AWARD

- Haruyuki Inui, June 2021, THERMEC' 2021 Distinguished Award, THERMEC' 2021, Vienna, Austria.
- Kodai Niitsu, Makoto Asakura, Koretaka Yuge and Haruyuki Inui, September 2021, The 1st Best Paper Award for Budding Author, The Japan Institute of Metals and Materials, Japan.
- Shuhei Yoshida, Takuto Ikeuchi, Yu Bai and Nobuhiro Tsuji, September 2021, The 1st Best Paper Award for Budding Author, The Japan Institute of Metals and Materials, Japan.
- Kaveh Edalati, September 2021, A Highly Cited Author of Materials Transactions, Japan.
- Nobuhiro Tsuji, November 2021, 70th Anniversary Distinguished Achievement Award, The Japan Institute of Light Metals, Japan.
- Takeshi Nagase, Mitsuharu Todai and Takayoshi Nakano, September 2021, The 69th Best Paper Award, The Japan Institute of Metals and Materials, Japan.
- Haruyuki Inui, November 2021, Humboldt Research Award, Alexander von Humboldt Foundation, Germany.
- Takeshi Fujita, November 2021, Highly cited researcher 2021, Clarivate Analytics Co.,Ltd.
- Saeid Akrami, Parisa Edalati, Masayoshi Fuji and Kaveh Edalati, January 2022, Top 3 Highly Read Manuscript of Materials Science and Engineering: R, Elsevier.
- Shuhei Yoshida, February 2022, Inoue Research Award for Young Scientists, Inoue Foundation for Science, Japan.
- Akihiko Chiba, March 2022, The 28th Masumoto Hakaru Award, The Japan Institute of Metals and Materials, Japan.
- Akihiko Chiba, March 2022, The 61st Tanikawa-Harris Award, The Japan Institute of Metals and Materials, Japan.
- Nobuhiro Tsuji, March 2022, The 61st Tanikawa-Harris Award, The Japan Institute of Metals and Materials, Japan.
- Takeshi Wada, March 2022, The 80th Meritorious Award, The Japan Institute of Metals and Materials, Japan.
- Masanori Enoki, Yohei Ohsawa and Horoshi Ohtani, March 2022, The Best Paper Award (Tawara Award), The Iron and Steel Institute of Japan.
- Katsunari Oikawa, March 2022, Ferrum Contribution Award, The Iron and Steel Institute of Japan.

PRESS

1. Press Release, 23 June 2021, "Decoupling between calorimetric and dynamical glass transitions in high-entropy metallic glasses", J. Jiang, Z. Lu, J. Shen, T. Wada, H. Kato, M. Chen, Nikkei Inc. URL: https://www.nikkei.com/article/DGXLRSP613072_T20C21A6000000/
2. Nature Index 2021 Materials Science, Nature Research., "Improving the mix for better control of nanocomposites", H. Muto. URL: https://www.nature.com/articles/d42473-021-00151-1
3. Press Release, 20 August 2021, "Nanoporous ultra-high-entropy alloys containing fourteen elements for water splitting electrocatalysis", Takeshi Fujita. URL: https://www.jst.go.jp/pr/announce/20210820/index.html.
4. Kyoto University HP: Latest research news, 31 August 2021, "Direct observation of local chemical ordering in a few nanometer range in CoCrNi medium-entropy alloy by atom probe tomography and its impact on mechanical properties", K. Inoue, S. Yoshida, N. Tsuji. URL: https://www.kyoto-u.ac.jp/ja/research-news/2021-08-30-1
5. The Science News (No. 3843), 1st October 2021, "Direct observation of local chemical ordering in a few nanometer range in medium-entropy alloy", K. Inoue, S. Yoshida, N. Tsuji.

LATEST INFORMATION

International Meeting

- High-Entropy Materials II-From Fundamentals to Potential Applications (MRS 2022 Spring Meeting), May 8-13, 2022, Honolulu, HI, USA (Hybrid). https://www.mrs.org/meetings-events/spring-meetings-exhibits/2022-mrs-spring-meeting
- Symposium "High Entropy Alloys: Potential for industrial applications", May 12, 2022 | Dresden & Online (Hybrid Event). https://www.iws.fraunhofer.de/en/events/hea-symposium.html

Domestic Meeting

- The Japan Institute of Metals (JIM) Symposium "Materials Science of High-Entropy Alloys", March 15-17, 2022, Online meeting, Japan. https://jim.or.jp/MEETINGS/me_index.html
- 2022 Startup Meeting of All Research Groups, May 17-18, 2022, Online meeting, Japan. https://highentropy.mtl.kyoto-u.ac.jp/members
- The Japan Institute of Metals (JIM) Symposium "Materials Science of High-Entropy Alloys", September 21-23, 2022, Fukuoka Institute of Technology, Japan. https://jim.or.jp/MEETINGS/me_index.html
- 2023 Final Meeting of All Research Groups, March, 2023, Japan. https://highentropy.mtl.kyoto-u.ac.jp/members
- The Japan Institute of Metals (JIM) Symposium "Materials Science of High-Entropy Alloys", March, 2023, Tokyo City University, Japan. https://jim.or.jp/MEETINGS/me_index.html

HEAs
High Entropy Alloys
Science of New Class of Materials Based on Elemental Multiplicity and Heterogeneity

