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THE 4th JOINT WORKSHOP ON ADVANCED MATERIALS (2022)

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Dalian University of Technology–Tohoku University
The 4th Joint Workshop on Advanced Materials (2022)
May 23, 2022 On-line

Technical Program

13:00 (13:00@Dalian) Chairs: Profs. From IMR and DUT	14:00 (JST)	Opening Addresses Prof. Tadashi Furuhara Prof. Mingliang Huang
13:10 Chairs: Prof. H.G. Dong Prof. A. Chiba	14:10	DUT: Fangyuan Hu, Xigao Jian Structure Design and Electrochemical Performance Regulation of Polymer-Based Electrochemical Energy Materials
13:35	14:35	IMR: Takeshi Wada, Soo-Hyun Joo, Hidemi Kato Beating Thermal Coarsening in Nanoporous Metals by High-Entropy Design
14:00	15:00	DUT: Xufeng Dong, Yu Tong, Min Qi, Ning Ma and Jinping Ou Preparation and Application of Magneto/Electro-rheological Composites
14:25	15:25	IMR: Satoshi Semboshi Development of high-strength and high-electrical conductive Cu-Ti alloy wires
14:50	15:50	DUT: Zhiyong Qiu Investigation of the Invar effect via anomalous Hall effect
15:15-15:25	16:15-16:25	Coffee Break
15:25 Chairs: Prof. H. Huang Prof. H. Kato	16:25	IMR: Takeshi Seki, Koki Takanashi Enhanced Anomalous Nernst Effect in Metallic Superlattices
15:50	16:50	DUT: Yanhui Li, Wei Zhang Improvement of magnetic softness of high-B_s Fe-based nanocrystalline alloys by forming pre-existing α-Fe nanoparticles in their amorphous precursors
16:15	17:15	IMR: Akihiko Chiba, Kenta Aoyagi, Yufan Zhao, Kenta Yamanaka Optimum alloy powder characteristics for powder-bed fusion type electron beam additive manufacturing
16:40	17:40	DUT: Qing Wang, Zhenhua Wang, Jinlin Li, Chuang Dong Formation of BCC/B2 coherent microstructure in high-entropy superalloys and their properties
17:05	18:05	IMR: Rie Y Umetsu Detecting the electronic structures of half-metallic ferromagnets in Heusler alloys by resonant inelastic soft-X-ray scattering under magnetic field
17:30	18:30	Closing Remarks Prof. Hidemi Kato Prof: Honggang Dong

Structure Design and Electrochemical Performance Regulation of Polymer-Based Electrochemical Energy Materials

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Keywords: Polymer-based electrode, Electrolyte, Intrinsic doping, Electrode process

Abstract:

Porous frameworks, as potential electrodes, have been widely applied in the energy storage devices including supercapacitors and secondary batteries. However, traditional porous carbon materials were mainly prepared through physical activation or chemical activation. Limited by the synthesis conditions, it is difficult to control the pore structure and element composition of porous materials at the same time. Recently, we developed a series of hierarchical porous frameworks with multiple heteroatoms (N, S, O, *etal*) intrinsic doping, by designing the molecular structure of the precursors of dinitrile monomers with aromatic heterocycles. The pore structure and heteroatoms of the framework can be effectively adjusted by tailoring the aromatic heterocycles in the monomers. This design philosophy realized the directional control of the structure and compositions of the materials. Under this guidance, dinitrile monomers containing benzene rings, thiophene rings, bithiphene, and pyridine rings have been designed and synthesized successfully. Porous frameworks, which are suitable for supercapacitors, sodium ion batteries, sodium ion capacitors, and lithium sulfur batteries, respectively, have been fabricated. All the electrodes exhibit satisfactory electrochemical performance, as well-developed porous structure can promote the transportation of ions, while abundant heteroatoms could provide active sites for ions adsorption and storage. Besides, we have verified that increasing the heteroatoms contents could improve the utilization rates of active substance as well as reducing the nucleation and polarization potential of the lithium sulfide in lithium sulfur batteries.

