AWARD

Tadashi Furuhara
July 2018, THERMEC '2018 Distinguished Award.

Haruyuki Inui
March 2019, The 25th Masumoto Hakaru Award, The Japan Institute of Metals.

Haruyuki Inui
March 2019, The 69th Japan Institute of Metals Micrograph Award, The Japan Institute of Metals.

PRESS

1 Kyoto University Academic Day 2018, 22 September 2018, "Advanced Materials Design: High-Entropy Alloys", Haruyuki Inui.

2 Kyoto University Academic Day 2018, 22 September 2018, "Bulk Nanostructured Metals: Innovation beyond conventional materials developments", Nobuhiro Tsuji.

3 Nikkei XTECH, 26 February 2019, "Innovation to Realize Strengthening Mechanism of Steels by Thermo-Mechanical Processing", Akinobu Shibata and Nobuhiro Tsuji.

LATEST INFORMATION

International Meeting

- Novel Structural Materials Based on New Principles Symposium (Materials Research Meeting 2019), December 10-14, 2019, Yokohama, Japan.
  https://mrm2019.jmru.org
- High-Entropy Alloys and Other Novel High-Temperature Structural Alloys (MRS 2019 Fall Meeting), December 1-6, 2019, Boston, MA, USA.
  https://www.mrs.org/fall2019
- World Congress on High Entropy Alloys (HEA 2019), November 17-20, 2019, Seattle, Washington, USA.
  https://www.tms.org/HEA2019
- The 10th Pacific Rim International Conference on Advanced Materials and Processing, August 18-22, 2019, Xi'an, China.
  http://www.medmeeting.org/7482?lang=en
- Beyond Nickel Based Superalloys III, June 11-14, 2019, Nara, Japan.
  http://web.apollon.nta.co.jp/bnbs2019/
- TOPICAL SYMPOSIUM 1 (TS-1):"High Entropy and Other Multi-principal-element Materials", 46th International Conference on Metallurgical Coatings and Thin Films (ICMCTF-46), May 19-24, 2019, San Diego, CA, USA.
  http://www2.avs.org/conferences/ICMCTF/2019/tutorialsession_1.htm

Domestic Meeting

- The Japan Institute of Metal (JIM) Symposium "Materials Science of High-Entropy Alloys", November 11, 2019, Tokyo, Japan.
  https://jim.or.jp/EVENTS/event_index.html#02
- Fall Meeting of the Japan Institute of Metals, September 11-13, 2019, Okayama, Japan.
  https://jim.or.jp/MEETINGS/me_index.html
- Spring Meeting of the Japan Society of Powder Metallurgy, June 4-6, 2019, Tokyo, Japan.
  https://confit.atlas.jp/guide/event/jspm2019s/top?lang=ja
- 2019 Startup Meeting of All Research Groups, May 29, 2019, Kyoto, Japan,
  Meeting of All Research Groups, March 23, 2019, Tokyo, Japan.
  https://highentropy.mtl.kyoto-u.ac.jp/members
- Annual Meeting of the Japan Institute of Metals, March 20-22, 2019, Tokyo, Japan.
  https://jim.or.jp/MEETINGS/me_index.html
- Meeting of A03(e) Research Group March 30, 2019, Kyoto, Japan,
  Meeting of A01(a) Research Group January 30, 2019, Tokyo, Japan,
  Meeting of A01(b) Research Group December 26, 2018, Sendai, Japan,
  Meeting of A02(c) Research Group December 14-15, 2018, Kyoto, Japan,
  Meeting of A02(d) Research Group December 11, 2018, Sendai, Japan.
  https://highentropy.mtl.kyoto-u.ac.jp/members

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
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HEAS

High Entropy Alloys

Science of New Class of Materials Based on Elemental Multiplicity and Heterogeneity