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Ministry of Education, Culture, Sports, Science and Technology Grant-in-Aid
"Scientific Research on Innovative Areas" for FY2018-22

HEAs
High Entropy Alloys
Science of New Class of Materials Based on Elemental Multiplicity and Heterogeneity

NEWSLETTER Vol. 4
2022 MAY

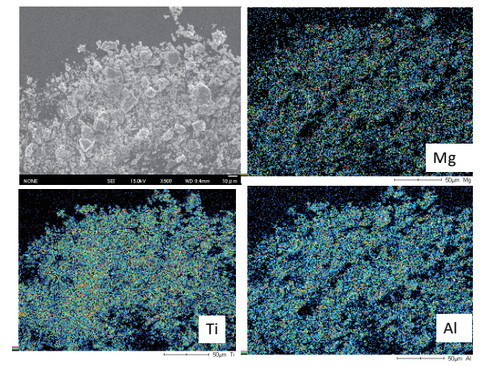
Introduction to Publicly Offered Research Teams

New Teams Boost up the Second Half of the HEA Project

A01 Low-density high entropy alloys composed of Group 1 and 2 elements

Shigehito Isobe (Hokkaido University), Hirotada Hashimoto (Hokkaido University), Hiroshi Oka (Hokkaido University), Naoyuki Hashimoto (Hokkaido University)

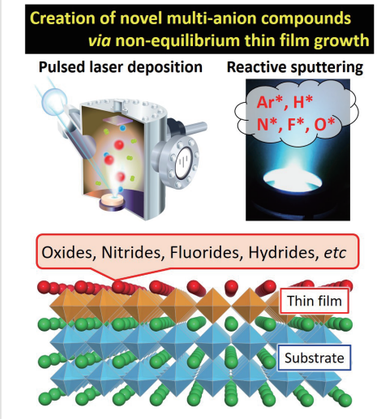
Our target is low-density high entropy alloys (HEAs) mainly composed of Group 1 and 2 elements. Most of the existing or currently researched high-entropy alloys, including Cantor alloys, are mainly composed of transition metal elements. There are few reports on the HEAs mainly composed of alkali metals and alkaline earth metals, because the alloys with alkali metals and alkaline earth metals are less likely to form solid solution. In this research, we try to synthesize low-density HEAs by mechanical alloying. As an example, we have succeeded to synthesize new alloys composed of Li, Mg, Al, and Ti. From the results of XRD and SEM-EDS (Figure), it has been indicated that a solid solution single phase (FCC structure) of $LiMg_{0.5}AlTi_{1.5}$ was obtained. As applications, functional materials such as next-generation light metal materials and hydrogen storage materials can be considered. Now, we are trying to synthesize quinary HEAs composed of light elements.



A01 Development of novel functional materials in multi-anion high-entropy compounds

Ryota Shimizu (Tokyo Institute of Technology)

We study the novel functionalities in high-entropy compounds of ionic crystals. Using non-equilibrium epitaxial thin-film growth techniques such as pulsed laser deposition and reactive magnetron sputtering, we aim for the creation of novel materials that cannot be synthesized in bulk. There are three topics as follows. (1): synthesis of layered oxide epitaxial thin films containing four or more transition metal elements[1], (2): synthesis of high-entropy fluoride epitaxial thin films with perovskite and rutile structures, and (3): synthesis of high-entropy multi-anion compounds simultaneously containing four anions (F, N, H, O). We expect this study to develop electrochemical applications such as high-performance electrode materials and solid electrolytes for lithium and fluoride batteries, and catalysts for oxygen-evolution reactions in water electrolysis.

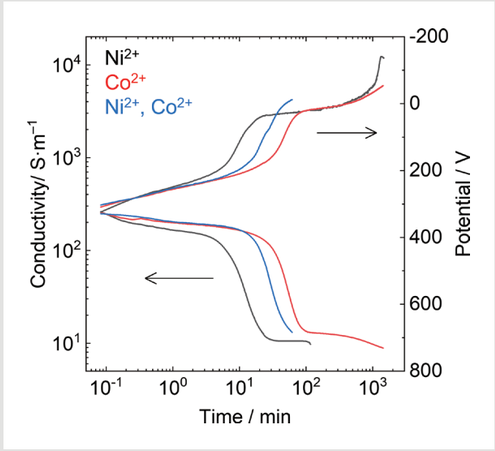


Reference:
[1]: Wang *et al.*, "Synthesis of High-Entropy Layered Oxide Epitaxial Thin Films: $LiCr_{1/6}Mn_{1/6}Fe_{1/6}Co_{1/6}Ni_{1/6}Cu_{1/6}O_2$", Cryst. Growth Des. **22**, 1116 (2022).