Beating Thermal Coarsening in Nanoporous Metals by High-Entropy Design

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Keywords: Nanoporous metals, High-entropy alloy, Dealloying, Surface area

Abstract:

Minimizing the ligament sizes of nanoporous metals is technically challenging because the coarsening follows a universal empirical correlation with homologous temperature. Ligament coarsening is a surface-diffusion-dominated process, and the relationship between the melting point and diffusion is apparent in the conventional metallic materials. Although nanoporous metals produced by dealloying have outstanding physical properties due to their unique bicontinuous structure, the undesirable coarsening leads to degradation of physical properties. To overcome this intrinsic thermal coarsening, we utilized high-entropy design into the dealloying process.

The high-entropy alloys (HEAs), which is characterized by the nearly equiatomic composition of more than five components, are attracting much attention in metallurgy. In such compositionally complex alloys, configuration entropy is maximized and the disordered solid-solution phase become thermodynamically stable rather than the ordered compound phase. The HEAs possess attractive mechanical properties such as high strength, ductility, superplasticity, etc. at an elevated temperature. The main reason of such unique characteristics is considered as the high thermal stability of fine microstructure. The grain growth in HEAs is exceptionally slow because of the sluggish diffusion, namely, the increase the activation energy due to the variety of atomic size in the constituents. As the ligament coarsening in nanoporous metals is analogous to the grain growth of polycrystalline materials, we expected the high-entropy design in nanoporous materials has a potential for achieving an exceptional fine porous structure and high stability against the coarsening.

To synthesize the nanoporous HEA, we utilized liquid metal dealloying (LMD), a unique technique to fabricate non-noble porous materials. The composition of the nanoporous HEA is carefully established among elements immiscible with the Mg melt, and then the selected TiVNbMoTa HEA is alloyed with miscible Ni. During LMD in the Mg melt, it is expected that Ni selectively dissolves while the five immiscible elements rearrange their atomic configuration into a ligament. The precursor $(Ti, V, Nb, Mo, Ta)_{25}Ni_{75}$ was immersed in Mg melt for 10 min at 837 K. The average ligament size achieved in a unimodal porous structure is just 10 nm and the corresponding specific surface area reached as high as 55.7 m^2/g. The diffraction pattern proves that the porous metal forms BCC lattice with its chemical composition of $Ti_{13.29}V_{26.67}Nb_{19.91}Mo_{27.77}Ta_{12.16}Ni_{0.2}$ (at.%), falling into the HEA. This is the smallest ligament size ever reported in the dealloyed nanoporous metals. The activation energy for coarsening of nanoporous HEA was calculated to be 301.8 kJ/mol, being much higher than those reported for surface diffusion of each element. Previously developed porous metals follow the general linear relationship of ligament size versus homologous temperature in a log–log scale, however, the linear relationship shifts down by one order of magnitude in smaller-size regime for the developed nanoporous HEAs. It is therefore concluded that by using high-entropy design, we overcome the universal effect of temperature on the coarsening of nanoporous metals.

Preparation and Application of Magneto/Electro-rheological Composites

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Keywords: Smart materials, Magnetorheological, Electrorheological, Composites, Vibration control

Abstract:

It is a crucial issue to reduce the vibration of civil structures, mechanical structures and space structures. Passive energy dissipation devices based on elastomers, metal dampers, and viscous dampers only can control the vibration of structures in a narrow frequency. Smart materials with tunable stiffness or tunable damping could actively control the vibration of structures within a wider frequency. Magneto/electro-rheological composites, including magnetorheological fluids, electrorheological fluids, magnetorheological elastomers, and electrorheological elastomers, are such a kind of smart materials. These smart composites are prepared by dispersing electric polarized or magnetic polarized particles within carrier liquids or polymer matrix. Under an applying electric or magnetic field, their viscosity, yield stress or dynamic viscoelasticity change fast and reversibly. During the past decades, we investigated the mechanisms of magneto/electro-rheological composites. By controlling the morphology of the active particles and by modifying the interfaces between the particles and the matrix, we developed some high performance magneto/electro-rheological composites. Several representative works will be introduced in this presentation. Figure 1 shows the structure, mechanism and enhanced electrorheological properties of electrorheological elastomers containing TiO_2/urea core−shell particles. We have used these smart composites to fabricate smart devices that could reduce the vibration of various structures in wide frequency.