NEWSLETTER Vol. 1
2019 MAY

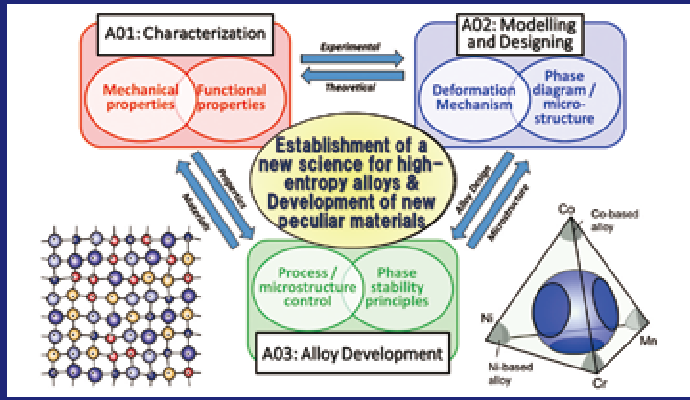
New Science for High-Entropy Alloys

Materials Design Based on Elemental Multiplicity and Heterogeneity

High-Entropy Alloys

Project Leader: Haruyuki Inui (Kyoto University)

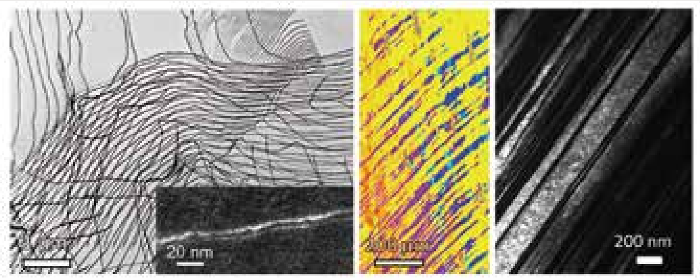
Since September 2018, we have launched a new research project "High-Entropy Alloys: Science of New Class of Materials Based on Elemental Multiplicity and Heterogeneity" supported by the Ministry of Education, Culture, Sports, Science and Technology. The program is categorized in the Innovative Area of the Grant-in-Aid for Scientific Research (*Kakenhi*, in Japanese), and a five-year project ending in March 2023. We will publish 'News Letters' periodically as a part of the activity of this program.
This project aims at establishing a new science concerning high-entropy alloys that exhibit new and peculiar materials properties by elucidating nonlinear interactions among various constituent elements through intensive and interdisciplinary cooperative research among research groups of various research fields within the project. 'High-entropy alloys' is defined in a narrow sense as equiatomic solid-solution alloys formed with constituent elements more than five kinds, the subjects of research have recently been expanded to include concentrated alloys with chemical compositions in the middle of multi-component phase diagrams, even they are deviated from the equiatomic compositions and contain precipitates of the secondary phase. Many of these high-entropy alloys of broader sense exhibit peculiar mechanical properties, such as abnormally high strength and high toughness at low temperatures, high strength retention at high temperatures, which are not observed in conventional alloys. These peculiar materials properties are considered to arise from the so-called 'cocktail' effects (nonlinear interactions among various constituent elements), and the identification of materials property expression behind the cocktail effects is one of the most challenging topics in materials science. Through establishing new scientific principle for controlling variety and inhomogeneity of elements, we aim at creating a new scientific area, in which the basis is established for developing new peculiar materials beyond conventional ones.
Unlike conventional alloys (such as Ni- and Al-based alloys) that are developed with a particular principal element at a corner of the phase diagram, high-entropy alloys are to be developed in the middle of multi-component phase diagrams, which have been undiscovered. Many unknown alloys with excellent properties are therefore expected to be discovered. Some particular combinations of elements may generate a cocktail effect that is not predictable only from the combination, and we expect a paradigm shift to occur in materials development, so that a best combination of elements and their fractions is searched, departing from conventional ways with one particular principal element and some minor alloying elements.
The goal of the research project is to systematically clarify the relationship between the peculiar properties of high-entropy alloys (HEAs) and their structures and to identify materials property expression behind the cocktail effects through close collaboration of researchers in various fields. During the research period, the project focuses on three topics shown below;
(1) Identification of Materials Property Expression and Materials Development of HEAs (Group A01), (2) Modelling and Designing of Materials Property of HEAs (Group A02), (3) Controlling of Phase Stability and Microstructures of HEAs (Group A03). The targets of the groups A01, A02 and A03 in the project and the relationship between the groups are illustrated in the figure shown below. The project also aims at establishing new and innovative areas of materials science through integrating the experimental results and theoretical/numerical results. Recently, the development of the state of the art nanostructure analysis in materials science, such as three dimensional transmission electron microscopy, three dimensional atom probe tomography, etc., is remarkable, and the project is intended to involve such novel techniques. Large-scale computer simulation based on atomic models is used within the project as well. Each of A01, A02 and A03 groups consists of 2 sub-groups. As a whole, the research project aims to creating new methodology and research fields in novel materials science through integrating advanced experimental and theoretical/simulation studies.