A01 Synthesis of nanostructured high entropy alloys by using multicomponent hydroxide nanoparticles

Naoki Tarutani (Hiroshima University), Yuka Hiragi (Hiroshima University), Kazumasa Suzuki (Shiga Prefecture University), Kiyofumi Katagiri (Hiroshima University)

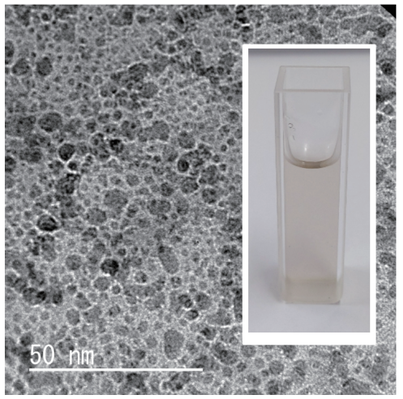
Synthesis of high-entropy alloys (HEAs) with controlled nanostructures has been attracted attentions towards highly functional materials. Although HEA nanoparticles were found to prepare through chemical ion reduction and thermal decomposition of salts, chemical composition are still limited and hard to design the nanostructures. Here we focus on developing a novel approach to synthesize HEAs with controlled nanostructures using multicomponent hydroxide nanoparticles as precursors. Metal hydroxides are known to form crystals including multi metal elements with homogeneous distribution by coprecipitation. The figure shown in right panel is a result of tracing the coprecipitation process in the case of Co and Ni hydroxide nanoparticles. Conductivity and potential correspond to ion concentration and solution pH, respectively. With increasing the solution pH triggered by the addition of reaction initiator, ion concentration decreased, which means formation of metal hydroxide. Co-Ni system showed intermediate trend of the change of solution pH and ion concentration compared to the respective Co and Ni systems. This indicates formation of binary metal hydroxides. Based on the solution conductivity and potential measurements, we found to achieve quinary metal hydroxide nanoparticles. It is expected to obtain HEAs by reducing the quinary metal hydroxide nanoparticles.



A01 Production of High-Entropy Alloy Nanoparticles by Top-Down and Bottom-Up Laser Processes

Tomoyuki Yatsuhashi (Osaka City University)

High-entropy alloy nanoparticles (NPs) have been increasingly recognized as important catalysts in chemical processes. Various synthetic methods have been proposed, but there are difficulty originating from the use of complex templates as well as low production yield. The goal of this study is to synthesize alloy NPs by top-down and bottom-up laser processes in liquid phase. In bottom-up synthetic process, alloy NPs are obtained by the confinement and fusion of desired elements. Laser-induced nucleation is known as fast-heating and fast-cooling processes that enables to produce noble metal alloy NPs from the corresponding metal ion mixture solution. However, this method is not applicable to transition metal ions. We succeeded to synthesize transition metal NPs by using metal complex solution as reactants, but the synthesis of alloy NPs is underway. In the case of top-down laser process, NPs are obtained by the ablation of bulk alloy materials in liquid medium. We constructed new optical set-up using a galvamo mirror system to scan the laser beam. FeCoNi medium entropy alloy that was produced by electrodeposition was chosen as a sample for laser ablation in water. Colloidal solution of NPs smaller than 10 nm in diameter was easily separated from bulk starting materials (picture).

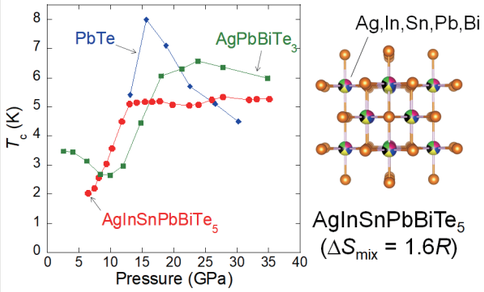


A01 Robustness of superconductivity in HEA-type metal telluride $AgInSnPbBiTe_5$ under high pressures

Yoshikazu Mizuguchi (Tokyo Metropolitan University), Md. Riad Kasem (Tokyo Metropolitan University), Yuki Nakahira (Tokyo Metropolitan University), Aichi Yamashita (Tokyo Metropolitan University), Ryo Matsumoto (NIMS), Hitoshi Yamaoka (RIKEN)

Recently, material development and studies of physical properties of HEA-type superconductors have been one of hot topics in the field of superconductors. We observed anomalous superconducting states in $AgInSnPbBiTe_5$ under high pressure; the transition temperature (T_c) of $AgInSnPbBiTe_5$ does not change with pressure in the high-pressure (CsCl-type) phase, which is clearly different from the pressure dependence of T_c for PbTe, the zero-entropy counterpart [1]. Since the crystal and electronic structures for $AgInSnPbBiTe_5$ and PbTe are similar under high pressures, we propose that the robust superconductivity is induced by local disordering at the metal-Te bonding states.

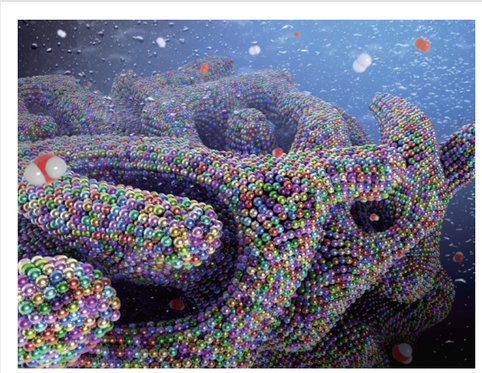
[1] Md. Riad Kasem et al., “Robustness of superconductivity to external pressure in high-entropy-alloy-type metal telluride $AgInSnPbBiTe_5$”, arXiv:2112.06461.