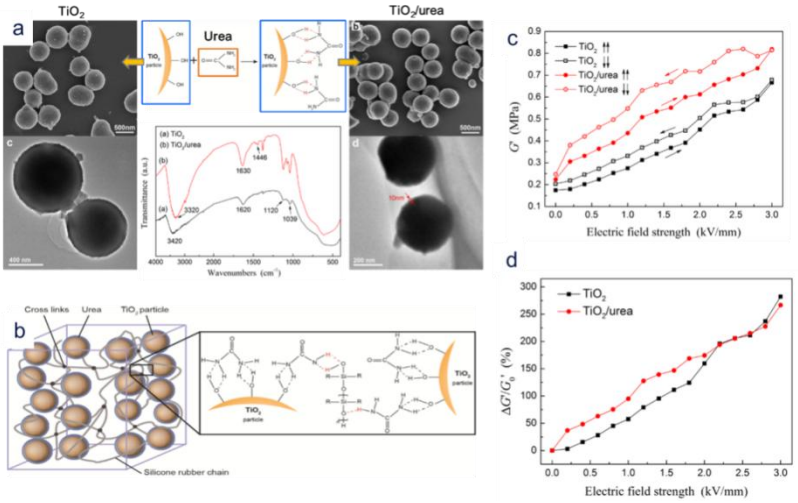

Figure 1. (a) Morphology and structure of TiO_2/urea core−shell particles, (b) mechanism, (c) dependence of storage modulus on electric field and (d) dependence of relative ER effect on electric field of electrorheological elastomers containing TiO_2/urea core−shell particle.

Development of high-strength and high-electrical conductive Cu-Ti alloy wires

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Keywords: Cu alloy, precipitates, aging, severe plastic deformation, microstructure, strengthening, electrical conductivity

Abstract:

Age-hardenable Cu-Ti alloys, which usually contain 3–5 at.% Ti, are attractive for use in advanced electrical devices, such as conductive lead wires and suspension guide springs, because their strength and stiffness are comparable to those of widely used Cu-Be alloys (containing 10 to 12 at.% Be), although their electrical conductivity is inferior to the latter. Against recent background of downsizing and streamlining electrical devices, further enhancement in the mechanical and electrical properties of Cu-Ti alloys is strongly required. In this study, we attempted to prepare Cu-Ti alloy wires with an improved strength and electrical conductivity. To achieve this goal, not only a conventional peak-aged alloy with a high strength and low electrical conductivity, but also an over-aged alloy with a degraded strength but high electrical conductivity were subjected to severe drawing at room temperature. Then, the variations of the microstructure, strengths and electrical conductivity during severe drawing were systematically investigated.

When drawing the peak-aged Cu-3.6 at.% Ti alloy, the Vickers hardness increased rapidly at an initial deformation by drawing, and then saturated to around 325 HV. On the contrary, when drawing the over-aged Cu-3.6 at.% Ti alloy, the Vickers hardness increased steadily during drawing, and eventually exceeded the value of the wires drawn from the peak-aged alloy. The electrical conductivity of the over-aged alloy increased slightly by drawing to an equivalent strain of 3.2. Then, it dropped by furthermore drawing, although the value was always higher than that from the peak-aged alloy. This means, both the strength and the electrical conductivity were improved by the procedure of over-aging and then drawing severely rather than that of conventional peak-aging and then drawing process, as shown in Fig. 1[1]. Fig. 1 also indicated that the performance of Cu-Ti wires in this study was competitative with that of commercial Cu-Be wires. The improvement of the strength for the over-aged alloy can be explained by the microstructural evolution during severe drawing. Before drawing, the over-aged alloy was entirely occupied by cellular components of terminal Cu solid solution and β-Cu_4Ti laminates by a discontinuous precipitation reaction at grain boundaries. In an initial stage of drawing, the cellular components containing the β-Cu_4Ti laminates preferentially arranged in parallel to the drawing direction. On furthermore drawing, the thickness and inter-laminate distance of the β-Cu_4Ti laminates were reduced, and eventually the β-Cu_4Ti laminates transformed into nano-sized fibers. The fine β-Cu_4Ti fibers promoted the formation of dislocations and the refinement of subgrains unlike the case of drawing from the peak-aged alloy. As the result, the over-aged alloy was strengthened significantly without much degradation of electrical conductivity during severe drawing.

