NIMS AWARD
National Institute for Materials Science

NIMS Award Symposium 2023

Structural Materials × Carbon Neutral

Abstracts

National Institute for Materials Science

Contents

The National Institute for Materials Science (NIMS) is one of the three designated national research and development agencies in Japan. The mission of NIMS is to conduct basic research in materials science and translate the results into innovations that contribute to solving societal problems.

On April 1, 2023, NIMS began its 5th 7-year medium-term plan. To meet the timely demands of society, we will continue our efforts with the goal of achieving world-class research results in materials science. In order to make technological contributions to a carbon-neutral society, NIMS has identified research on storage battery materials, hydrogen-related materials, and ultra-high-temperature materials as priority research areas. Therefore, it is very significant to hold NIMS Award Symposium under the theme "Structural Materials × Carbon Neutral".

NIMS Award Symposium is one of the largest and most important events organized by NIMS each year, consisting of NIMS Award Ceremony and an academic symposium related to the recipient's field of research. NIMS Award is an international award given to outstanding researchers who have conducted innovative research in materials science. The award areas are selected in the following order: Materials for Environment and Energy, Functional Materials, Structural Materials and Basic Materials Science. This year, the selection committee selected the winner in the area of "Structural Materials" based on the recommendations of world-renowned researchers. This year's recipient is Professor Dierk Raabe, Director of the Max-Planck-Institut für Eisenforschung GmbH, for his outstanding academic achievements in the field of alloy design. A detailed citation of NIMS Award winner is included in the abstract booklet. In addition, a poster session is planned to provide an opportunity for the awardee to present their research in their areas of expertise.

Through this NIMS Award Symposium, we hope that you will also see the results of research in related fields at NIMS through oral and poster presentations.

Kazuhiro Hono
President, National Institute for Materials Science

Programs (Day1 & 2)

Nov. 6 (Monday)

9:30- Registration

10:00- Opening Remarks by NIMS President Dr. Kazuhiro Hono, and Greeting from MEXT

10:05 - 10:20 NIMS Introduction by NIMS President Dr. Kazuhiro Hono

10:20 - 10:40 **NIMS Award 2023 Ceremony**

10:40 - 11:40 [Chair: Dr. Kaneaki Tsuzaki]

NIMS Award 2023 Winning-lecture
Prof. Dierk Raabe (Max-Planck-Institut für Eisenforschung GmbH, Germany)
"The Materials Science Behind Hydrogen-Based Green Steel Making"

11:40 - 13:00 Photo Session & Lunch Break

NIMS Award Session

[Chair: Dr. Takahito Ohmura]

13:00 - 13:40 Invited Talk **NA-1**
Prof. Sudarsanam Suresh Babu (University of Tennessee, Knoxville, USA)
"Microstructural Heterogeneity in Metal Additive Manufacturing"

13:40 - 14:20 Invited Talk **NA-2** **Prof. Simon P. Ringer** (The University of Sydney, Australia)
"Towards a New Class of Alpha-beta Ti-O-Fe Alloys via Additive Manufacturing - a case study in atomic-scale microstructural control"

14:20 - 14:40 NIMS Talk **NA-3** **Dr. Makoto Watanabe** (RCSM, NIMS)
"Materials Integration for Understanding Process-Structure-Property Linkage of Additive Manufacturing"

14:40 - 15:00 Poster / Coffee

[Chair: Dr. Kota Sawada]

15:00 - 15:40 Invited Talk **NA-4** **Prof. Sung-Joon Kim** (POSTECH, Korea)
"Understanding Material Factors on Liquid Metal Embrittlement Sensitivity of Zn-coated AHSS"

15:40 - 16:20 Invited Talk **NA-5** **Prof. Tadashi Furuhara** (Tohoku University)
"Sublattice Alloy Design for Application of Solute Clustering in High-strength Steels"

16:20 - 16:40 NIMS Talk **NA-6** **Dr. Hideki Katayama** (RCSM, NIMS)
"Corrosion Risk Prediction Map for Maintenance of Infrastructure"

16:40 - 18:00 Poster/ Refreshment

18:00 - 19:30 NIMS Award Reception (1F Multi-purpose Hall)

Nov. 7 (Tuesday)

8:30- Registration

Session 1: Deformation and Fracture

[Chair: Dr. Hideki Katayama]

9:00-9:30 Invited Talk **S1-1** **Prof. Nobuhiro Tsuji** (Kyoto University)
"Possibilities of Advanced Steels Managing Both Ultra-High Strength and Large Ductility"

9:30-10:00 Invited Talk **S1-2** **Prof. Manabu Enoki** (The University of Tokyo)
"Microstructure Based Prediction/Design of Mechanical Properties and Damage Monitoring of Structural Materials"

10:00-10:30 Invited Talk **S1-3** **Prof. Masaki Tanaka** (Kyushu University)
"Understanding the Brittle-to-ductile Transition Based on Shielding Theory"

10:30-11:00 Poster / Coffee

[Chair: Dr. Yuuji Kimura]

11:00-11:30 Invited Talk **S1-4** **Associate Prof. Motomichi Koyama** (Tohoku University)
"Interactions among Hydrogen-transformation-crack in Metastable Austenitic Steels"

11:30-12:00 NIMS Talk **S1-5** **Dr. Akinobu Shibata** (RCSM, NIMS)
"Hydrogen-related Fracture in High-strength Martensitic Steels"

12:00-13:30 Lunch Break

Session 2: High-temperature Materials

[Chair: Dr. Makoto Watanabe]

13:30-14:00 Invited Talk **S2-1** **Prof. Eiichi Sato** (Institute of Space and Astronautical Science, JAXA)
"Multi-material Designed Satellite Thruster through Ceramics/metal Dissimilar Joining"

14:00-14:30 Invited Talk **S2-2** **Prof. Yuichiro Koizumi** (Osaka University)
"Digital Twin Science of Powder Bed Fusion Metal Additive Manufacturing"

