive *ab initio* simulations. Included in the database for potential fitting are atomic configurations that cover large phase space of the systems. For example, for the Zr-Cu-Ag system, around 600 configurations have been generated. The final interatomic potentials, employing the embedded atom formalism, were developed by fitting the pre-defined energy landscape. The finalized potentials were then verified and validated against *ab initio* MD data. More validations involving structure characterization, such as high-energy XRD and EXAFS will be considered in the future. The interatomic potentials as developed will have many implications and great applicability; more computational work is currently under way.

2. Molecular dynamics study of the Zr-Cu-Ag system. By using the newly developed interatomic potentials, the glass formation of the Zr-Cu-Ag system was systematically studied. The atomic structure of the ZrCuAg metallic glass resulting from large-scale MD (> 8,000 atoms) were characterized, atomic packing details revealed. The structural features of the computer-generated ZrCuAg BMGs are consistent with the recent findings of Dr. Fujita that Ag atoms tend to form lone pairs and strings in Ag-lean compositions, (e.g., Ag < 10 at.%). It is also found that the spatial extension and the connectivity of Ag-Ag pairs change as functions of cooling rates and alloy compositions. When the concentration of Ag reaches as high as 20 at.%, atomic segregation of Ag on the nano-meter scale has been identified. The results will be further corroborated and explored by using synchrotron X-ray scattering to be conducted at SPRING-8. Our MD simulation on the ZrCuAg system complements the experimental work done at WPI.
   To investigate the structural origin of the greatly enhanced glass forming ability of the ZrCuAg system, slow dynamics of the supercooled liquids has been studied. While dynamic heterogeneity of the supercooled liquids has been identified, structural analysis of the role of Ag in the dynamically immobile regions has yet to be performed. More computational work in this direction is expected.

3. Large-scale computer simulation of the deformation of BMGs. Deformation mechanisms of BMG remain largely unresolved so far. One of the puzzles lies in how the sample size determines the plasticity as well as shear-banding of BMGs. To this end, by taking advantage of the unique supercomputing capability at WPI, Prof. Sheng has attempted the first ever computer experiments on the mechanical behavior of "real" BMG samples, herein, ZrCuAg, using ~20 million atoms (corresponding to sample size of 50 nm x 50nm x 100 nm). Also studied are the mechanical behavior of small samples, where the size varies from 5~10 nm in diameter. It has been found that those small samples (~10 nm) undergo uniform deformation under mechanical loading. During the deformation, a new phenomenon of atomic segregation /clustering was found. For the 20 million-atom sample, the deformation process on the supercomputer is still in progress, and no conclusive results

can be reached yet.

Last but not least, Prof. Sheng has worked together with researchers (students and postdocs) at WPI, familiarized them with concepts in computational materials science, and taught them computational techniques to deal with various problems. During several tutorials given to them, the researchers were able to learn how to visualize and analyze computational data, how to build semi-empirical potentials from first-principle calculations. Prof. Sheng has worked them through a number of computational packages, varying form ab initio calculations (VASP, WIEN2k) to classical molecular dynamics (lammps) to physical property evaluation (e.g. phonon calculations). He has also helped them to practice on in-house structural analysis and X-ray analysis codes, which will greatly facilitate their future work on high-energy X-ray diffraction.

In summary, Prof. Sheng has mainly worked on computer simulation of bulk metallic glasses during his visit at WPI. While some publishable preliminary results have been obtained, he expects to use more time to iron out the details and hopes to continue the collaboration with WPI (Prof. M.W. Chen) after his returning to the US. Some scientific papers will be written and dissimilated to technical journals such as APL.

WPI Activity Report of Prof. Feng
July 2, 2008 – August 30, 2008
Host professors: Prof. Ming-wei Chen, Prof. Sadamichi Maekawa

During my stay at IFCAM, I have collaborated with local groups, especially Prof. Min-wei Chen's group, on various projects, which are listed in the following.

1. Inelastic x-ray scattering (IXS) experiments on nanoporous gold film. The size effects on the Plasmon dispersion of confined systems is one of the active subjects in the field of plasmonics. During my stay, I conducted IXS experiments at Spring8 on nanoporous gold film samples, which were provided by Dr. Lang in Prof. Chen's group. The pore sizes were 5nm, 10nm, 20nm. During the experiments, we have observed the Plasmon dispersion. Because the signal is quite weak, we decide to grow much thicker samples, and will continue the measurements in the next beamtime.

2. Collaboration on the newly discovered Iron based high temperature superconductors. My group has succeeded in synthesizing $NdO_{1-x}F_xFeAs$, $BaFe_2As_2$, $Ba_{1-x}K_xFe_2As_2$ samples. During my stay, Prof. M. W. Chen and Dr. L. Zhang at IMR has conducted XRD, Raman, EELS, EDX, TEM experiments on these samples, and obtained interesting results. I myself have conducted photoemission measurements on these samples at UVSOR, and HiSOR synchrotrons in Japan. I have helped with data analysis and interpretation. We set up a discussion session with Prof. Maekawa, Dr. Mori, and Prof. Toyama on these data. As results of this collaboration, Prof. Chen has submitted a research proposal to JST (Prof. Maekawa and myself as co-PI). Two manuscripts have been written and will be submitted to academic journals soon. We will continue the collaborative research along this line in the years to come.