A01(a) Peculiar Mechanical Properties and Their Mechanisms of High-Entropy Alloys

Haruyuki Inui (Kyoto University), Koichi Tsuchiya (National Institute for Materials Science), Hiroyuki Sato (Hirosaki University), Masaki Tanaka (Kyushu University), Kyosuke Kishida (Kyoto University), Kodai Niitsu (Kyoto University)

The aim of this group is to identify the mechanisms of peculiar mechanical properties of high-entropy alloys, such as abnormally high strength and high toughness at low temperatures, high strength retention at high temperatures, which are not observed in conventional alloys. One of the interesting and unknown subjects in high-entropy alloys is mechanisms of solid-solution hardening. Conventional theories based on the interaction strength between dislocation and spherically symmetric strain filed around isolated solute atoms cannot be simply applied to high-entropy alloys because solute and solvent atoms cannot be defined and the resultant strain filed around each solute may not be so simple. The deduction of deformation mechanisms of high-entropy alloys is thus very important. The group involves specialists of nanostructure analysis using various advanced techniques such as TEM, HREM, 3D Atom-Probe, and so on. Quantitative analysis of the mechanisms behind peculiar mechanical properties through advanced analytical techniques experimentally obtained in this group will be correlated with the results of theoretical analysis in groups A02 and A03.



A01(b) New Material Synthesis with Novel Properties using High-Entropy Effect

Hidemi Kato (Tohoku University), Norimasa Nishiyama (Tokyo Institute of Technology), Hiroyuki Muto (Toyohashi University of Technology), Takeshi Wada (Tohoku University), Izumi Muto (Tohoku University), Akira Takeuchi (Tohoku University)

The aim of this group is to synthesize new materials not only in metallic but also non-metallic systems with novel properties using the concept of High-Entropy Alloy (HEA) by employing the advanced techniques originated in Japan. In the metallic system, nanoporous / nanohetero HEA and bulk metallic glassy HEA will be developed respectively by Liquid Metal Dealloying (LMD: Kato) and Rapidly Quenching (RQ: Wada) techniques. In the non-metallic system, HEA ceramics of Oxides, Nitrides and Carbides, of which studies have just been started in the world, will be developed by ultrahigh pressure (UHP: Nishiyama) synthesis and electrostatic nano-assembly (ESNA: H. Muto) techniques. In addition, fundamental investigation on improving corrosion resistance in FeCrNiMnCo HEA system will be performed by the micro-electrochemical (MEC: I. Muto) system to synthesize novel HEA alloys with ultrahigh corrosion resistance and establish its design theory. A01 (b) group was organized with active scientists in different scientific research fields with their own techniques. Each member will proceed his own research and make interplay simultaneously with the other members to novel achievements, which the research group consisting of members in similar research fields never get to.

