NIMS NOW

National Institute for Materials Science

Vol.1 No.7 December, 2003 English Edition

RESEARCH FRONTLINE

Development of Simulation Method for Nano-scale Microstructure Evolution in Practical Materials

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Because material properties such as strength and magnetic properties largely depend on the nano-scale material structure, microstructure control at the nano-scale level is indispensable for developing materials with excellent properties. The PST Group therefore developed a computer simulation system which makes it possible to predict and analyze the nano-scale structure based on the phase-field method. This is a new method in which microstructure morphology is expressed in terms of variables such as concentration, degree of order, etc., and the microstructure evolution process is analyzed by calculating changes in these variables over time.

The figures at the right show calculated examples of the γ' precipitate formation process in a heat-resistant Ni-Al alloy (Fig.1), the microstructure evolution process in a ZrO_2-Y_2O_3 system, which is popular as a partially stabilized zirconia (Fig.2), microstructure evolution during film formation with a Co-Cr alloy hard disk material (Fig.3), and evolution of a nano-granular structure including FePt particles and the order-disorder phase transition of the FePt phase (Fig.4). In all cases, the simulations closely reproduced experimental results.

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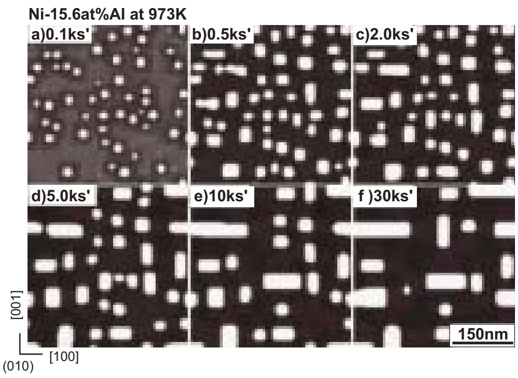

Fig.1 Phase decomposition during isothermal aging of Ni-Al alloy (white: γ ' phase).

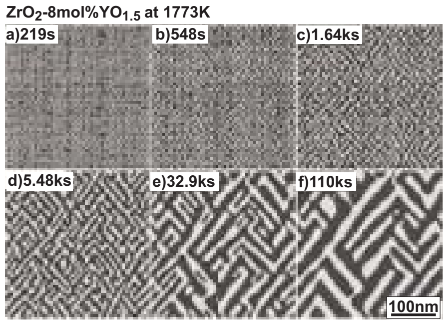

Fig.2 Microstructure evolution process during isothermal aging of ZrO_2-Y_2O_3 system (dark phase: Y-enriched phase formed by phase decomposition in tetragonal crystals).

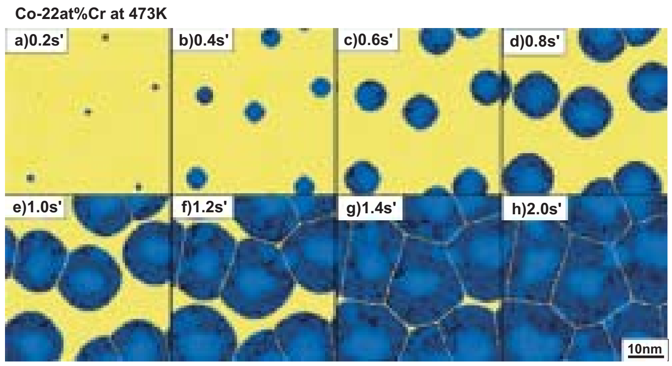

Fig.3 Microstructure evolution process of Co-Cr film during sputtering (yellow: substrate, blue: Co-Cr phase; lighter blue corresponds to Co enrichment).

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Multi-functional 3-Dimensional Nanostructures

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Advanced Materials Laboratory(AML)

Three-dimensional nanostructures hold great promise in a wide variety of applications. The Functional Glass Group is conducting research on these materials by applying anodizing technology, which improves durability by oxidizing the surface of aluminum.