3. Collaboration on the electronic structure of BiBaKCoO. BiBaKCoO is a kind of misfit structured system with a highly strained interface. We have conducted photoemission measurements and found some very interesting charge transfer across the internal oxide interface. However, since the oxygen nonstoichiometry at the interface will directly affect the electronic structure, it is unclear the charge transfer is due to doping or strain. In order to determine the oxygen concentration, Prof. Chen has conducted WDS measurements on BiBaKCoO, and provided the critical data of oxygen concentration, which helped me to interpret the measured electronic structure.

4. Setting up collaboration on Photoemission measurements of various bulk metallic glasses (BMG). I have learnt about BMG during my visit. It is a new field to me, and I am quite fascinated by some of the physics there, and interested to combine my specialty of photoemission spectroscopy with BMG. Prof. Chen, Nieh, Sheng and I had a lot of discussion on these materials. Prof. Chen has provided me samples of several BMG's, we will conduct photoemission measurements soon.

5. Setting up more collaborations with other IMR professors. Prof Maekawa has helped to introduce Prof. Y. Iwasa to me. Prof. Y. Iwasa and I will collaborate on measuring the electronic structure of ZrNCl compounds synthesized by Prof. Y. Iwasa's group.

During the period of my stay at IFCAM, I also had the opportunity to interact with Prof. Shimada at Hiroshima university, and with visiting Professors H. Sheng, and T. G. Nieh.

This visit at IMR is really a fruitful one, I have enjoyed the collaboration with several groups here, particularly Prof. Ming-wei Chen and his group.

Finally, I would like to thank WPI, IMR, Tohoku University and Prof. **M. W. Chen** and Prof. **S. Maekawa** for giving me this opportunity. I am very grateful for their kindness and hospitality during my stay in Sendai.

Announcement

Junior Faculty/Post-doctoral Positions

Tohoku University
WPI-AIMR

Effective October 1, 2007, Tohoku University created a new Research Institute, the Advanced Institute for Materials Research (AIMR), based on an initiative of the Japanese Department of Education (MEXT) for World Premier International Research Center Initiative (WPI) to bring together scientists involved in research on nano-science and technology.

In the 21st century, material science, broadly defined as the study of how complex/novel properties arise in matters/materials from the interactions of individual components, will comprise of inter-discipline collaboration.
(HTTP://WWW.WPI-AIMR.TOHOKU.AC.JP).

Over the next few years, as many as one hundred new appointments at the levels of post-doctoral fellows and junior faculty will be available. All innovative researchers are welcome as active promoters of basic/applied sciences in the fields of physical metallurgy, physics, chemistry, precision mechanical engineering and electronic / informational engineering.

We are continuously looking for excellent applicants throughout the year.
Please submit
1) **a curriculum vitae,**
2) **research proposal (<3,000 words),**
3) **summary of previous research accomplishments (<2,000 words),**
4) **copies of 5 significant publications, and**
5) **2 letters of recommendation**

by email to **yoshi@mail.tains.tohoku.ac.jp,**
sakurai@imr.tohoku.ac.jp, and
wpi-office@bureau.tohoku.ac.jp.
All files must be submitted electronically in pdf or Word format.

Applications from, or nominations of, women and minority candidates are encouraged. Tohoku University WPI-AIMR is an affirmative action / equal opportunity employer.

Graduate Student scholarship
In Materials Science/Engineering

WPI-AIMR
Graduate Student scholarship

Effective October 1, 2007, Tohoku University created a new Research Institute, the Advanced Institute for Materials Research (AIMR), based on an initiative of the Japanese Department of Education (MEXT) for World Premier International Research Center Initiative (WPI) to bring together scientists involved in research on nano-science and technology.
In the 21st century, material science, broadly defined as the study of how complex/novel properties arise in matters/materials from the interactions of individual components, will becomes an essential and most important research topics
(HTTP://WWW.WPI-AIMR.TOHOKU.AC.JP).
TU WPI-AIMR is now looking for young motivated Ph.D. graduate student candidates in the fields of physical metallurgy, physics, chemistry, mechanical engineering and electronic / informational technology. All innovative M. S. students are welcome as active promoters of basic/applied sciences in these fields.

Applications are continuously screened throughout the year.
Please submit

1) **a curriculum vitae,**
2) **research proposal (<1,000 words),**
3) **2 letters of recommendation,**

by email to
yoshi@mail.tains.tohoku.ac.jp,
sakurai@imr.tohoku.ac.jp, and
wpi-office@bureau.tohoku.ac.jp.
All files must be submitted electronically in pdf or Word format.

WPI-AIMR

Workshop Guideline

Tohoku University's new Research Institute, the Advanced Institute for Materials Research (WPI-AIMR) solicits several applications per year for International Workshops in the field of "broadly defined Materials Science."