14:30-15:00 Invited Talk **S2-3** **Associate Prof. Yuhki Tsukada** (Nagoya University)
"Grain Boundary Segregation and Creep Rupture Strength of High-temperature Materials"

15:00-15:30 Poster / Coffee

[Chair: Dr. Ryoji Sahara]

15:30-16:00 NIMS Talk **S2-4** **Dr. Toshio Osada** (RCSM, NIMS)
"Development of Ni-based Superalloys for Jet Engine Applications"

16:00-16:30 NIMS Talk **S2-5** **Dr. Taisuke Sasaki** (CMSM, NIMS)
"On the Role of Atom Probe Tomography in Understanding of Microstructural Origin of High Strength in Metallic Alloys"

16:30-16:35 Closing Remarks by Director of RCSM, Dr. Takahito Ohmura

16:35-19:00 Poster Session [Core Time 17:00 - 19:00]

P1 Process

No.	Name	Affiliation/ Company	Presentation Title
P1-01	Yoshiaki Toda	NIMS	New Microstructure Design of Heat-resistant Titanium Alloys with Property Improvements Using Super Thermal Field
P1-02	Satoshi Emura	NIMS	Introduction of Millefeuille-like α/β Layered Structure into Ti-Mo Alloy through Thermomechanical Treatment
P1-03	Phuangphaga Daram	NIMS	Compositionally Graded Titanium to Aluminum Processed by Laser Powder Bed Fusion Process: Microstructure Evolution and Mechanical Properties
P1-04	Sachiko Hiromoto	NIMS	Development of Apatite and LDH Coatings of Mg Alloys Depending on the Application
P1-05	Yusuke Tsutsumi	NIMS	Improvement of Corrosion Resistance of Type 420J2 Martensitic Stainless Steel by Laser thermal Processing
P1-06	Akitsu Shigetou	NIMS	Low-Temperature and Non-vacuum Surface Modification for Anti-Hydrolysis Hybrid Bonding
P1-07	Machiko Ode	NIMS	Observation and Numerical Prediction of Concentration Distribution at Cast Coating Interface of Solid Pt, Ir, Re Using Liquid Ni-Based Alloys
P1-08	Yuuji Kimura	NIMS	Delayed Fracture of Ultra-high Strength Steel Processed by Warm Tempforming
P1-09	Susumu Takamori	NIMS	Microstructures and Mechanical Properties of Fe–15Mn–10Cr–8Ni–4Si Seismic Damper Cast Alloy
P1-10	Hiroshi Honda	NIMS	Evaluation of Laser Absorptivity of Titanium Powder by Using Ray Tracing
P1-11	Takuma Saito	NIMS	Effect of Cooling Rate From Sub-Solvus Solution Treatment Temperature on Hardness in Powder Metallurgy Ni-Co-base Superalloy
P1-12	Masahiro Kusano	NIMS	Three-Dimensional Cellular Automaton for Grain Growth of Inconel 738LC in Laser Powder Bed Fusion
P1-13	Tomonori Kitashima	NIMS	Fabrication of Single Crystals in Laser Powder Bed Fusion Using a Flat-Top Laser
P1-14	Makoto Watanabe	NIMS	Materials Integration for Laser Powder Bed Fusion Process
P1-15	Rintaro Ueji	NIMS	Anisotropy of Uniaxial Yield Stress of Pearlitic Steel Caused by Compressive Deformation
P1-16	Ryuta Yurishima	University of Ibaraki	High-throughput Search for High-performance Materials Using Composition-graded Bulk Specimens
P1-17	Naoe Hosoda	NIMS	Biomimetic Reversible Interconnection

P2 Characterization

No.	Name	Affiliation/ Company	Presentation Title
P2-01	Takahito Ohmura	NIMS	Nano-mechanical Characterization for Multi-scale Modeling in Mechanical Behavior of Metallic Materials
P2-02	Tomotaka Hatakeyama	NIMS	Microstructure of Modified 9Cr-1Mo Steel Manufactured by Laser Powder Bed Fusion
P2-03	Fumiyoshi Yoshinaka	NIMS	Hierarchical Fatigue Damage Mechanism and Development of Fatigue-resistant Alloy
P2-04	Mainak Saha	Indian Institute of Technology Madras	On the Three-dimensional Atomic Scale Characterisation of Nano-Scale B2 Phase in Ni-Alloyed Fe-Mn-Al-C Low-density Steel
P2-05	Hidetoshi Somekawa	NIMS	Effect of Grain Boundary Segregation On Mechanical Properties in Mg Alloys
P2-06	Viola Paul	NIMS	Effect of Yttrium Addition on the Nanoindentation Behavior at Mg–Y Alloy Grain Boundaries
P2-07	Tomoya Nagira	NIMS	Application of Friction Stir Welding for Fe-Mn-Si Alloy
P2-08	Silvia Pomes	NIMS	Elevated Temperature Exploration of Mechanical Behavior in Zr-based Bulk Metallic Glass through Nanoindentation Testing
P2-09	Susumu Meguro	NIMS	Thermoelectric Generation by Joining Interface Control of thermocouple Metals
P2-10	Digvijay Singh	NIMS	Unveiling the Transformation Pathways of Hierarchical γ90 – εtwin – α′ Triple Phase Structure Formation at ε-ε Martensite Intersection
P2-11	Norimitsu Koga	Kanazawa University	Tensile Properties and Deformation Behavior at Low Temperatures in Ferrite and Austenite Duplex Stainless Steel With Various Grain Sizes
P2-12	Wenqi Mao	Japan Atomic Energy Agency	Excellent Combination of Strength and Ductility of an Ultrafine-grained Stainless Steel at Cryogenic Temperatures Studied by in Situ Neutron Diffraction
P2-13	Seiichiro Ii	NIMS	Static and Dynamic Characterization of Grain Boundary-dislocation Interaction
P2-14	Wu Gong	Japan Atomic Energy Agency	Microstructure Characterization through *in Situ* Neutron Diffraction with Diffractometer TAKUMI
P2-15	Kazuho Okada	NIMS	Improvement of Resistance Against Hydrogen Embrittlement by Carbon Segregation at Prior Austenite Grain Boundary in As-Quenched Martensitic Steels
P2-16	Ivan Gutierrez	NIMS	Development of Analysis Methods for SEM-based Techniques and X-Ray Contrast Tomography: Application to Strain Localization Phenomena and Hydrogen-induced Effects on Plasticity in High-strength Steels
P2-17	Tatsuya Ito	Japan Atomic Energy Agency	In Situ Neutron Diffraction Study on Deformation Behavior of Hydrogen-charged SUS310S Austenitic Steel