Figure 1 shows the method of fabricating the structure which will be used as the basic pattern. First, a thin aluminum film is applied to a glass plate with a transparent, electro conductive thin film of the type used in liquid crystal displays. The Al film is then electrolyzed in an aqueous solution of acid, forming a thin film of aluminum oxide (Al_2O_3) with an array of pores several nanometers to 10s of nanometers in size opening perpendicular to the glass surface. This corresponds to the process by which an Al film is oxidized to form alumina. Here, the conductive film serves as an electrode, promoting electrolysis of Al until the end of the process. The pore size can be increased up to several 100s of nanometers by slightly dissolving the Al_2O_3 with acid. The fact that pores can be enlarged using acid to form through-thickness pores is an unprecedented feature and is closely related to multi-functionality. The pore size varies greatly depending on the type of acid solution used in electrolysis. The number of pores is inversely related to the voltage during electrolysis and can be controlled in the range of roughly 100 million to 1 trillion/mm2. This completes the basic pattern.

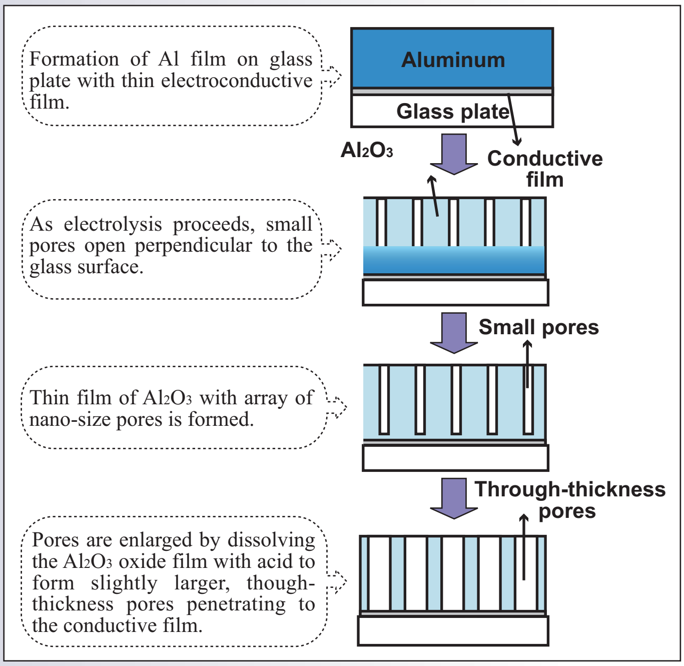

Fig.1 Procedure for forming nanostructure pattern on glass surface.

Next, an even wider variety of 3-dimensional nanostructures can be created by introducing various substances into the pores. The main methods used to introduce substances into these micropores, which have diameters of several 10s of nanometers, are a leak-type process, in which the substance is conveyed to the pore wall in liquid form, and a plating-type process, in which a metal is layered on the conductive film, which serves as an electrode. Examples can be seen in the electron microscope image of nickel-nanorod array (Fig. 2), which was formed by introducing metallic Ni into the pores by the plating method and then dissolving the Al_2O_3 film with acid, and the image of a tubular titanium dioxide (TiO_2) nanostructure fabricated by introducing a Ti-containing solution, shown below (Fig. 3).

We are now involved in developmental research on magnetic disks with ultra-high recording capacities, parts for optical telecommunications, new-type solar cells, high performance catalysts, and other potential products using this method.

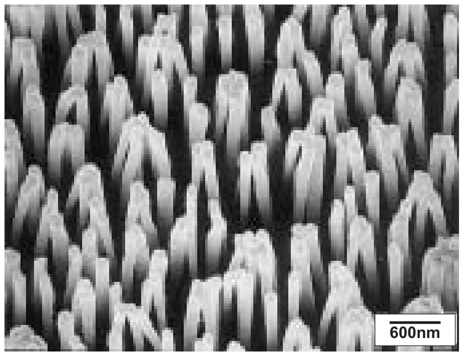

Fig.2 Electron microscope image of nickel-nanorod array.

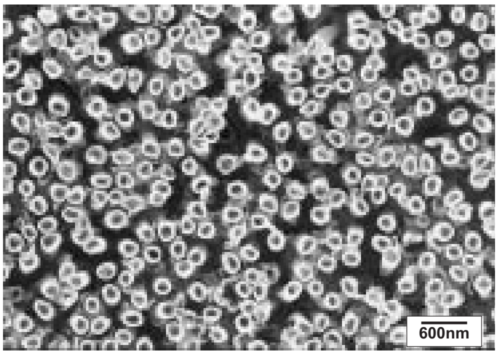

Fig.3 Electron microscope image of tubular-shaped nanostructure of TiO_2.