Guidelines:

1) Organizers

Qualified research staff of academic institutions and public or private research establishments can submit the application for an international workshop to be held at WPI-AIMR or its Satellite branches, jointly with the WPI-AIMR principal investigator(s) whose research interest overlaps with the scope of the workshop.

2) Financial support

Under normal circumstances, WPI-IMR supports up to 2/3 of the workshop budget, while the organizer is expected to cover the rest.

3) deadline

The application must be received at least four months in advance

to

yoshi@mail.tains.tohoku.ac.jp,
sakurai@imr.tohoku.ac.jp, and
wpi-office@bureau.tohoku.ac.jp.

All files must be submitted electronically in pdf or Word format.

Appendix

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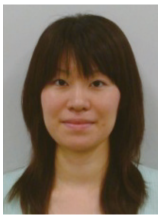

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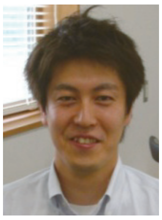

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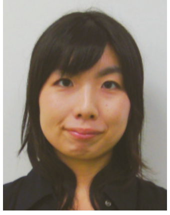

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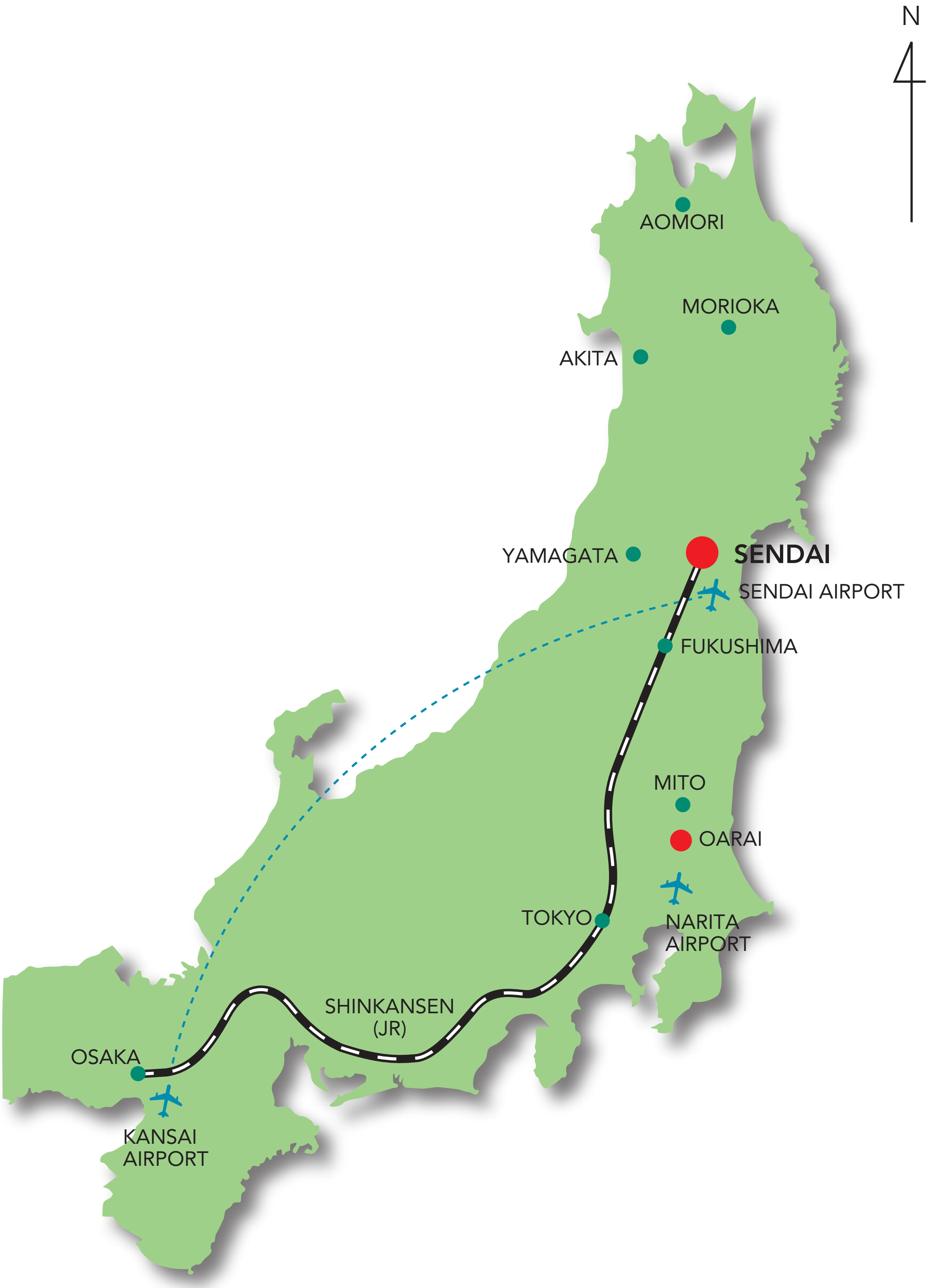

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