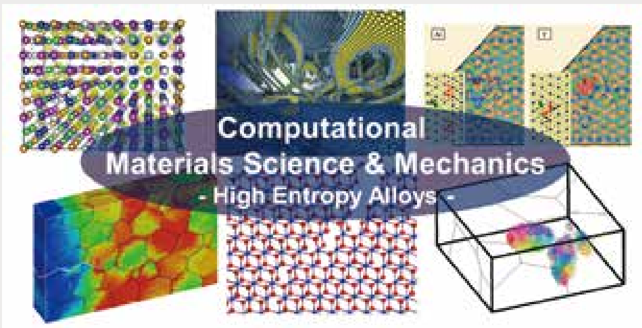
	H. Kato Tohoku Univ.	T. Wada Tohoku Univ.	N. Nishiyama Tokyo Inst. Tech.	H. Muto Toyohashi Univ. Tech.	I. Muto Tohoku Univ.
Techniques	Dealloying	Rapid Quenching	Ultra High Temp. & Pressure Synthesis	Electrostatic nano-assembly Technique	Micro-electrochemical System
Target Products	Metals, Alloys		Ceramics		
	Nanoporous Nanohetero	Bulk Metallic Glasses	Perovskite Oxides Spinel Nitrides	Integrated Composite Ceramic Particles	Ultra Corrosion Resistant Alloy and its Designing Theory
A. Takeuchi (Co-investigator, Tohoku Univ.) Advising Material Design Based on Thermodynamics					

Fig.1 Member and research target and technique in A01(b) group

A02(c) Computational Materials Science and Mechanics of High-Entropy Alloys

Shigenobu Ogata (Osaka University), Tomohito Tsuru (Japan Atomic Energy Agency), Tomotsugu Shimokawa (Kanazawa University), Momoji Kubo (Tohoku University), Yoshiteru Aoyagi (Tohoku University), Koretaka Yuge (Kyoto University)

The aim of this group is to reveal the origin of the excellent and unusual mechanical properties of high-entropy alloys, such as high strength, high fracture toughness, high ductility, high fatigue life, good corrosion resistance and so on, by means of the state-of-the-art computational materials science techniques, that is very large-scale first-principles electronic structure and atomic structure calculations, accelerated molecular dynamics, database driven grand canonical Monte Carlo methods, atomistically informed dislocation dynamics and crystal plasticity, the other various spatial and temporal multiscale modeling. The fundamental understanding of mechanical properties together with novel plasticity and nano-mechanics theories, and machine learning methods would lead to a non-empirical prediction and design of high performance high-entropy alloys by tuning the chemical composition, chemical ordering, microstructure, and so on. The group involves world-leading specialists of mechanics, chemistry, statistical physics, and multiscale modeling and simulation.



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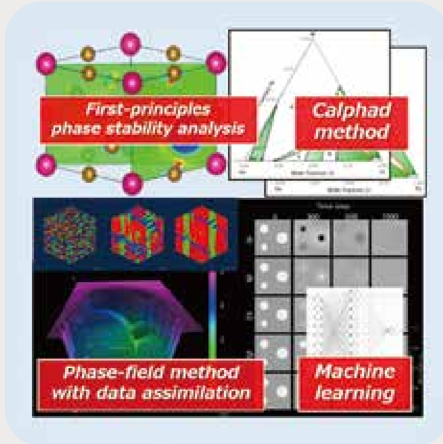
2019 MAY

A02(d) Materials Design of High-Entropy Alloys Accelerated by Computational Thermodynamics and Kinetics with Data Science Techniques

Toshiyuki Koyama (Nagoya University), Hiroshi Ohtani (Tohoku University), Ying Chen (Tohoku University), Katsunari Oikawa (Tohoku University), Taichi Abe (NIMS), Ikuo Ohnuma (NIMS), Nobufumi Ueshima (Tohoku University)