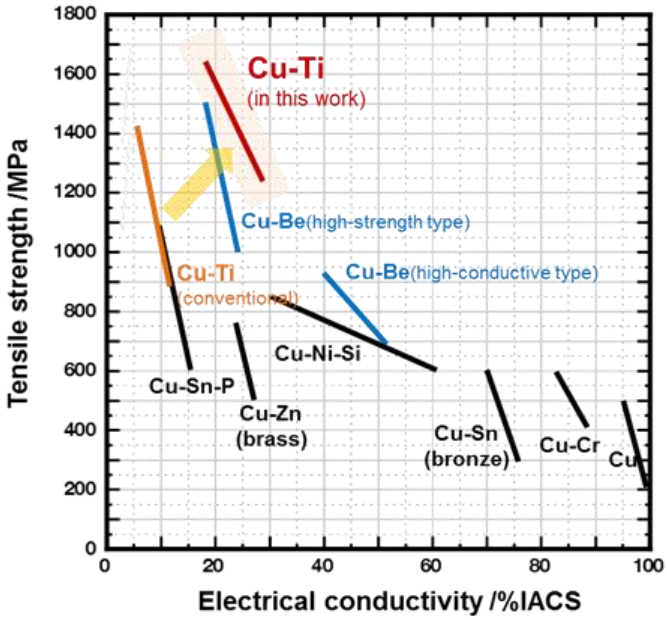

Fig. 1. Relationship between the tensile strength and electrical conductivity of Cu-Ti wires fabricated in this study, together with commercial Cu-based alloy wires.

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Investigation of the Invar effect via anomalous Hall effect

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Keywords: Invar effect, Anomalous Hall effect, Invar alloy, Spintronics

Abstract:

Invar effect refers to extraordinarily low thermal expansion coefficient in some alloys e.g. $Fe_{65}Ni_{35}$, which has been discovered and widely used for more than one hundred years. However, the mechanism of the Invar effect is still an enigmatic problem that has resisted theoretical and experimental assaults. Here, we demonstrated a systematic study of the Invar effect utilizing the anomalous Hall effect. In a typical commercial Invar alloy, it is found that not only the band-structure-originated intrinsic but also the external scattering related extrinsic anomalous Hall resistivities deviate from their ordinary trend when the thermal expansion anomaly occurs. Our results suggest that a structural change accompanying with forming and growing of nano-size domains should be more appropriate than a electronic state transition between high spin and low spin for the explanation of the Invar effect, which can also be supported by the analysis of the normal Hall effect. This work offers an innovative thought for the understanding of the Invar effect, which can be a guideline for the application and exploration of new type Invar materials.

Enhanced Anomalous Nernst Effect in Metallic Superlattices

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Keywords: Metallic Superlattice, Anomalous Nernst Effect, Ordered Alloy, Flexible Substrate

Abstract:

Spin caloritronics, the field studying the interconversion between charge current ($\boldsymbol{J}_c$) and heat current ($\boldsymbol{J}_q$) mediated by spin current ($\boldsymbol{J}_s$) and/or magnetization ($\boldsymbol{M}$), has attracted much attention not only for academic interests but also for practical applications. The newly discovered spin caloritronic phenomena have stimulated the renewed interest in the thermoelectric phenomena in ferromagnets. One of the thermoelectric phenomena in ferromagnets is the anomalous Nernst effect (ANE), in which $\boldsymbol{J}_c$ appears in the cross-product direction of $\boldsymbol{M}$ and a temperature gradient (∇T). Although ANE has been known for a long time, the microscopic physical picture for ANE has not fully been understood. In addition to the fundamental point of view, this magneto-thermoelectric effect is possibly beneficial for thermoelectric conversion applications. The key for the ANE-based thermoelectric conversion is to find a material with a large anomalous Nernst coefficient (S^{ANE}).