P2 Characterization

No.	Name	Affiliation/ Company	Presentation Title
P2-18	Toru Hara	NIMS	Advanced FIB-SEM Serial-sectioning Techniques Dedicated for 3D-EBSD Analysis
P2-19	Jiangwei Liu	NIMS	High Thermal Stability for Boron-Doped Diamond Field-effect Transistors
P2-20	Ryunosuke Harada	University of Hyogo	Effects of Temperature and Strain Rate on Mechanical Properties in FeMnNiCoCr High Entropy Alloy
P2-21	Sangmin Lee	NIMS	Deformation Behavior and Microstructure of Dual-phase CoCuNi Alloy Processed by High-pressure Torsion and Subsequent Annealing
P2-22	Kaito Kikuchi	Nagaoka University of Technology	Development of a New Age-hardenable Magnesium Alloy Sheet with Excellent Room Temperature Formability and Corrosion-resistance
P2-23	Hideaki Nishikawa	NIMS	Short Fatigue Crack Growth Mechanism in Ni-Co Based Superalloy at Elevated Temperatures and in Oxidative Atmospheres
P2-24	Dayuan Liu	NIMS	Estimation of Mechanical Properties of Alloys Using Neighboring Indentation Test
P2-25	Takahiro Sawaguchi	NIMS	Evidence Supporting Reversible Martensitic Transformation under Cyclic Loading on Fe–Mn–Si–Al Alloys Using in Situ Neutron Diffraction
P2-26	Seunghyeon Kim	NIMS	Corrosion Behavior of $Gd_2Si_2O_7$/ $Sc_2Si_2O_7$ with CMAS Melts for Environmental Barrier Coatings
P2-27	Nozomu Adachi	Toyohashi University of Technology	Mechanical Response of Pure Fe Having Different Grain Sizes under Tensile Stress
P2-28	Kyoko Kawagishi	NIMS	Construction of a Materials Database for Aeroengine Materials

P3 Evaluation

No.	Name	Affiliation/ Company	Presentation Title
P3-01	Kimiyoshi Naito	NIMS	Anisotropic Properties of Polyacrylonitrile- and Pitch-based Carbon Fibers
P3-02	Sheng Xu	Tohoku Univeristy	Examining the Cryogenic Elastocaloric Effect in A Cu-Al-Mn Alloy
P3-03	Kota Sawada	NIMS	Effect of Segregation of Alloying Elements on Creep Strength in Heat Resistant Steels
P3-04	Ayako Ikeda	NIMS	High-throughput Evaluation Methods for Ni Based Superalloys Using Composition and Process Temperature Graded Bulk Samples
P3-05	Hideki Katayama	NIMS	Development of Prediction Technology for Corrosion Damage Risk of Infrastructures
P3-06	Jonathon Tanks	NIMS	Durable Biomass/Polypropylene Composites for Improving Sustainability in Structures
P3-07	Kentaro Wada	NIMS	Gaseous Hydrogen Embrittlement of Pure Nickel and Copper Nickel Alloys
P3-08	Satoshi Morooka	Japan Atomic Energy Agency	Magnetic Order and Phase Transformation in Fe-Mn-C Alloy at Cryogenic Temperature
P3-09	Elango Chandiran	NIMS	Activation of Non <a> Type Dislocations and Damping Capacity Improvement by Deformation Induced Martensitic Transformation in Mg-Sc Alloy
P3-10	Rion Abe	Iwate University	3D Visualization of Hydrogen Trapping Sites in Al-Zn-Mg Alloys
P3-11	Christopher Mercer	NIMS	Evaluation of the Mechanical Response of Functional Lattice Structures
P3-12	Chihiro Tabata	Waseda University	Measurements of Interfacial Strength between Sulfur-segregated Al_2O_3 and Ni-Al Single Crystal Alloy Using Nanoindentation
P3-13	Hiroyuki Oguma	NIMS	Elucidation of Fatigue Fracture Mechanism Focusing on the Environment and Interface in Materials
P3-14	Yuhei Ogawa	NIMS	Beneficial Aspect of Hydrogen on the Mechanical Property of Fe-Cr-Ni Austenitic Steels
P3-15	Kensuke Miyahara	NIMS	Small Ball Rebound Hardness Tester and Progress for Japanese Industrial Standards (JIS)
P3-16	Houichi Kitano	NIMS	Advancement of Welding Technology through the Use of AI Technology
P3-17	Masao Hayakawa	NIMS	Review of Damage Evaluation and Remanufacturing for Material Sustainability
P3-18	Yoshinori Ono	NIMS	Developing a Foundation for Material Evaluations to Support R & D on Liquefied Hydrogen-related Equipment
P3-19	Yoshiharu Murase	NIMS	Corrosion Resistance Evaluation of Structural Materials by Multimodal KFM-EBSD-EDS Analysis
P3-20	Kazuya Shimoda	NIMS	High Temperature Fatigue Properties of SiC/SiC Composites via Novel Production Route Using Sandwich Prepreg Sheets
P3-21	Kotaro Doi	NIMS	Electrochemical Measurement of Hydrogen Diffusion Coefficient for Mg-based Materials