Receiving of Graduate Students from Charles University

Beginning in 2002, NIMS received doctoral-level students from Charles University in Prague, Czech Republic, which has the richest tradition among the universities in central Europe, under the memorandum on International Joint Graduate University Program with that university. NIMS also began receiving five new graduate students this year. Students from Charles University are expected to engage in research at NIMS for 6 months to one year and write a thesis for a degree based on the results.

Development of Atmospheric Corrosion Test Devices

Hiroyuki Masuda
Corrosion Analysis Group
Materials Engineering Laboratory (MEL)

Although necessity may be the mother of invention, seven years after the start of research on atmospheric corrosion in the STX-21 (Ultra-Steels) Project, the true nature of atmospheric corrosion is at last gradually being revealed. This report describes three recently-developed devices for research on atmospheric corrosion.

The first is a portable surface reaction measuring device (shown in photo). In Japan, some steel structures such as bridges are constructed using weathering steel, which is used without painting. The steel surface forms a stable protective rust film, preventing further corrosion, but the protective property cannot be judged by visual inspection. Based on the principle that electric potential shifts from noble to base (becomes lower) when corrosion occurs, this device enables in situ judgment of the protective property of the rust film from the potential behavior when water is dripped on the structure surface. In spite of its low cost, a built-in CPU gives the device high expandability. For example, when used in combination with an X-Y stage, basic research work such as measurement of potential distribution is possible.

The second device is a new atmospheric corrosion tester. In actual environments, corrosion progresses most rapidly when sea salt particles with diameters of approximately 10 μm accumulate on a metallic surface which is subject to a cyclical process of condensation and drying (evaporation). However, atmospheric corrosion testers currently available in the market have various disadvantages. For example, the equipment is expensive, with prices of ¥10 million or higher, but because the saltwater spray method is used, it cannot reproduce actual environments. With the new tester, any desired condensation/drying process can be simulated while controlling the generated quantity of sea salt particles. Accuracy is high, and the cost of a test-manufactured unit was extremely reasonable, at less than ¥500,000.

The third item is a portable measuring device for airborne sea salt particles. Because the corrosion rate of steel materials depends on the number of airborne sea salt particles, when constructing steel structures, it would be extremely useful in deciding the need for higher grade steel and/or painting if the concentration of airborne salt could be known in advance. However, no existing device was capable of measuring the airborne salt concentration in a short period of time. Using a silver-coated quartz resonator (piezoelectric resonator), this device measures the salt concentration, distinguishing salt particles from other airborne matter, based on frequency changes in the quartz resonator when the humidity in a simple closed container is changed. High accuracy measurements can be obtained by exposing the quartz resonator for as little as 2-3 days.

Fig. Portable surface reaction measuring device.

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RESEARCH FRONTLINE

Development of Simulation Method for Nano-scale Microstructure Evolution in Practical Materials

Because results can be obtained in several minutes, even with an ordinary personal computer, trial-and-error computer experiments in microstructure evolution are possible. The chemical composition and heat treatment conditions for obtaining the optimum microstructure can be determined efficiently, providing a powerful tool for material design.

On September 12, researchers at NIMS, the National Institute of Advanced Industrial Science and Technology (AIST), Tohoku University, and Kyushu Institute of Technology launched a venture company called Material Design Technology Co., Ltd. to handle the full range of material design problems using a system which combines this simulation method and a thermodynamic database of alloy phase diagrams, and applied to NIMS and AIST for recognition as an approved venture business.

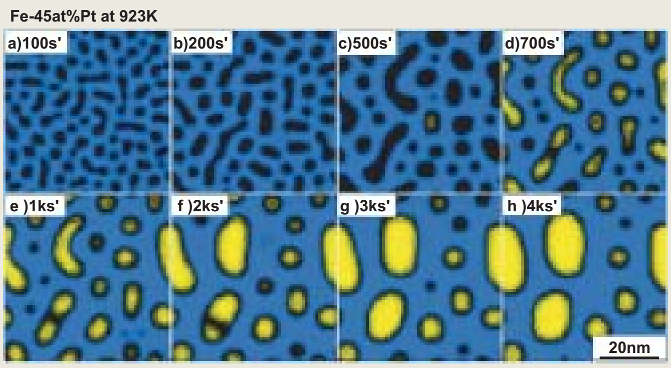


Fig.4 Phase separation process in FePt granular structure (blue: amorphous alumina phase, black: disordered fcc phase of FePt, yellow: $L1_0$ ordered phase of FePt.).