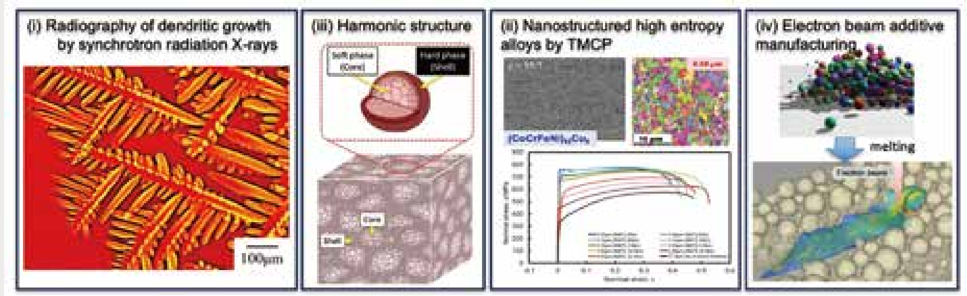
The fundamental issues to boost up materials design in the field of high-entropy alloys (HEAs) are (1) the effective and accurate assessment of phase diagrams and Gibbs energies in the wide composition range of multi-component systems, and (2) the rapid optimization of materials properties within the diverse space of materials and process parameters. In order to overcome these issues, the group A02(d) focuses on the following three targets: (i) First-principals calculation on the phase diagram of HEAs with Calphad approach and re-assessment of the Gibbs energy database, (ii) Comprehensive evaluation of materials parameters in Gibbs energy functions and diffusion mobility functions from the microstructural kinetic data by means of the phase-field method with data assimilation techniques, and (iii) Effective optimization of materials properties on HEAs, which is accelerated by various machine learning techniques. The aim of this group is to provide the efficient strategy in materials science and engineering to handle HEAs on a daily basis. The methodologies and database accumulated in this group are shared with other groups in the project, which would contribute to the enhancement of entire research activities.



A03(e) Nano-/Micro-Structure Control of High-Entropy Alloys by Advanced Processing

Nobuhiro Tsuji (Kyoto University), Kei Ameyama (Ritsumeikan University), Akihiko Chiba (Tohoku University), Hideyuki Yasuda (Kyoto University), Stefanus Harjo (JAEA J-PARC Center)

Properties of metallic materials can be widely controlled by changing their microstructures. The aim of this group is to establish the guiding principle for fabricating high-entropy alloys (HEAs) having desirable properties based on fundamental understanding of nano- and micro-structures evolution during processing. Four kinds of important processes are involved in the group: i.e., solidification, thermo-mechanical processing (TMCP), powder metallurgy, and additive manufacturing. Using state-of-the-art technologies in processing and characterization, mechanisms of microstructure evolution will be clarified. It is expected to acquire various kinds of new findings on metallurgical phenomena, structure evolution, and resultant properties characteristics of HEAs. Obtained knowledge and fabricated HEAs are provided to other group in the project, in order to realize the synergism and to progress the research activities.



A03(f) Experimental Clarification of Intrinsic Elemental Interaction and Principles of Phase Stability in High-Entropy Alloys

Tadashi Furuhara (Tohoku University), Kazumasa Sugiyama (Tohoku University), Koji Inoue (Tohoku University), Hideki Araki (Osaka University), Masataka Mizuno (Osaka University)

The aim of this group is to establish the guiding principles in stabilization of high-entropy alloys (HEA). One of the interesting and unknown subjects in this field is complex elemental interaction and phase decomposition of multi-component high alloys where solid solution becomes more unstable against ordering reaction and compositional phase separation.

This group involves specialists of nanostructure analysis using various advanced techniques, i.e., high-resolution XRD and TEM, 3D atom probe and positron annihilation and so on. Quantitative analyses of nano-hetero structures are performed for multi-component alloys (MCA) including high-entropy alloys (HEA) which undergo various kinds of thermal cycles. Governing principles of phase stability clarified in the group are correlated with design of fabrication processes in A03(g) and theoretical analyses in A02(d) and further, would contribute to drive the research in the other groups in A01 and A02.