Laboratory for Advanced Materials

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I-1. Development Research Division
Nanoscale Structure-Controlled Materials Group

【Research Activities】

Controlling structure in the nanometer scale range by raising the purity of elements, alteration in the casting methods, and optimization of additional elements are necessary to obtain glassy alloys possessing a tough nature and an outstanding functionality. High-resolution transmission electron microscope showed the existence of atomic arrangement at nanometer scale, and correlated the excellent features and characteristics exhibited by the glassy alloys. Our aim is to develop a high performance, and low cost hydrogen permeable film using amorphous materials, instead of high cost Pd-based alloys. We have successfully developed a Ni-Nb-Zr ternary alloy in which Nb and Zr are used for acquiring the high hydrogen permeability, while the Ni controls the hydrogen embrittlement.

1. H. Kato, K. Yubuta, D.V. Louzguine, A. Inoue and H.S. Kim: Influence of Nanoprecipitation on Strength of $Cu_{60}Zr_{30}Ti_{10}$ Glass Containing μm-ZrC Particle Reinforcements, Scripta Materialia, **51** (2004), 577-581.

2. Y. Yokoyama, K. Fukaura and A. Inoue: Effect of Ni Addition on Fatigue Properties of Bulk Glassy $Zr_{50}Cu_{40}Al_{10}$ Alloys, Materials Transactions, JIM, **45** (2004), 1672-1678.

3. W. Zhang, D.V. Louzguine and A. Inoue: Synthesis and Magnetic Properties of Fe-Pt-B Nanocomposite Permanent Magnets with Low Pt Concentrations, Appl. Phys. Lett., **22** (2004), 4998-5001.

4. S. Yamaura, Y. Shimpo, H. Okouchi, M. Nishida, O. Kajita and A. Inoue: The Effect of Additional Elements on Hydrogen Permeation Properties of Melt-Spun Ni-Nb-Zr Amorphous Alloys, Materials Transactions, **45** (2004), 330-333.

【Plan】

Various examinations are required to increase the reliability of metallic glasses as an engineering material. We aimed to establish a quality-controlled method for fabrication of glassy alloys. A new solidification-controlled process is developed, which can control the glassy structure at atomic scale. Scanning penetration electron microscopy, and EDS/EELS methods were used to clarify the structure, atomic arrangement, elemental distribution with in the material, and their correlation with material's characteristics. Development of glassy alloy possessing high hydrogen permeability, and high resistance of hydrogen embrittlement is also one of the objectives of this work. Furthermore, thin films of the alloy will be produced in order to obtain an improvement in the actual penetration flux.

I-2. Development Research Division
Microscale Structure-Controlled Materials Group

【Research Activities】

We have carried out the basic research for the development of highly efficient energy materials, electronic information materials, and social welfare bio-materials. Following remarkable results were obtained in year 2004:

(1) We have examined the effects of addition of transition metals on the corrosion resistance of Cu-based bulk metallic glasses. Corrosion resistance of Cu-based bulk metallic glasses is found to improved significantly by the addition of a small amount of Nb.

(2) We have developed Ni-Nb-Zr-based metallic glass/amorphous alloy in wide-ribbon form, which can be used as a hydrogen permeable film and a fuel cell element.

(3) We have studied the structural stability of Zr-based metallic glasses against the heavy compression. It was found that the Zr-Al-Ni-Cu metallic glass is extremely stable against the deformation. Based on the above results, we have developed a Fe-based metallic glass for shot peening.

(5) Ferromagnetic Fe-Pt nano-particles were obtained by etching boundaries in the rapidly quenched Fe-Pt-B amorphous alloy ribbons.

(6) We have succeeded in the improvement of bone-compatibility of an implanted titanium material by calcium titanate coating.

(7) We have developed Cu-Zr alloys having higher tensile strength compared to commercially available Cu-Be based alloys with electrical conductivity ~ 30%IACS.

(8) We have developed quasi-crystalline particles dispersed in Al-Fe-Cr-Ti-Co alloy having high-specific strength, and high-heat resistance by using an extrusion method.

1. K. Asami, C.-L Qin, T. Zhang and A. Inoue: Effect of Additional Elements on the Corrosion Behavior of a Cu-Zr-Ti Bulk Metallic Glass, Mater. Sci. Eng., **A375-377** (2004), 235-239.