P4 Modeling

No.	Name	Affiliation/ Company	Presentation Title
P4-01	Taichi Abe	NIMS	Computational Phase Diagrams and their Database Based on CALPHAD
P4-02	Taiyo Maeda	Yokohama National University	Numerical Prediction of Strength Scatter in Ceramics Based on Microstructural Information
P4-03	Mariko Kadowaki	NIMS	Numerical Simulations to Analyze the Corrosion Behavior of Metallic Materials
P4-04	Ikuo Ohnuma	NIMS	Segregation Engineering of Structural Materials by CALPHAD Method
P4-05	Arkapol Saengdeejing	NIMS	Developing Thermodynamic Database from First-principles Calculations Data
P4-06	Mostafizur Rahman	Yokohama National University	Kinetic Parameters for Strength Recovery in Self-healing Ceramics
P4-07	Dmitry S. Bulgarevich	NIMS	Representative Volume Element Reconstruction and Crystal Plasticity Modeling of Stress-strain Curves for Additively Manufactured Hastelloy X
P4-08	Ryoji Sahara	NIMS	Design of High Temperature Materials Using a Multiscale Simulation Without Empirical Parameter
P4-09	Xiaoyang Zheng	NIMS	Reprogrammable Mechanical Metamaterials
P4-10	Aaditya Manjanath	NIMS	Probing Chemical Reaction Dynamics through Excited-state Time-dependent *GW* Simulations
P4-11	Jiaxin Zhou	NIMS	Computational Morphology Design of Duplex Structure Considering Interface Debonding
P4-12	Masato Wakeda	NIMS	Atomistic Modeling of Nanoscale Interaction between Dislocation and Grain Boundary in BCC and FCC Metals
P4-13	Sukeharu Nomoto	NIMS	Seamless Numerical Simulation for Laser Powder Bed Fusion Process by Lattice Boltzmann and Multi-phase Field Methods
P4-14	Junping Du	Osaka University	A Neural Network Accelerated Kinetic Monte Carlo Simulation of the Evolution of Chemical Order in CrCoNi Medium-entropy Alloy
P4-15	Vickey Nandal	NIMS	Artificial Intelligence and Expert Cooperative Design of Non-isothermal Aging Heat Treatment Schedules for Improving 0.2% Proof Stress in γ – γ' Binary Ni-Al Alloys
P4-16	Shihao Zhang	Osaka University	Highlier Efficient Neural Network Interatomic Potential of α-iron and Hydrogen System
P4-17	Hitoshi Izuno	NIMS	Tandem Bayesian Model: Connection of Weld Joint Creep Performance and Welding Conditions Considering HAZ Shape Factor
P4-18	Shinnosuke Yanagawa	NIMS	Multiscale Finite Element Analysis of Yield Point Phenomenon In Ferrite-pearlite Duplex Steels
P4-19	Keiya Sugiura	Nagoya University	3D Microstructure Reconstruction of Metallic Materials Using Generative Adversarial Networks

NIMS Award 2023

NIMS Award 2023 Winner

This year's NIMS Award targeted basic research in the field of structural materials that has led to profound benefit for society and industry and created impactful results that have changed the world. Prof. Dierk Raabe's "Pioneering research on the sustainability and microstructure-based design of advanced metallic alloys" was selected to receive the NIMS Award 2023 as an outstanding global achievement.

Professor Dierk Raabe

Department Microstructure Physics and Alloy Design
Sustainable Synthesis of Materials
Max-Planck-Institut für Eisenforschung GmbH, Germany

[Field of Research]
Structural Metals, Sustainability, Metallurgy,Metal Physics, Computational Science

Research Summary and Impact on the Academic and Industrial Sectors

[Research Achievement Title]
Pioneering research on the sustainability and microstructure-based design of advanced metallic alloys

[Outline of Awarded Research Achievement]
Prof. Dierk Raabe has focused on the relation among lattice defects, their defect chemistry, mechanical properties and sustainable fabrication processes in structural metallic materials. Also, he has used state-of-the-art multiscale analysis techniques such as atom probe tomography, transmission electron microscopy, field ion microscopy, and machine learning for correlative atomic-scale characterization of microstructure developments, such as dislocations and interfaces, and chemical properties due to phase transformation. He has then applied this approach to the trade-off problem between strength and ductility, controlling structural phase transformation by chemically adjusting thermomechanical stability, and has developed new materials with both high strength and durability.

[Ripple Effects of Achievements on Academia and Industry]
Prof. Dierk Raabe's research achievements to date have conspicuously contributed to the latest research that is identifying pathways for the sustainability of metallic materials. It is now globally recognized that the production and manufacturing of materials must become more sustainable, particularly the associated high carbon dioxide emissions must be urgently reduced. In this context, Prof. Raabe's work particularly addresses primary production with less carbon dioxide, high-performance alloys based on metal recycling, alloy design for enhanced scrap compatibility, improved impurity- and hydrogen-tolerance of alloys, green steel production by hydrogen plasma, direct reduction of iron ore by hydrogen etc., all contributions with highest urgency and benefit to academia and industry.