We previously reported the enhancement of ANE in the Fe-based metallic multilayers [1], implying that the low dimensionality of layer and/or the existence of interface plays a role for the increase in ANE. This means that metallic multilayers or superlattices with a number of interfaces are promising for achieving large ANE.

In this talk, we introduce our recent studies on the ANE using the Ni / Pt metallic superlattices [1] and the Co_2MnGa / AlN multilayers [2]. For the former, the perpendicularly magnetized Ni/Pt (001) epitaxial superlattices were fabricated directly on a non-conductive $SrTiO_3$ substrate [3], and the Ni layer thickness dependence of ANE was investigated for [Ni (t nm) / Pt (1.0 nm)]$_{\times N}$. We found that the values of S^{ANE} for the Ni/Pt superlattices are one order of magnitude larger than that for the bulk Ni. The enhanced ANE is attributable to the large transverse thermoelectric conductivity.

For the latter, the polycrystalline Co_2MnGa / AlN multilayer films were deposited on an amorphous substrate, which shows $S^{ANE} = 4.9\ \mu V\ K^{-1}$. This large S^{ANE} is comparable to the values reported for the single crystal Co_2MnGa bulks. The detailed structural analysis and the transport measurement suggest that the effect of interfacial strain on the Seebeck coefficient plays an important role for enhancing the ANE. Since the AlN layer is available on any substrate materials, even on a flexible polyimide substrate, large ANE is successfully achieved for the Co_2MnGa / AlN stack.

References

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Improvement of magnetic softness of high-Bs Fe-based nanocrystalline alloys by forming pre-existing α-Fe nanoparticles in their amorphous precursors

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Keywords: Fe-based nanocrystalline alloy, Cu-cluster, Pre-existing α-Fe nanoparticle, Crystallization behavior, Nanostructure, Soft magnetic property

Abstract:

Thedemand for energy saving and device miniaturization drives the development of soft magnetic materials to the direction of high saturation magnetic flux density (B_s), high permeability (μ), and low core loss (P). Fe-based Fe-Si-B-Nb-Cu nanocrystalline alloys have been widely used as core materials due to their high μ and low P, while their B_s of only ~1.24 T is not conducive to the miniaturization of the devices. Fe-based Fe-Si-B-(P)-Cunanocrystalline alloys exhibit high B_s of over 1.80 T but their fine nanostructure and good magnetic softness are obtained by annealing under a high heating rate and precise temperature control because of the absence of Nb and other large-sized elements, which brings challenge for industrial production. Due to the positive mixing enthalpy between Cu-Fe atom pair, Cu atoms tend to segregate from Fe atoms and aggregate to form Cu clusters, which provide heterogeneous nucleation sites to promote the nucleation of α-Fe primary crystals. A higher content of Cu would facilitate the formation of sufficiently dense nuclei/nanocrystals in a suitable Fe-based amorphous alloy matrix during melt-spinning, which are favor to obtaining a fine nanostructure by subsequent heat treatment. In this work, the effect of Cu content on the melt-spun structure, crystallization behavior, and annealed structure and magnetic properties of $Fe_{83-x}Si_4B_{13}Cu_x$ (x = 1.3–2.3) alloys have been investigated. Three-dimensional atom probe and transmission electron microscopy analyses reveal that high number-density (N_d) Cu-clusters and *Pre-existing Nano-sized α-Fe Particles (PN-α-Fe)* are coexistence in the melt-spun amorphous matrix for the alloys with Cu≥1.7at.%, and the PN-α-Fe form by manners of one-direction adjoining and enveloping the Cu-clusters. Two-step crystallization behavior associated with growth of the PN-α-Fe and subsequent nucleation and growth of newly-formed α-Fe is found in the primary crystallization stage of the alloys. The strong competitive growth among the high-N_d PN-α-Fe effectively inhibits the excessive growth of the α-Fe grains even under a low-heating-rate annealing, resulting in a fine nanostructure and excellent soft magnetic properties. A $Fe_{81.3}Si_4B_{13}Cu_{1.7}$ nanocrystalline alloy with an average α-Fe grain size ($D_{α\text{-}Fe}$) of 14 nm possesses a high B_s of 1.77 T and low coercivity (H_c) of 7.1 A/m, which is much superior to that of a $Fe_{81.7}Si_4B_{13}Cu_{1.3}$ alloy ($D_{α\text{-}Fe}$ = 53 nm, B_s = 1.73 T, and H_c = 379 A/m). In addition, the effects of Nb addition on the melt-spun and annealed structure and magnetic properties of the high-Cu-content nanocrystalline alloy have been investigated as well.