2. S. Sobu, H. Kimura, D.V. Louzguine and A. Inoue: Formation, Thermal Stability and Mechanical Properties of Aluminum-Based Glassy Alloys Containing Boron, Mater. Trans., **45** (2004), 1204-1209.

3. T. Yamamoto, M. Taya, Y. Sutou, Y. Liang, T. Wada and L. Sorensen, Magnetic Field-induced Reversible Variant Rearrangements in Fe-Pd Single Crystals, Acta Materialia, **52** (2004) 5083-5091.

【Plan】

We have carried out the research and development of the novel substances, and materials applicable as energy, electronic, and bio-materials based on the results obtained in year 2004. Especially, the priority was given to the following research topics:

(1) Investigation of relationship between the microstructure and the ultra low-coercive force observed in Fe-based soft magnetic bulk metallic glasses.
(2) Preparation of large sized bulk specimen of Fe-based metallic glasses.
(3) Development of metallic glass/amorphous alloys having excellent hydrogen permeability.
(4) Development of metallic glass for portable electronic equipments.
(5) To study the influence of Fe addition on the undercooled liquid region of Zr-based metallic glass.
(6) Improvements in the magnetic properties of ferromagnetic Fe-Pt nano-particles obtained from Fe-Pt-B amorphous ribbons.
(7) Direct preparation of Fe-Pt-M-B nano-crystalline alloy with $L1_0$-phase by rapid quenching.
(8) To investigate the mechanism involved in the improvement of bone-compatibility by calcium titanate coating.
(9) Development of Cu-Zr alloy wires having good electrical conductivity and high tensile strength.
(10) Development of quasi-crystalline particles dispersed in Al-Fe-Cr-Ti-Co alloy having high-specific strength and high-heat resistance by extrusion method.
(11) To study the mechanism of a rubber-like behavior in single crystal Fe-Pd ferromagnetic shape memory alloy.

I-3. Development Research Division
Materials Design and Development Group

【Research Activities】

For many years, progress in microelectronics has been associated with a reduction in the minimum feature size of integrated circuits. However, this trend, as described by Moore's Law, seems to be ending due to process and physical limitations, and therefore a new paradigm shift has been expected. Our group has covered a wide range of molecular systems which have potential application in molecular electronics using first-principles calculations; molecular rectifiers, supramolecular enamel wires (covered wires), connection between organic molecules and metal electrodes, electronic transport through small molecules for a building block, self-assembled nanowires on silicon surface, bent carbon nanotube, and so on.

1. R. V. Belosludov, A. A. Farajian, H. Mizuseki, K. Ichinoseki and Y. Kawazoe: Electron Transport in Molecular Enamel Wires, J. J. Applied Physics, **43** (2004), 2061-2063.

2. M. Khazai, A. A. Farajian, G-H Jeong, H. Mizuseki, T. Hirata, R. Hatakeyama and Y. Kawazoe: Dynamical Criteria for Cs Ion Insertion and Adsorption at Cap and Stem of Carbon Nanotubes: Ab Initio Study and Comparison with Experiment, J. Phys. Chem., **B108** (2004), 15529-15535.

【Plan】

The structure, dynamical and thermodynamical properties of metallic glasses (so-called amorphous) will be determined using reverse Monte Carlo (MC), molecular dynamics (MD), and lattice dynamics (LD) simulations [4,5]. This combined approach leads to a more accurate and detailed structural description of amorphous solids when compared to experiment than was previously possible [5]. Using the supercell approach (possible by supercomputer) the initial model of metallic liquid with random atomic distribution but with experimental density will be constructed using reverse MC method. After that, the MD modeling of supercooling process will be provided in the following way. First, the optimized structure and thermodynamic functions (such as entropy, enthalpies) of alloy will be obtained at experimental temperature and the temperature dependence of supercell parameters will be constructed. Second, this atomic configuration will be compressed by reducing the volume of supercell and will be relaxed again at low temperature. The procedure can be repeated with temperature decreasing and cooling rate can be modeled by selected temperature step. The final structures of metallic glasses will be relaxed to eliminate possible imaginary modes using a conjugate-gradient method. The final results can be compared with experimental radial distribution functions.

II. Applied Research Division

【Research Activities】

The demand to metallic implant materials for biomedical applications is greatly increasing nowadays because of the rapid growth of population ratio of the aged people in the representative countries. Recent research has attempted to overcome the long-term health problem caused by the release of Ni and V ions from the alloy.