Profile

History

1983～1984	Study of Music, Konservatorium Rheinland, Institut Wuppertal
1984～1989	Study of Physical Metallurgy and Metal Physics, RWTH Aachen, supervised by Prof. Dr. K. Lücke, summa cum laude
1992	Doctoral thesis, Institute for Physical Metallurgy and Metal Physics, RWTH Aachen, supervised by Prof. Dr. K. Lücke, summa cum laude
1997	Habilitation, Physical Metallurgy and Metal Physics, RWTH Aachen
1992～1997	Research assistant, group leader, Institute for Physical Metallurgy and Metal Physics, RWTH Aachen, Germany
1997～1999	Postdoctoral researcher, Dept. Materials Science & Engineering, Carnegie Mellon University, USA
1999～today	Director, Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Awards and Honors

2012 & 2022	2 ERC Advanced Grants of the European Union
2022	Acta Materialia Gold Medal
2022	Doctor Honoris Causa, Norwegian Technical University Trondheim
2021	Kelly Lecture, University of Cambridge, 100th anniversary year lecture of the Department of Materials Science & Metallurgy
2014	Honorary Professor, Katholieke Universiteit Leuven, Belgium
2013	Member and vice-senator of National Academy Leopoldina
2004	Gottfried Wilhelm Leibniz Award of the German Research Foundation
1995, 2015, 2016	3 best paper awards
1997	Heisenberg Award of the German Research Foundation

Selected Publications

1) B. Sun, W. Lu, B. Gault, R. Ding, S. K. Makineni, D. Wan, C.H. H. Wu, H. Chen, D. Ponge, D. Raabe, Chemical heterogeneity enhances hydrogen resistance in high-strength steels, Nature Materials, 20, 1629 (2021)

2) H. Zhao, P. Chakraborty, D. Ponge, T. Hickel, B. Sun, C.-H. Wu, B. Gault, D. Raabe, Hydrogen trapping and embrittlement in high-strength Al-alloys, Nature, 602, 437 (2022).

3) L. Han, F. Maccari, I. R. S. Filho, N. J. Peter, Y. Wei, B. Baptiste, O. Gutfleisch, Z. Li, D. Raabe, A mechanically strong and ductile soft magnet with extremely low coercivity, Nature 608, 24 (2022).

4) D. Raabe, C. C. Tasan, E. A. Olivetti, Strategies for improving the sustainability of structural metals, Nature 575, 64 (2019).

5) Z. Rao, P.-Y. Tung, R. Xie, Y. Wei, H. Zhang, A. Ferrari, T.P.C. Klaver, F. Körmann, T. P. Sukumar, A. Kwiatkowski da Silva, Y. Chen, Z. Li, D. Ponge, J. Neugebauer, O. Gutfleisch, S. Bauer, D. Raabe, Machine learning-enabled high-entropy alloy discovery, Science 378, 78–85 (2022).

6) D. Raabe, D. Ponge, P. Uggowitzer, M. Roscher, M. Paolantonio, C. Liu, H. Antrekowitsch, E. Kozeschnik, D. Seidmann, B. Gault, F. De Geuser, A. Dechamps, C. Hutchinson, C. Liu, Z. Li, P. Prangnell, J. Robson, P. Shanthraj, S. Vakili, C. Sinclair, L. Bourgeois, S. Pogatscher, Making sustainable aluminum by recycling scrap: The science of “dirty” alloys, Progress in Materials Science, 100947 (2022).

7) D. Raabe The Materials Science behind Sustainable Metals and Alloys. Chem. Rev. 123(5):2436–2608 (2023).

"The Materials Science Behind Hydrogen-Based Green Steel Making"

Dierk Raabe
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Abstract
1.85 billion tons of steel are produced per year, making it the most important alloy in terms of volume and impact. While steel is a sustainability enabler, through lightweight car parts, wind farms and magnets, its primary production is the opposite. Its reduction from oxides by use of fossil carbon carriers produces 2t CO_2/t of steel, qualifying it as the largest single cause of global warming [1].
The presentation introduces basic research questions associated with producing steel more sustainably, particularly with lower CO_2 emissions [1-5]. It opens a critical discussion on the question what the basic science topics behind green steel making are and which key research questions must be tackled, to reinvent a 3000-year-old industry within a few years, considering both, advanced experimental and in-situ experiments [2-4] as well as theory and simulations [5]. Also it is discussed which reduction methods are the most promising ones and which scientific bottleneck questions must be solved to make Green Steel become reality. Therefore, the presentation addresses some recent progress and open issues in understanding the key mechanisms of hydrogen-based direct reduction and hydrogen-based plasma reduction including topics such as the kinetics of the solid state and plasma-based reduction reactions, mass transport kinetics, nucleation during the multiple phase transformations, the oxide's chemistry and microstructure, as well as the roles of plasticity, damage and fracture associated with the phase transformation [6].

[1] Raabe D, Tasan CC, Olivetti EA. Strategies for improving the sustainability of structural metals. Nature. 2019 Nov; 575 (7781): 64-74.
[2] SH Kim, X Zhang, Y Ma, IR Souza Filho, K Schweinar, et al. Influence of microstructure and atomic-scale chemistry on the direct reduction of iron ore with hydrogen at 700° C, Acta Materialia, 2021
[3] IR Souza Filho, Y Ma, M Kulse, D Ponge, B Gault, et al. Sustainable steel through hydrogen plasma reduction of iron ore: Process, kinetics, microstructure, chemistry, Acta Materialia, 2021
[4] Souza Filho IR, Springer H, Ma Y, Mahajan A, da Silva CC, Kulse M, et al. Green steel at its crossroads: Hybrid hydrogen-based reduction of iron ores. J Clean Prod 2022;340:130805.
[5] Bai, Y. et al. Chemo-Mechanical Phase-Field Modeling of Iron Oxide Reduction with Hydrogen. Acta Mater. 231, 117899 (2022).
[6] D. Raabe The Materials Science behind Sustainable Metals and Alloys. Chem. Rev. 123(5):2436–2608 (2023).

NIMS Award Session

Invited Talk NA-1

Microstructural Heterogeneity in Metal Additive Manufacturing

Sudarsanam Suresh Babu
UT/ORNL Governors Chair in Advanced Manufacturing, Department of Mechanical, Aerospace, Biomedical Engineering, The University of Tennessee, Knoxville, USA

Abstract

Additive manufacturing has emerged as a robust technology for producing components of various sizes, featuring intricate geometries. The interplay between geometry and processing methods with arc, laser, and electron beam results in dynamic changes in melt pool shapes. Consequently, these changes lead to variations in thermal gradient (G) and liquid-solid interface velocity (V) during the solidification process. These variations are further compounded by repeated heating and cooling cycles, each characterized by distinct heating rates, peak temperatures, and cooling rates. These thermal factors drive the evolution of non-equilibrium microstructures, involving complex phase selection phenomena and transitions from columnar to equiaxed grain formation due to the instability of the liquid-solid (L/S) interface.