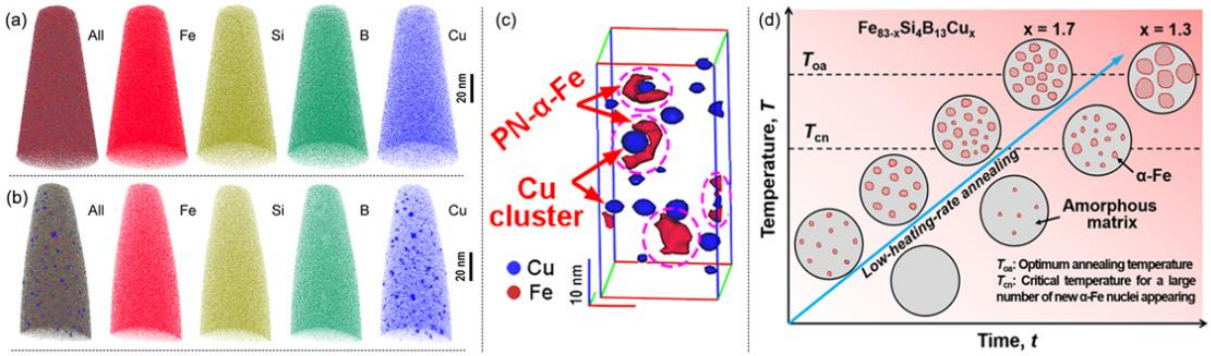

Fig. APT element maps of melt-spun $Fe_{83-x}Si_4B_{13}Cu_x$ alloys with x = 1.3 (a) and x = 1.7 (b), enlarged portion illustrating Cu and Fe with 7 at% Cu and 85 at.% Fe iso-concentration surfaces of the x= 1.7 alloy (c), and microstructure schematics at different heating stages for the two alloys under a low-heating-rate annealing.

Optimum alloy powder characteristics for powder-bed fusion type electron beam additive manufacturing

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Keywords: Additive manufacturing, Electron beam melting, Inconel 718 alloy

Abstract:

Powder morphology makes an essential impact on powder flowability and, consequently, on the spreading uniformity of powder layer during electron beam powder-bed fusion (EB-PBF). Notably, as powder particles undergo a thermal interaction with an electron beam, the surface characteristics of the powder layer correlated to the powder morphology will inevitably influence the heat transfer and consolidation process. In the present study, the Inconel 718 samples were fabricated using (i) imperfect spherical and (ii) spherical powders, under the same process parameters domain determined by uniform experimental design. The forming qualities were characterized in terms of surface topography, density, and internal defect. The samples processed with the optimal parameters were also evaluated and characterized to highlight the decisive role of powder in forming quality.

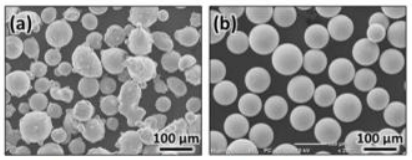

Fig. 1. Morphologies of powders fabricated by (a)GA and (b)PREP.