We have succeeded in developing shape memory Ti-Nb-Sn alloy consisting of non-cytotoxic elements, with excellent cold formability. For example, the superelastic Ti-Nb-Sn alloy at human body temperature, which is applicable to orthodontics arch-wire, is developed by the optimization of alloy composition and heat treatment conditions.

(2) Ti-Nb-Sn alloy for orthopeadic implants such as knees, hips and shoulder is developed with low Young's modulus of 40～50 GPa and high strength of ～1000 MPa by microstructural control via thermo mechanical processing.

1. T.Ozaki, H.Matsumoto, S.Watanabe and S.Hanada: Beta Ti Alloys with Low Young's Modulus, Mat. Trans, **45** (2004), 2776-2779.

【Plan】

(1) The behavior of martensitic transformation in super elastic Ti-Nb-Sn alloy is strongly affected by relatively low temperature aging. Therefore, this work would aim at examining the structural change of the alloy under aging in detail, and then examining the mechanism of super elasticity.

(2) In Ti-Nb-Sn alloy with low Young's modulus and high strength for biomedical implant such as stems for artificial hip joints and orthopedic bone plates, this work aims at examining the mechanism of Young's modulus and strength based on micro structural change under thermo mechanical processing.

III. Research Station

【Research Activities】

Research Station consists of three parts, Materials Synthesis, Evaluation and Analysis, and Crystal Preparation. There are following examples of research activities conducted in three stations.

1) Station of Materials Synthesis :

β-alumina type compounds are useful materials because they show high ion conductivity. Nonstoichiometric Ba β–alumina single crystals, $Ba_{1-0.25x}Mg_{1-x}Al_{10+x}O_{17+0.25x}$, were grown in the range from x=0 to 1 using a floating zone (FZ) method. The composition and oxygen partial pressure effects on the electrical conductivity both in parallel and perpendicular conduction plane were clarified.

2) Station of Evaluation and Analysis :

In development of biomaterials, evaluation of the materials in simulated body fluid is inevitable. Especially, information from their surface is important. The surface film composition on titanium under culturing murine fibroblast L929 was investigated by XPS, and found calcium phosphate precipitaion, but the amount of the calcium phosphate was smaller than those in Hanks' solution, MEM, and MEM+FBS.

3) Station of Crystal Preparation :

Single crystals of higher borides $AlMgB_{14}$ and $AlMgB_{22}$ were grown from a molten aluminum flux in an Ar stream. The optimum conditions for growing these borides were established. The hardness and oxidation resistivity for these borides were investigated.

1. A. Y. Zhang, T. Akashi and T. Goto: Electrical Conductivity of Nonstoichiometric Baß-alumina Single Crystals Prepared by a Floating Zone Method, Solid State Ionics, **166** (2004), 77-82.

2. S. Hiromoto, T. Hanawa, K. Asami: Composition of Surface Oxide Film of Titanium with Culturing Murine Fibroblasts L929, Biomaterials **25** [6] (2004) 979 –986.

3. S. Okada, K. Kudou, T. Shishido, I. Higashi, N. Kamegashira, K. Nakajima and T. Lundstrom: Crystal Growth of Aluminum Magnesium Borides from Al-Mg-B Ternary System Solutions and Propeties of the Crystals, Materials Science Forum, **449-452** (2004), 368.

【Plan】

Three stations have active collaborative programs with research groups from this center as well as from others. Synthesis of new functional materials, preparation of crystals for many applications, evaluation and analysis of various materials are now in progress. The present research include the following theme.

1) Station of Materials Synthesis :

1. Development of efficient energy materials and electronic information materials such as soft magnetic Fe-base metallic glasses, formation of large-sized bulk metallic glasses of Fe-and Co-base alloys by flux method, the high hydrogen penetration glassy alloys, etc.
2. Preparation of zirconia film by liquid source ECR plasma CVD method.

2) Station of Evaluation and Analysis :

1. Evaluation of corrosion resistance of bulk metallic glasses by X-ray photoelectron spectroscopy, electron probe micro analysis, *etc.*
2. Evaluation of biomaterials by X-ray photoelectron spectroscopy, Auger electron spectroscopy, *etc.*

3) Station of Crystal Preparation :

1. FZ-growth of single crystalline β-Ga_2O_3 and fabrication of GaN by nitridation
2. Hydrothermal growth of high quality ZnO single crystalline.