SPECIAL REPORT

Technology Evolution and Technical Cooperation at NIMS

Hidetoshi Nakamura
Technology Evolving Office (TEO)
Research Promotion Division

1. Joint Research with Private Companies

NIMS actively promotes joint research with private companies, carrying out a total of 113 such projects in fiscal 2002. In fiscal 2003, NIMS inaugurated the following new types of joint research to encourage closer cooperation with private companies, and has already received several tens of millions of yen in funding from the private sector.

Type of research	Outline
Joint research with partial funding from private companies	Private companies bear part of the cost required to implement joint research at NIMS.
Joint research with matching funds	Private companies bear part of the cost required to implement joint research at NIMS, and NIMS pays costs necessary for the joint research under a separate framework.

2. Technical Consulting

In fiscal 2002, NIMS began providing technical consulting services by researchers when requested by private companies. The scope and content, cost, and conditions of these technical consulting services are decided contractually through discussions with the client. NIMS provided technical consulting services in 9 cases in fiscal 2002.

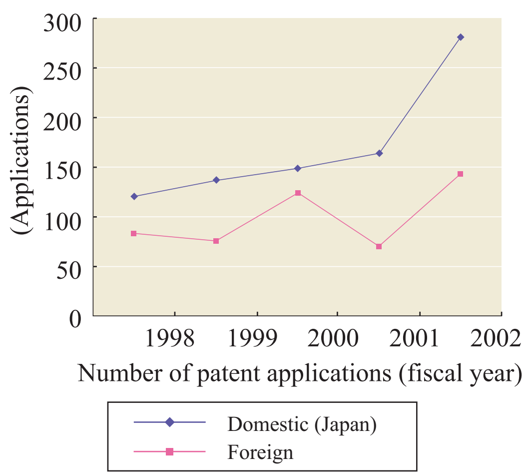
3. Consigned Research

Upon request by outside organizations, NIMS performs research, testing, etc. on consignment.

4. Patent Applications/Licensing

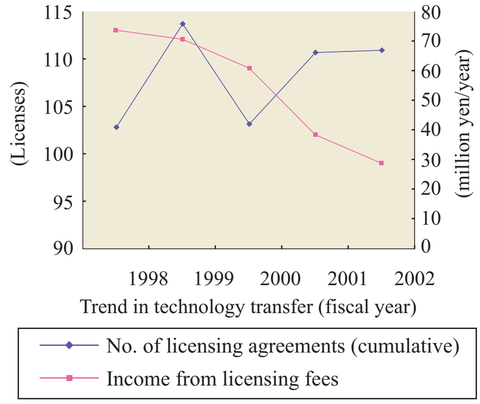
(1) Patent applications

NIMS actively protects the results of its research by applying for patents, and submitted a total of 424 applications in fiscal 2002 (domestic: 282, foreign: 142).



(2) Licensing

Licensing negotiations are conducted with private companies, principally by the Technology Evolving Office. In some cases, the licensing process is consigned to the Japan Science and Technology Agency (JST). In fiscal 2002, NIMS concluded 9 new licensing agreements and had income from licensing fees totaling approximately ¥67 million.



5. Support for Venture Businesses

As part of its effort to encourage practical application of research results, NIMS created NIMS Venture Business Support System in fiscal 2002. Firms approved as NIMS Venture Business are also eligible to use NIMS facilities and equipment at low cost.

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Visit by Deputy Vice-Chancellor of the University of Queensland

On August 7, NIMS concluded an agreement with the five main Australian universities (Sydney, Melbourne, New South Wales, Queensland, and Western Australia) based on a system of international cooperation among graduate schools in the field of materials science. Commemorating this event, Prof. David Siddle, Deputy Vice-Chancellor (Research) at the University of Queensland, visited NIMS on October 14. Prof. Siddle has also served as Pro-Vice-Chancellor (Research) at the University of Sydney, and thus is a central figure among the Deputy Vice-Chancellors of the five leading universities. During his visit, he met with NIMS' President Kishi and discussed ways of promoting the development of the new system. Beginning next year, NIMS plans to receive approximately five graduate students from Australia.