We use two types of Inconel 718 alloy powders (Fig. 1), namely, (i) imperfect spherical and (ii) spherical powders fabricated by gas atomization (GA) and plasma-rotating electrode process (PREP), respectively. The Inconel 718 cuboid samples were produced on a SUS304 substrate using an EB-PBF machine. Meanwhile, mesoscale numerical simulations were applied to analyze the fusion process on powder layers composed of two types of powders, thereby clarifying the significance of powder characteristics in defect suppression of EB-PBF-built Inconel 718.

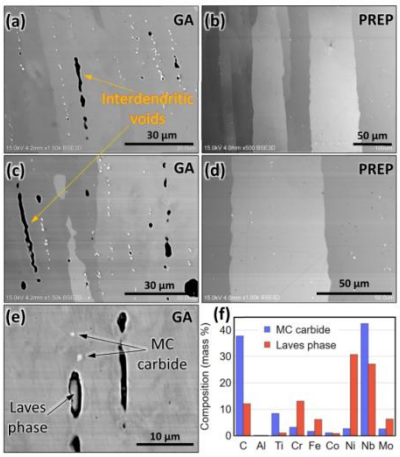

Fig.2[1] SEM (BSE) image of the cross section parallel to the building direction of the EBMed material obtained under the optimum building conditions by machine learning. (c)(e) A sample formed with GA powder. (b)(d) A sample formed by PREP powder. (E) (f) MC carbide and Laves phase.

1) Processing with the PREP powders had a relatively broad process window suppressing defect. 2) Based on simulation results and theoretical analysis, low energy absorption rate and thermal conductivity made the GA powders likely to evoke lack–of–fusion and excessive melting under low and high energy conditions, respectively. 3) The suppression of interdendritic voids forming in the sample built with the PREP powders (Fig. 2) was due to the high cooling and solidification rates evaluated by numerical simulation.

In the EBMed material obtained using GA powder, as observed in Figs. 2 (a) and 2 (c), voids are formed along the building direction in the same manner as the precipitate in which the voids are connected in a chain. It is distributed in the dendrite boundary region. Generally,

it is considered that these voids are formed because the dendrite contracts during solidification and the melt is not sufficiently supplied to the dendrite-dendrite space. In addition, as shown in Figs. 2 (e) nd 2 (f), in the sample obtained by using GA powder, MC carbides formed in the dendrite space due to micro segregation during solidification-(Nb,Ti)C Laves phase-$(Ni, Cr)_2(Nb,Ti)$ is observed. On the other hand, in the EBMed material obtained from PREP powder, no precipitates such as voids and MC carbides at the dendrite boundary and the Laves phase, which are observed in the GA powder sample, are observed. Thus, there is a clear difference in the solidification process when building with GA powder and PREP powder. It is worth noting that this difference in the solidification process is due to the difference in the powder shape (spherical or irregular shape) used for EBM manufacturing.

References

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Formation of BCC/B2 coherent microstructure in high-entropy superalloys and their properties

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Keywords: superalloys, high-entropy alloying, coherent microstructure, materials design, phase-field simulation, properties

Abstract:

It is difficult to tailor the BCC/B2 coherent microstructure in simple systems due to a relatively-large difference in compositions between the ordered B2 phase and its parent BCC solid solution. The present work applies the cluster-formula approach and high-entropy (HE) alloying principle to design alloy compositions for tuning the lattice misfit between BCC/B2 phases in multi-principal superalloy systems. And spherical and cuboidal coherent precipitations are achieved in the designed BCC/B2 HEAs, in which the weave-like microstructure could be avoided by composition design. The phase-field simulation was preformed to study the microstructural evolution of BCC/B2, in which the key parameters to determine the BCC/B2 coherent microstructure are found. The property results show that the cuboidal B2 nanoprecipitation in the BCC matrix would render the HE superalloys with prominent mechanical properties (high strength and large ductility). While the spherical BCC nanoprecipitation in the B2 matrix would result in an excellent soft-magnetic property, which has a great potential for the application of electromagnetic wave-absorption materials. Both precipitation strengthening mechanism and soft-magnetic mechanism are also discussed. The design of BCC/B2 coherent microstructure will open a new way to develop novel high-performance HEAs.