A01 Nanoporous ultra-high-entropy alloys containing fourteen elements for water splitting electrocatalysis

Takeshi Fujita (Kochi University of Technology)

The dealloying method was applied as a facile synthetic route to nanoporous ultra-high-entropy alloys (np-UHEAs) containing up to 14 elements (Al, Ag, Au, Co, Cu, Fe, Ir, Mo, Ni, Pd, Pt, Rh, Ru, and Ti). TEM analysis of the alloys indicated a hierarchical, nanoporous, and nanocrystalline fcc structure with uniformly distributed elements. The dealloying strategy shows great potential for the design and preparation of np-UHEAs as it can accommodate a far greater number of elements than the 14 used in this study. Furthermore, they exhibit high catalytic activities and electrochemical stabilities in the hydrogen evolution reaction and oxygen evolution reaction in acidic media, superior to that of commercial Pt/graphene and IrO_2 catalysts. This study not only provides the basis for prospecting and designing np-HEAs with diverse compositions and structures, but also provides unprecedented opportunities for element selection for fabricating an omnipotent catalyst for various applications [1].

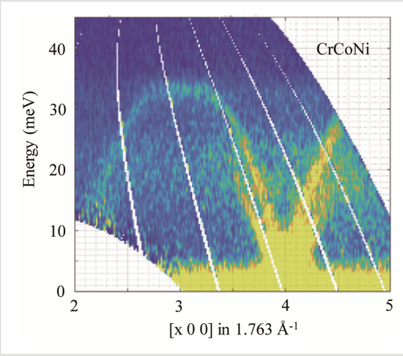


[1] Z. X. Cai, H. Goou, Y. Ito, T. Tokunaga, M. Miyauchi, H. Abe, T. Fujita, Nanoporous ultra-high-entropy alloys containing fourteen elements for water splitting electrocatalysis, Chemical Science **12** (2021) 11306-11315.

A01 Atomic Dynamics in High-Entropy Alloys Investigated by Inelastic X-ray and Neutron Scattering

Satoshi Tsutsui (JASRI), Kazuki Iida (CROSS), Ryoichi Kajimoto (JAEA), Masato Matsuura (CROSS), Takeshi Teramoto (Kobe University), Mohamad Qayyumbin Mohamad Izlan (Kobe University), Ryota Shimohara (Kobe University), Katsushi Tanaka (Kobe University)

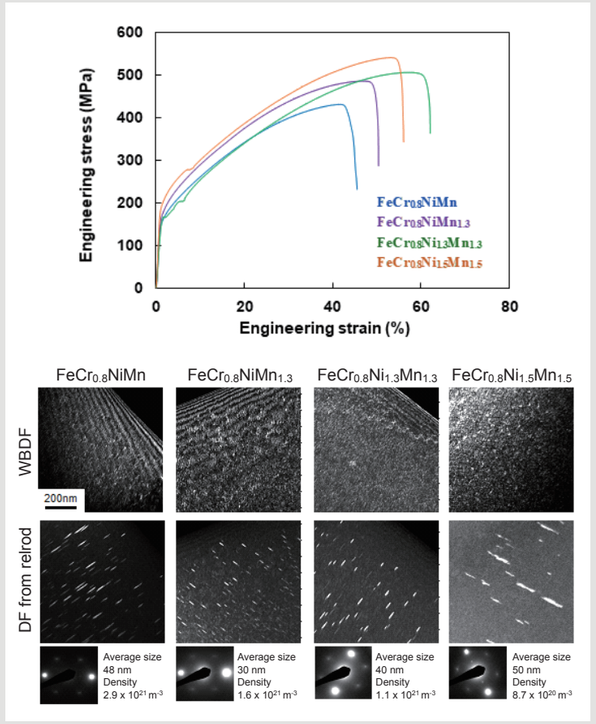
Phonon dispersion relations reflect elasticities of materials on microscopic viewpoints. Inelastic X-ray scattering (IXS) and inelastic neutron scattering (INS) techniques are complementary to investigate phonon dispersion relations. Since X-rays (neutrons) are scattered by electrons (nuclei), comparison of dynamical structure factor corresponding to phonon dispersion relations between IXS and INS techniques sometimes provides element-specific phonon dispersion relations. In particular, the comparison of dynamical structure factors between IXS and INS is helpful to understand contributions of each element to the elasticities of high-entropy alloys consisting of atoms whose atomic numbers are close among them. We have successfully obtained the dynamical structure factors in CrCoNi and CrMnFeCoNi with IXS at BL35XU in SPring-8 and INS at BL01 in J-PARC MLF. The microscopic elasticity estimated from the dynamical structure factors quantitatively agree with the macroscopic elasticity reported previously.



A01 Effect of stacking fault energy on irradiation damage in Co-free high entropy alloys

Naoyuki Hashimoto (Hokkaido University), Eyo Wada (Hokkaido University), Keisuke Fukumoto (Hokkaido University), Hiroshi Oka (Hokkaido University), Shigehito Isobe (Hokkaido University)