Nano-Structured Porous Catalyst Material Using High Polymer Base

—Development of bio-inspired technology—

Junzo Tanaka
Toshiyuki Ikoma
Regeneration Materials Group
Biomaterials Center(BMC)

PRESS RELEASE

Porous silver materials are used as catalysts, electrochemical materials, heat-radiating materials, and biological filters. Porous materials are produced by impregnating metal ions in a porous substance such as alumina or pumice, followed by chemical reduction under heating. As one particular advantage, they have an extremely large specific surface area in comparison with ordinary metallic powders. Thus, for example, catalysts are especially effective when used with a porous carrier.

In the present work, which was carried out with the cooperation of the University of Bristol (Prof. Stephen Mann) in the UK, we succeeded in developing a porous material with an extremely large specific surface area by the method called "bio-inspired technology." Because materials of this type can be used not only with metals such as gold and silver, but also with oxides and oxide/metal composites (e.g. silver/copper oxides, silver/titanium oxides), development is currently in progress in a variety of fields with the aim of effectively utilizing the properties of high polymers.

As a high polymer, the polysaccharide dextran was used. This substance is glutinous and has the advantage of low cost. Dextran and metallic salts were mixed well to produce a paste, which was then heated to a temperature from 500℃ to 900℃, oxidizing and burning the high polymer component to form a porous body. The porous material thus obtained is shown in the figure.

Pores form in the material when dextran swells due to thermal decomposition at high temperature. In some cases, interconnected pores with sizes of 1〜20μm were observed. The structure of these pores varied depending on the baking temperature.

The bio-inspired method developed in this work can be employed to synthesize oxide substances with a wide-range of nano structures. Furthermore, the fact that it is not necessary to use alumina or pumice as the base material for producing a porous structure, as with conventional techniques, offers numerous practical advantages, including economy, larger scales of production, and simplicity in the manufacturing process.

(These research results were reported in the June issue of the English journal "Nature Materials," and have also been presented in various Japanese-language newspapers, including the Nikkan Kogyo Shimbun, Japan Industrial Journal, Nikkei Industrial Shimbun, and Chemical Daily.)

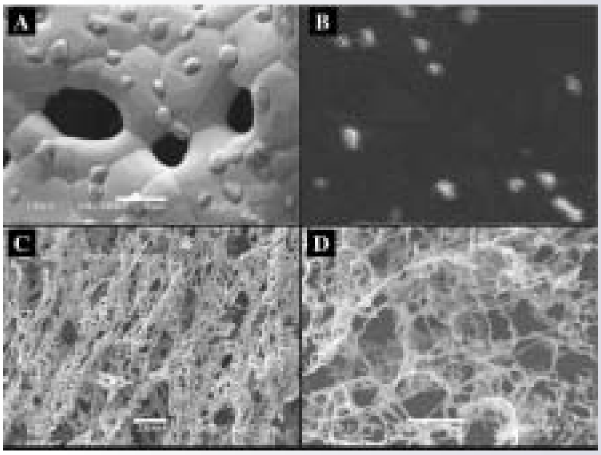

Fig. Structure of porous material. A: Porous material of silver with uniformly dispersed CuO (baking temperature: 800℃), B: Distribution of Cu at same location as in A (EDS analysis), C: CuO baked at 800℃, D: Ferric oxide (γ Fe_2O_3) baked at 600℃.

NIMS NEWS

Visit to NIMS by Prince and Princess Akishinomiya

NIMS was honored with a visit by Prince and Princess Akishinomiya on October 14 as part of a regional inspection tour in Ibaraki Prefecture. The royal couple also attended the opening ceremony of the 6th International Asia Design Conference. They visited the 1st Floor Exhibition Room at NIMS' Sengen Site Central Building and a display area of the Steel Research Center at Structure Control Laboratories.

Explanation of research and development in STX-21 (Ultra-Steels) Project (Structure Control Laboratories).

Talk by President Kishi Marks Mid-point in NIMS Mid-term Plan

Talk by President Kishi (Sengen Site Lecture Hall).

In October 2003, NIMS reached the mid-point in its first 5-year Mid-term Plan following its establishment as an independent administrative institute. On October 1, which marked the actual mid-point, the President of NIMS, Prof. Teruo Kishi, spoke to the assembled staff, reflecting on the history and achievements of the organization in the past 2 1/2 years and offering his beliefs on the direction NIMS should take in the future. At the same gathering, a booklet entitled "At the Mid-point in the Mid-Term Plan" was distributed to all participants.

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