In this presentation, a review of the foundational solidification theories based on interface response functions (IRF) derived from simple binary systems will be presented. Subsequently, an extension of these concepts to address the highly transient L/S interface motions observed during pulsed arc welding of Fe-C-Al-Mn alloys will be discussed. Given that additive manufacturing essentially involves welding with complex boundary conditions, one can explore the applicability of IRF models in explaining the fish-scale type structures observed in 316 AM components. Furthermore, the correlation between spatially varying G and V within the melt pool and the phase selection observed in Al-Ce-Mn alloys will be examined. In this alloy, the outcomes can range from the formation of the fcc phase to intermetallic compounds or eutectic microstructures. Additionally, research on cascading stability of these solidification microstructures, considering the barriers to nucleate a third phase at the interfaces formed during solidification, will be presented. Finally, the relevance of these findings in the context of qualifying metal additive manufacturing components, particularly in conjunction with in-situ monitoring techniques, will be outlined.

Dr. Babu obtained his bachelor's degree in metallurgical engineering from PSG College of Technology, Coimbatore, India, and his master's degree in industrial welding metallurgy-materials joining from Indian Institute of Technology, Madras. He obtained his PhD in materials science and metallurgy from University of Cambridge, UK in 1992. He also worked as a research associate in the Institute for Materials Research, Sendai, Japan before joining ORNL in 1993. From 1993 to 1997, he held joint researcher position with ORNL, University of Tennessee and The Penn State University. From 1997 to 2005, he worked as an R&D staff at ORNL. From 2005 to 2007, Suresh held a senior level technology leader position in the area of engineering and materials at Edison Welding Institute, Columbus, Ohio. From 2007 to 2013, Suresh served as Professor of Materials Science and Engineering at The Ohio State University. In 2013, Suresh was appointed as UT/ORNL Governor's chair of advanced manufacturing at the University of Tennessee, Knoxville, TN. In 2020, Suresh was appointed to the National Science Board by the President of the United States of America for a six-year term.

Invited Talk NA-2

Towards a New Class of Alpha-beta Ti-O-Fe Alloys via Additive Manufacturing—a Case Study in Atomic-scale Microstructural Control

Simon P. Ringer
Pro-Vice-Chancellor (Research Infrastructure), and
Professor of Materials Engineering, The University of Sydney, Australia

Abstract

Thermal gyrations and compositional inhomogeneities brought about during metal additive manufacturing (AM) significantly change the microstructural evolution during processing compared to conventional processing routes. The rapid heating and cooling cycles over extended periods of time during AM create metallurgical opportunities through the associated novel solid-state phase transformation phenomena. This presentation showcases selected recent results from an international research project—AUSMURI (Australia-US Multidisciplinary Research Initiative)—to highlight the power and impact of international research centres. The international inter-agency synchronisation of funding is challenging but very valuable. This is notable given the alignment of the strategic priorities of Japan and Australia. The presentation also provides a detailed expose of our efforts to combine AM process design and alloy design to achieve a new microstructural opportunities and new levels of performance in titanium alloys, including a new class of AM-enabled titanium-oxygen-iron alloys via laser directed energy deposition. The potential for sustainable AM materials streams is very when this aspect is placed at the centre of the process and alloy design.

Simon P. Ringer is a metallurgist specialising in the relationships between the microstructure of materials and their engineering properties and performance. His research focuses on understanding materials from the atomic-scale to gain insights that can shape the design of the materials themselves, and the processes by which they are made. His work spans the development of structural alloys, semiconductors and functional materials. He is an expert in microscopy and computational materials simulations, and several examples of his fundamental research have been translated to industrial practice. He has held appointments in Australia, Sweden, Japan and the USA, led the establishment of a number of major research institutes and facilities, and has a global academic and industrial network. He was elected as Fellow of the Australian Academy of Technology and Engineering in 2020. He is professor of materials engineering at the University of Sydney and Pro-Vice-Chancellor for research infrastructure, where he is responsible the strategy, policy and operations of research infrastructure, research technology services, and research space management.

NIMS Talk NA-3

Understanding Process-Structure-Property Linkage of Additive Manufacturing

Makoto Watanabe

Field Director, Research Center for Structural Materials (RCSM),

National Institute for Materials Science (NIMS)

Abstract

Metal additive manufacturing (AM) has attracted a lot of interest as a new processing technique to realize complex geometries based on a computer-aided design (CAD). Laser Powder Bed Fusion (LPBF) is the most widely used powder bed metal AM process in the industry. In LPBF, it is important to suppress the formation of defects such as cracks and pores through rapid heating and cooling by a laser beam. In addition, since a characteristic anisotropic microstructure is formed, it is necessary to understand the process-microstructure-property correlation and establish microstructure control techniques to achieve the required mechanical properties. The geometry of a component has a large influence on the temperature field during the process, and so the microstructure can vary greatly depending on the position even under the same laser conditions. Therefore, in the development of new components, optimization by trial and error using only experiments is extremely inefficient, and the establishment of prediction techniques using computation is essential. We have studied heat-resistant alloys with the aim of accumulating process-microstructure-property correlation data in the LPBF process and establishing our own prediction technique.