In order to investigate the effect of stacking fault energy on microstructural evolution [1] in reduced activation high entropy alloys, electron and/or Au^{+} ion irradiation was performed to the Co-free FCC-type $FeCr_{0.8}Ni_xMn_y$ (x, y = 1, 1.3, 1.5) alloys. TEM observation of the 5%-deformed $FeCr_{0.8}Ni_xMn_y$ alloys revealed the increase in the stacking fault energy with increasing both Ni and Mn concentration. In addition, $FeCr_{0.8}Ni_{1.5}Mn_{1.5}$ had the highest stacking fault energy, which was much higher value than that of 316SS. Furthermore, the yield strength and the elongation of deformed $FeCr_{0.8}Ni_xMn_y$ also showed the Ni and Mn concentration dependence. It seems that $\sigma_{0.2}$, UTS, and ε_t are slightly increasing with increasing Mn and Ni contents, while, the 0.2% proof stress ($\sigma_{0.2}$), the ultimate tensile strength (UTS), and the total elongation (ε_t) were comparable to that of 316H stainless steel. The electron irradiation at 400 ºC resulted in the formation of black dots, self-interstitial atom faulted loops, but no observable voids in all the $FeCr_{0.8}Ni_xMn_y$ alloys. The comparison of microstructural evolution revealed less faulted Frank loop formation in $FeCr_{0.8}Ni_{1.3}Mn_{1.3}$ and $FeCr_{0.8}Ni_{1.5}Mn_{1.5}$ alloys. From these results, it is suggested that FeCrNiMn-based Co-free high entropy alloys would be developed as high irradiation resistant materials by controlling the stacking fault energy with optimized element concentration.

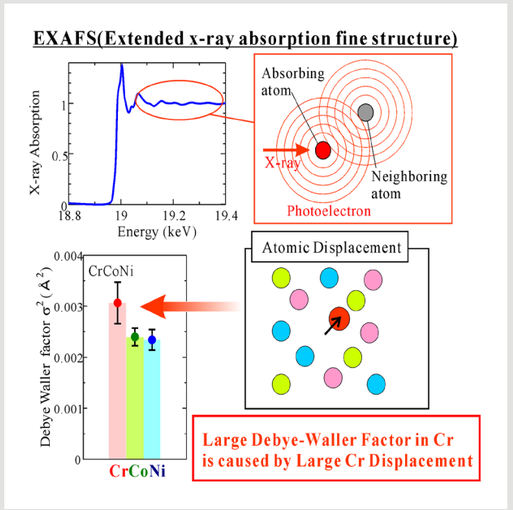


[1] N.Hashimoto, T.Fukushi, E.Wada, and W-Y.Chen: J. Nucl. Mater., **545** (2021), 152642.

A01 Local Structural Analysis in High-Entropy Alloys by using Synchrotron-radiation X-ray.

Noriaki Hanasaki (Osaka University)

The high/medium-entropy alloys (HEA/MEAs) are promising materials for their high strength. Since the HEA/MEAs contain many kinds of element in the same ratio, the conventional solvent-solute-atom concept cannot be applied. Recently, it is suggested theoretically that some specific elements such as Cr have large atomic displacement and their displacements have relation with the strength of the HEA/MEAs. In order to clarify the element's character and the local structure in HEAs experimentally, we observed the EXAFS (Extended x-ray absorption fine structure) in CrCoNi, and found that the local disorder in Cr sites is larger than in other constituent element sites [1]. This experimental result is consistent with the large Cr displacement predicted by the previous first-principle calculations. By the systematic study in various alloys, we will reveal a global element dependence of the local disorder and the atomic displacement.



[1] N.Hanasaki *et al.*, AIP Advances **11**, 125216 (2021).

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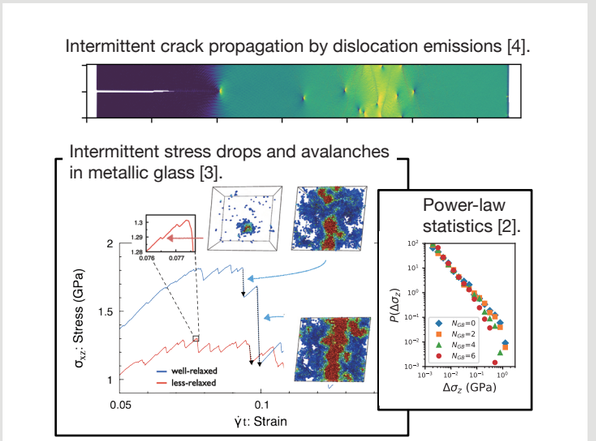
2022 MAY

A02 Intermittent Inelastic deformation in High-Entropy Alloys

Tomoaki Niiyama (Kanazawa University)

The inelastic deformation has an intermittent and critical nature characterized by power-law statistics. For instance, a wide range of acoustic emissions, stress drops, and strain bursts can be measured in plastic deformation. The fracture can also show intermittent behavior. Our molecular dynamics simulation revealed the details of the intermittent plasticity in crystals and metallic glasses [1–3]. The intermittent dynamics of cleavage failure (crack propagation in a single crystal) were also confirmed [4]. This study aims to elucidate the influence of the variety of atom sizes, a typical feature of high-entropy alloys (HEAs), on the intermittent dynamics of their inelastic deformation. This approach may bring a better understanding of the excellent mechanical properties of HEAs from the view of the critical feature and atomic-scale dynamics.



[1] T. Niiyama, T. Shimokawa, Physical Review E, **91**, (2015), 022401.
[2] T. Niiyama, T. Shimokawa, Physical Review B, **94**, (2016), 140102.
[3] T. Niiyama, M. Wakeda, T. Shimokawa, and S. Ogata, Physical Review E, **100**, (2019), 043002.
[4] T. Niiyama, T. Shimokawa, T. Fujimoto, Journal of the Society of Materials Science, Japan., **67** (2), (2018), 222–228.