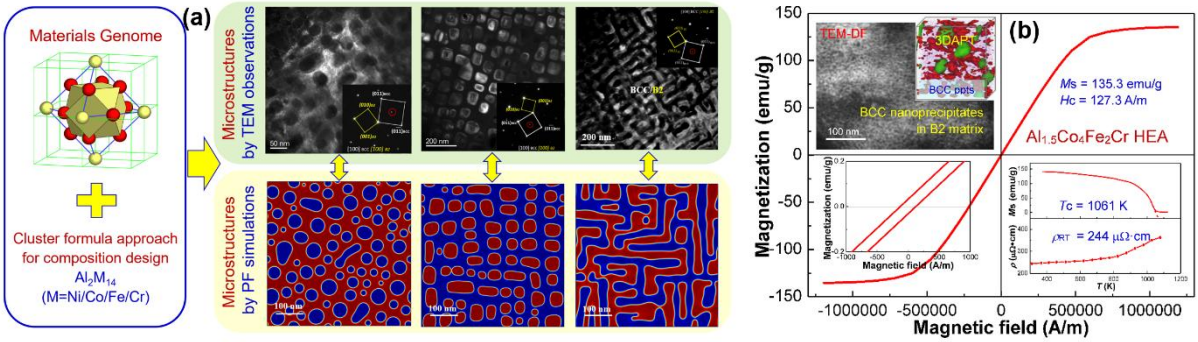

Fig. BCC/B2 coherent microstructures designed by the cluster-formula approach (a) and soft-magnetic property of Al-Fe-Co-Cr superalloy (b).

Detecting the electronic structures of half-metallic ferromagnets in Heusler alloys by resonant inelastic soft-X-ray scattering under magnetic field

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Keywords: Heusler alloys, electronic structures, RIXS

Abstract:

Many kinds of materials have been reported for the Heusler alloys denoted by the molecular formula of X_2YZ, here X and Y are transition metal elements or rare earth elements, Z is semimetal or semiconductor elements. When X and Y are composed of 3d transition metal elements, it is known to have many functions linked directly to applications such as superelasticity, shape memory effect, magnetocaloric effect, and huge thermoelectric power. Since half-metallic electronic structures were theoretically predicted in some Co- and Mn-based Heusler alloys in 1980's, the half-metallic ferromagnets have been intensively investigated in the field of spintronics. In recent years, materials related to spin gapless semiconductors and Weyl semimetals have also been reported in Heusler alloys, and they are more attracting attention.

Our group successfully detected the electronic structures of bulk single crystals of some Heusler alloys by resonant inelastic soft X-ray scattering (RIXS) in an external magnetic field and the magnetic circular dichroism (MCD) [1-3]. Because the RIXS is a photon-in/photon-out spectroscopy, experiments are not affected by any external perturbation such as magnetic field. Thus, it becomes to be powerful tool to probe the magnetic excitations in the magnetically ordered states and the spin-polarized electronic structures. In addition, by tuning the incoming photon energy to the core-level absorption edges, RIXS-MCD spectra can be observed and discussed element-specifically. The feature of the bulk sensitivity is also effective to our investigations. The experiments were performed using high resolution soft x-ray emission spectrometer installed at BL07LSU in Spring-8, Japan.

Clear RIXS-MCD spectra are observed in all Heusler alloys, and the difference of the spectral properties well reflects their electronic states. By comparing the obtained RIXS-MCD spectra and theoretically calculated ones by Kramers-Heisenberg formula, it was suggested the possibility of quantitative discussion on the existence of the band gap that characterizes the half-metallic electronic state, the relative position between the gap and the Fermi level, and the energy width of the Zeeman splitting, etc. It is said that the RIXS experiments are powerful tool to study the detailed electronic structures of various Heusler alloys and family materials.

Acknowledgments

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