The solidification microstructure and cracking behavior of the LPBF Ni-based alloys were investigated by controlling the temperature field through the constricted sample geometry [1]. In-situ temperature monitoring, part-scale and multi-track thermal analyses were performed. The correlations between the temperature gradient and solidification rate and the microstructures were quantitatively revealed. Microstructure control by a different type of a laser profile was investigated for pure Ni by inducing a planar melt pool with a flat-top laser [2]. The optimized process conditions succeeded to form a single crystal structure with a homogeneous near-{001}<100> texture and suppressed high-angle grain boundary. The melt pool morphology significantly affected solidification microstructure. The CFD simulation of melting behavior was developed to predict melt pool dimensions and gas pore formation [3]. Moreover, by developing in-house programs of Lattice Boltzmann method coupled with multiphase field method, the solidification microstructure was successfully predicted by considering the melt pool flow and grain anisotropy. Other research activities to understand and predict the process-structure-property linkage of LPBF will be introduced in the presentation.

[1] M. Kusano, M. Watanabe, Materials & Design, 222 (2022) 111016.
[2] D.E. Jodi, T. Kitashima, Y. Koizumi, T. Nakano, M. Watanabe, Additive Manufacturing Letters, 3 (2022) 100066.
[3] J. Katagiri, M. Kusano, S. Nomoto, M. Watanabe, Case Studies in Thermal Engineering, 50 (2023) 103477.

Makoto Watanabe is the Director of the Materials Manufacturing Field, Research Center for Structural Materials, National Institute for Materials Science (NIMS), Japan. He is also Group Leader of the Additive Manufacturing Group in the same field. He received his Ph.D. from the Department of Materials Engineering at the University of Tokyo in 2000. He worked at Princeton University (Postdoctoral Researcher (2000-2002)) and at the University of California Santa Barbara (Research Associate (2002-2004)), and then joined the Thermal Spray Coatings Group at NIMS in 2004. He also stayed at Stanford University as a visiting researcher (2011-2013), and worked at the University of Tokyo as an associate professor under the cross-appointment system (2017-2020). Recently, he has mainly studied about additive manufacturing (AM) of high temperature alloys by combining experimental and computational approaches to develop new alloys suitable for AM.

Invited Talk NA-4

Understanding Material Factors on Liquid Metal Embrittlement Sensitivity of Zn-coated AHSS

Sung-Joon Kim
Graduate Institute of Ferrous and Eco materials Technology (GIFT),
Pohang University of Science and Technology (POSTECH), Korea

Abstract

Most of automotive components are bonded by resistance spot welding of thin Zn-coated advanced high strength steel (AHSS) sheets. During the spot welding process Zn coating layer is molten by the heat generation, and often infiltrates into grain boundaries, causing intergranular cracking, known as liquid metal embrittlement (LME). Thus, the LME is a critical hurdle to apply the Zn-coated AHSS in automotive industries. Although there are many factors which affect LME, the effects of material factors such as alloying element (Si), and microstructural components will be introduced in this presentation. Among many elements in the steel sheets, Si is the most harmful one on LME. We found that Si in the steel delayed the dissolution of Fe into the coating from the steel, which suspended the active reaction of Fe-Zn and cannot prevent the steel from contacting the liquid Zn during welding. As a second factor, the importance of austenite fraction during spot welding is introduced and we suggest a novel method to prevent LME of Zn-coated twining induced plasticity (TWIP) steel, based on our findings.

Prof. Sung-Joon Kim is currently Dean of Graduate Institute of Ferrous and Energy Materials Technology (GIFT), POSTECH, Korea. He graduated from University of Illinois at Urbana-Champaign and received Ph.D in 1990. Before joining POSTCEH in 2011, he had been working in the Korea Institute of Materials Science (KIMS) in Changwon, Korea for more than 20 years as a principal researcher leading research and development of various kinds of steels, and later served as the vice president of the KIMS. for 3 years. He also served as the president of Korean Institute of Metals and Materials in 2019, and currently he is a member of the National Academy of Engineering of Korea. He is the author of more than 280 peer-reviewed publications. His major interest areas are alloy design of stainless steels, LME and hydrogen embrittlement, etc.

Invited Talk NA-5

Sublattice Alloy Design for Application of Solute Clustering in High-strength Steels

Tadashi Furuhara
Professor, Institute for Materials Research, Tohoku University, Japan

Abstract

Recent advances in high-strength steels for automobile applications or surface-hardened steels have attracted interest on controlling the nanoscale dispersion of alloy carbides/nitrides in ferrite. Particularly, B1-type carbide/nitride precipitation and metastable alloy clustering can be understood as the coupled ordering and compositional phase separation of interstitial alloying elements "i" and substitutional alloying elements "s". In this presentation, the behavior of i–s clustering and alloy carbide/nitride precipitation is introduced based on nanoscale characterization, theoretical calculations, and evaluations of mechanical properties. It is shown that strong i–s attractive interaction is responsible for metastable i–s clustering, which clearly indicated "hidden" nanoscale inhomogeneity in solid solutions. Further, a concept termed interstitial sublattice engineering in bulk and at interphase boundary for designing high strength steels will be discussed.

Tadashi Furuhara is a Professor, Tohoku University. He obtained his Bachelor and Master of Engineering degrees from Kyoto University, Japan. After he graduated with his Ph.D degree from Carnegie Mellon University, USA, he joined the faculty of engineering, Kyoto University in 1989 and made research and education as an assistant and associate professor. Then he became a professor at Tohoku University in 2005. His research activity covers a broad area in physical metallurgy of steels and non-ferrous alloys, such as phase transformations and precipitation, deformation and recrystallization, microstructure control by thermo-mechanical and thermo-chemical processings.
He also actively contributes to various academic societies in metallurgy field. He served as a Vice President of JIM between 2016-19 and is currently the President of ISIJ. He is also an editor of Acta and Scripta Materialia.