A03 High-Entropy Oxides as Active Photocatalysts for CO_2 Conversion

Saeid Akrami (Nagoya Institute of Technology), Yasushi Murakami (Kyushu University), Monotori Watanabe (Kyushu University), Tatsumi Ishihara (Kyushu University), Makoto Arita (Kyushu University), Masayoshi Fuji (Nagoya Institute of Technology), Kaveh Edalati (Kyushu University)

Photocatalytic conversion of CO_2 to reactive gasses such as CO and fuels under sunlight is a clean technology to reduce the amount of CO_2. In a recent study [1], a high-entropy oxide (HEO), $TiZrNbHfTaO_{11}$, was introduced as a new photocatalyst for CO_2 conversion. The HEO, which had dual phases and various structural defects, showed simultaneous photocatalytic activity for CO_2 to CO and H_2O to H_2 conversion without the addition of a co-catalyst. The photocatalytic activity of HEO for CO_2 conversion was better than conventional photocatalysts such as anatase TiO_2 and $BiVO_4$ and comparable with P25 TiO_2 as a benchmark photocatalyst. The study confirmed the high potential of HEOs as a new type of photocatalysts for CO_2 conversion.

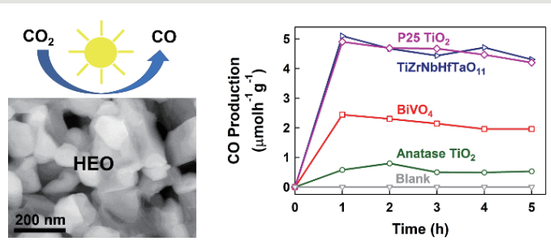


Fig. 1. High-entropy oxide with high photocatalytic activity for CO_2 to CO conversion.

[1] S. Akrami, Y. Murakami, M. Watanabe, T. Ishihara, M. Arita, M. Fuji, K. Edalati, "Defective high-entropy oxide photocatalyst with high activity for CO_2 conversion", Applied Catalysis B, **303** (2022) 120896.

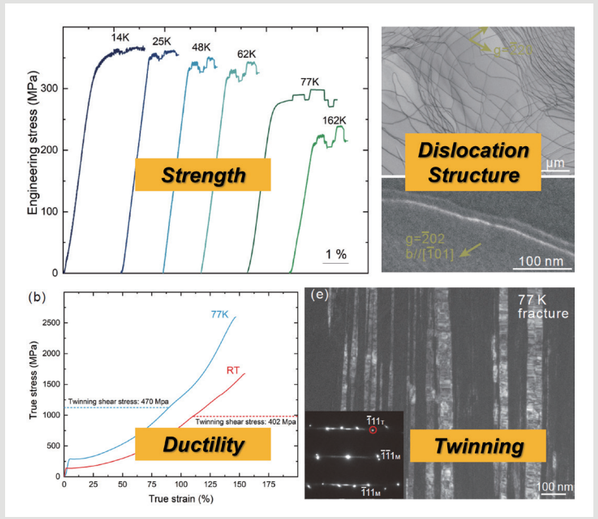
Activities of Young Researchers

Enthusiasm and flexible thinking of young researchers elucidate the essence of high-entropy alloys!

Fundamental investigation on deformation behavior of Cr-Co-Ni edium-entropy alloys

Zhenghao Chen (Kyoto University), Le Li (Kyoto University), Kyosuke Kishida (Kyoto University), Haruyuki Inui (Kyoto University)

The considerable interests in Cr-Co-Ni medium-entropy alloys (MEAs) with face-centered cubic (fcc) structure are (1) the highest strength among quaternary and ternary MEA derivatives of the Cr-Mn-Fe-Co-Ni HEA system, and (2) the excellent tensile ductility that increases with decreasing temperature. In order to figure out the origin of the fascinating mechanical properties, Group A01(a) makes comprehensive investigations on Cr-Co-Ni and derivative MEAs based on the knowledge of dislocation theory in following three parts: (i) The relationship between the novel solid solution parameter Mean Square Atomic Distance (MSAD) and the strength, (ii) The relationship among the Stacking Fault Energy (SFE), twinning deformation and the tensile ductility, and (iii) The effect of the Short Range ordering (SRO) on mechanical properties [1]. The aim of this group is to make comprehensive understanding on mechanical properties in H/MEAs based on dislocation theory and to hence establish an alloy-design guideline for structural fcc-H/MEAs achieving high strength and high ductility simultaneously.



[1] L. Li, Z.H. Chen, S. Kuroiwa, M. Ito, K. Kishida, H. Inui, E.P. George: "Tensile and compressive plastic deformation behavior of medium-entropy Cr-Co-Ni single crystals from cryogenic to elevated temperatures", International Journal of Plasticity, **148** (2022), 103144.

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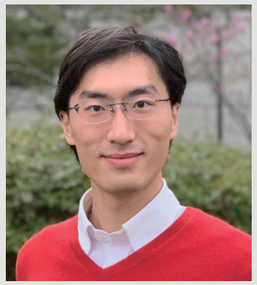
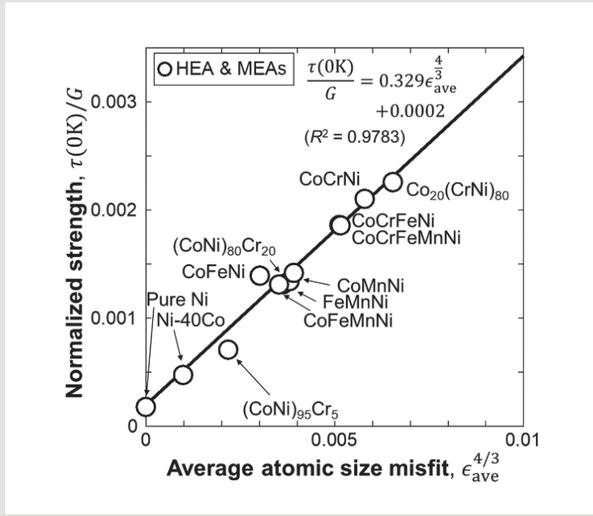


◆Our current interests are the origin of the chemical short range ordering (SRO) in fcc-H/MEAs and its influence on mechanical properties. The further in-depth understanding of SRO is believed to make contributions to achieving better strength-ductility balance in structural H/MEAs.

Essential characteristics of strengthening mechanisms in high/medium entropy alloys: From the viewpoint of heterogeneity on atomic-scale

Shuhei Yoshida (Kyoto University)

High entropy alloys (HEAs) and medium entropy alloys (MEAs) are novel classes of solid solution alloys having five or more and four or fewer constituent elements, respectively, with near equi-atomic fractions. Among them, HEAs and MEAs with face-centered cubic (FCC) structure have been known to exhibit an exceptional balance of strength and ductility in a wide range of temperatures ranging from room temperature to cryogenic temperatures. A series of our studies (Ref. [1] for instance) revealed that FCC HEAs and MEAs showed significantly high friction stress (fundamental resistance to dislocation motion in solid solutions), contributing to their high yield strength as well as high tensile strength. The high friction stress observed in FCC HEAs and MEAs was mainly attributed to elastic interaction between the elastic field of edge dislocations and large size misfits of alloying elements (severe lattice distortion) owing to the difference in the atomic sizes. The results suggest that the heterogeneity on atomic-scale (i.e., different elements with different sizes occupy different lattice sites) in HEAs and MEAs plays an essential role in determining their mechanical properties.



[1] S. Yoshida, T. Ikeuchi, T. Bhattacharjee, Y. Bai, A. Shibata, N. Tsuji: "Effect of elemental combination on friction stress and Hall-Petch relationship in face-centered cubic high / medium entropy alloys", Acta Materialia, **171** (2019), 201.

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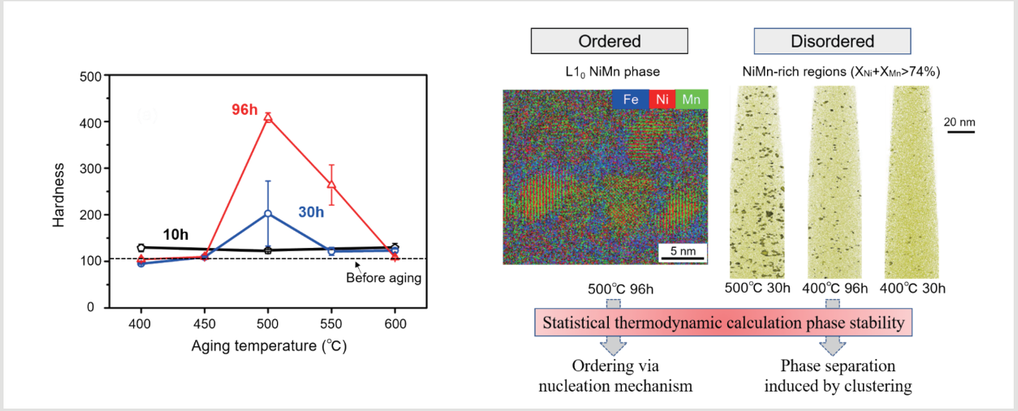
◆I'm currently working on experimental studies on physical metallurgy and mechanical/physical properties of various solid solution alloys including high/medium entropy alloys. I'm particularly interested in the relationship between microstructure evolution and macroscopic properties of alloys and in characterizing microstructures by using electron microscopy and quantum beam techniques.

Phase separation with ordering in aged Fe-Ni-Mn medium entropy alloy

Fei Sun (Nagoya University), Goro Miyamoto (Tohoku University), Yikun Liu (Tohoku University), Yuichiro Hayasaka (Tohoku University), Tadashi Furuhara (Tohoku University)

High- and medium-entropy alloys are currently receiving significant attention. Understanding short-range ordering and nano-scaled phase separation concerning elemental interaction is a key to controlling phase stability for designing high entropy alloys. To elucidate the interaction between elements and their relationship with ordering and phase separation, it is desirable to investigate ternary alloys with a small number of constituent elements. Phase separation and ordering behavior at the atomic scale have not been investigated in Fe-Ni-Mn alloys, and the effects of elemental interactions on them are still unknown. This study is focused on the ordering and phase separation during the decomposition of Fe-Ni-Mn medium entropy alloys. Based on the advanced characterization technologies (spherical aberration-corrected scanning transmission electron microscopy (Cs-corrected STEM) and three-dimensional atom probe (3DAP)) combined with statistical thermodynamics calculation, we aim to deepen the understanding of the interactions among constituent elements that affect solid solution stability in HEAs for alloy design and development. Obvious age hardening occurs after aging at 500 °C for 96 h due to the formation of the $L1_0$ ordered phase combined with phase separation. By aging at 400 °C or shorter time, obvious precipitation of the ordered phase is not detected but the radial distribution functions obtained by 3DAP present that enrichment of Ni and Mn nearby the same kinds of element is observed, and this tendency is stronger for Mn. This result suggests that phase separation is induced by Mn clustering in the early stage of aging. A statistical thermodynamic model of phase stability considering $L1_0$ ordered structure is developed. The analyses using the model suggest that phase separation is not possible in a disordered state at 500 °C, therefore, nucleation of the $L1_0$ phase should precede phase separation at this temperature. On the other hand, phase separation is possible even in a disordered state at 400 °C, and ordering further enhances phase separation.



[1] F. Sun, G. Miyamoto, Y. Liu, Y. Hayasaka, T. Furuhara: "Phase separation with ordering in aged Fe-Ni-Mn medium entropy alloy", Acta Materialia, **223** (2022), 117487.

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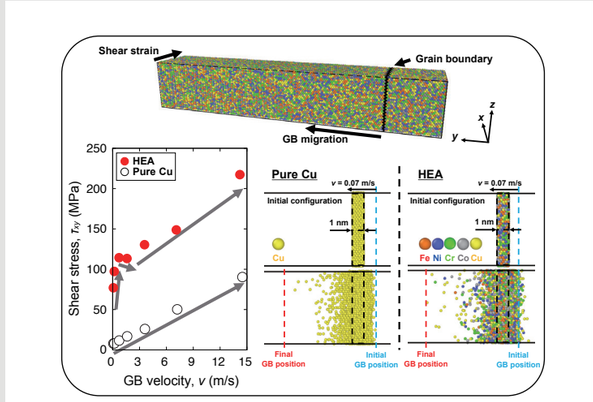
◆Our current interest focuses on the phase stability and elemental interactions of medium/high entropy alloys in terms of phase separation and ordering at nano-atomic scales using advanced characterization techniques (e.g. STEM, 3DAP, etc.) and thermodynamic calculations.

Atomistic Study on Dynamic Grain Boundary Segregation and Atom Drag due to Grain Boundary Migration in High-Entropy Alloys

Kohei Shiotani, Tomoaki Niiyama, Tomotsugu Shimokawa (Kanazawa University)

It has been reported that thermal stability of high-entropy alloys (HEAs) is better than that of pure materials and conventional dilute alloys, suggesting that activation of grain boundary (GB) migration can be suppressed in HEAs. In order to elucidate the mechanism for the excellent thermal stability of HEAs, understanding a detailed atomic-scale behavior of moving GBs is indispensable. Therefore, we perform molecular dynamics simulations about GB migration with model HEAs and investigate atomic-scale properties of moving GBs such as dynamic GB segregation in the HEAs. GB migration simulations by loading shear stress at temperature of 85% of melting point are conducted with equiatomic FeNiCrCoCu-HEAs at various GB velocities. For the comparison with the obtained results from the HEAs, we also conduct the same analyses with pure Cu as a representative of single-element materials. As shown in the bottom left figure, the applied shear stress as a driving force required for GB migration linearly increases with GB velocity in the whole velocity region in pure Cu, while the stress-velocity relation in the HEAs can be divided into two regions; low-velocity (v < 1 m/s) and high-velocity region (v > 1 m/s). In the low-velocity region, the increasing trend of the stress is clearly much stronger than that in the high-velocity region. The displacements of each atom within a crystalline region with 1 nm thick after being traversed by a moving GB are shown in the bottom right figure. We find that the atoms in pure Cu are displaced by the GB as well as the ones in the HEAs. However, through calculating the mean displacement of each element, we also find that no atom drag occurs in pure Cu, while Cu in the HEAs tends to be dragged by the moving GB over a long distance. The velocity region in which Cu is strongly dragged (< 1m/s) is coincidence to that in which the applied shear stress required for GB migration sharply increases. Importantly, we also confirm that Cu is the most segregable element to both stationary and moving GBs in the HEAs and the trend is stronger with a decrease in GB velocity. Therefore, the segregated and dragged atoms (that is Cu in this study) may make GB migration difficult in the HEAs.



[1] K. Shiotani, T. Niiyama, and T. Shimokawa, "Dislocation Emission from Grain Boundaries in High-Entropy Alloys: Influence of Atomic Composition at Grain Boundaries", Materials Transactions, **61** (2020), 1272-1279.

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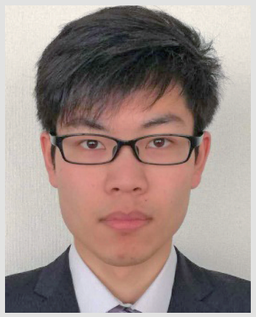

◆Our interest is to investigate the role of grain boundaries in excellent mechanical properties in high-entropy alloys. As one of the probable strengthening mechanisms relevant to grain boundaries, we reported the effect of grain boundary segregation on dislocation emission from grain boundaries in high-entropy alloys [1]. We now focus on how the atomic-scale characteristics of high-entropy alloys, e.g., atomic size difference and compositional heterogeneity of constitutional elements, have an impact on grain boundary migration behavior.