NIMS Talk NA-6

Corrosion Risk Prediction Map for Maintenance of Infrastructure

Hideki Katayama
Field Director, Research Center for Structural Materials (RCSM),
National Institute for Materials Science (NIMS)

Abstract

Many infrastructures were built intensively in Japan during the period of high economic growth (1960s), and in recent years, the damage and deterioration of infrastructure due to high aging have become apparent. Therefore, it is said that investments must be made in its repair and reconstruction in order to continue to use the infrastructures in the future. However, local governments manage most road bridges in Japan, and the current situation places a very high financial burden on them. In addition, local governments face the challenge of having few engineers engaged in bridge maintenance, which is an extremely serious situation in terms of the system. The universal and low-cost tool that enables prediction of the damage degree of infrastructure deterioration and its progression is indispensable to solve these problems. In particular, the number of cases of corrosion damage to main girders on road bridges is increasing every year, and a tool that can determine the corrosion environment of infrastructure in advance would be extremely useful. In this study, machine learning was used to link previously measured corrosion loss data with environmental data, and the model was constructed to predict corrosion from environmental data.

The one-year (September 2013 to August 2014) exposure test results for 150 x 70 x 2t (mm) size of carbon steels at six locations in Japan were used as the corrosion data for machine learning. Exposure test specimens were sampled every month, and the corrosion loss was measured. The one-month averages at each location were used for the environmental data. The investigation result of correlation coefficients between each environmental factor and the corrosion loss gave that wind speed and temperature showed relatively high correlations with the corrosion loss. As a result of examining each learning model for the accuracy of the correlation, it was found that the ensemble model using decision trees can estimate corrosion loss with the highest accuracy. The outdoor corrosion tests of 50 x 50 x 2t (mm) sized carbon steel specimens on three bridges in the coastal area verified the certainty of the corrosion prediction model constructed. The corrosion losses estimated by the corrosion prediction model based on environmental data at each bridge was compared with those obtained from outdoor corrosion tests. Relatively good correlations were observed for bridges in coastal areas, whereas for bridges in inland areas, the estimated values were larger than the measured ones.

Hideki Katayama is the Director of the Materials Evaluation Field, Research Center for Structural Materials, National Institute for Materials Science. He also concurrently serves as Group Leader of the Corrosion Research Group in the same field. He holds a Ph.D. in Metallurgical Engineering from the Tokyo Institute of Technology. He is also a visiting professor in the Department of Advanced Chemistry at Tokyo University of Science and a part-time lecturer in the Faculty of Bioscience and Applied Chemistry at Hosei University. He specializes in corrosion science and electrochemistry.

Session 1:
Deformation and Fracture

Invited Talk S1-1

Possibilities of Advanced Steels Managing Both Ultra-High Strength and Large Ductility

Nobuhiro Tsuji
Professor
Department of Materials Science and Engineering, Kyoto University, Japan.

Abstract

Structural metallic materials are required to have ultrahigh strength nowadays by social demands of light-weighting for huge constructions and transportation devices like automobiles. Ultrafine grained (UFG) metallic materials (or bulk nanostructured metals) with average grain sizes much smaller than 1 μm are candidates of ultrahigh-strength metals. Nanostructured metals and alloys usually show strength 2-4 times higher than that of conventional metals with coarse grain sizes larger than several tens micro-meter. However, their tensile ductility, especially uniform elongation, is limited in many cases, which is attributed to the early plastic instability caused by high flow stress and limited strain-hardening capability of the UFG materials. Therefore, an important strategy for managing both strength and ductility in nanostructured metals is to increase strain-hardening capability by controlling microstructures, such as, dispersing nano-particles in the UFG matrix, making the nanostructure multi-phased, etc. UFG metals fabricated by severe plastic deformation (SPD) naturally have characteristics of deformation structures. This is one of the main microstructural reasons of their limited ductility, as strain-hardened metals usually do not show large tensile elongation. In order to remove the deformed characteristics, annealing processes are usually applied. But in many cases of the SPD processed materials, the mean grain size becomes over 1 μm when fully annealed microstructures are obtained, so that their strength decreases very much. Recently, on the other hand, we have succeeded in obtaining fully recrystallized nanostructures in some alloys. The recrystallized nanostructured metals, especially some kinds of steels, show both high strength and enough strain-hardening ability, resulting in large uniform elongation. It has been found that the excellent mechanical properties of recrystallized nanostructured metals could be explained by enhancement of strain-hardening due to the activation of different (and unexpected) deformation modes. Examples of nanostructured steels managing both high strength and large tensile ductility will be introduced in the lecture.

Nobuhiro Tsuji received his PhD degree from Department of Materials Science and Technology, Kyoto University, Japan, in 1994. He worked as an assistant professor and then an associate professor in Osaka University, Japan, from 1994 to 2009. He has been a full professor for physical metallurgy of structural metallic materials at Department of Materials Science and Engineering in Kyoto University since March 2009. His research interests have been (i) correlation between nano/micro-structures and mechanical properties of structural materials; (ii) fundamental mechanisms of deformation, recrystallization, and phase transformation during thermomechanical processing of metals; and (iii) fabrication and properties of nanostructured metals. Particularly his works on bulk nanostructured metals (ultrafine grained metallic materials) are well recognized. Total citations for his 482 papers published in scientific journals are about 24,000 times and the *h*-index is 75 (according to *Scopus*).

Invited Talk S1-2

Microstructure Based Prediction/Design of Mechanical Properties and Damage Monitoring of Structural Materials

Manabu Enoki
Professor, The University of Tokyo, Japan

Abstract

The mechanical properties of metallic materials strongly depend on the microstructure. The strength properties are related to the average information of the microstructure, while the fatigue properties are related to the extreme values of the microstructural statistics. Crystal plasticity (CP) analysis can consider the influence of crystal orientation of microstructure, and finite element methods (FEM) for polycrystalline structures have made it possible to predict the mechanical properties of metallic materials. As material parameters in calculations must be determined based on reliable experimental results, and data assimilation methods can be used to obtain appropriate values and motels. CPFEM and data assimilation are very universal and general methods that can be applied to a wide range of problems. In this presentation, some examples will be presented such as optimization of strength-ductility balance of DP steels and optimization of weld geometry for fatigue properties of Mg alloy welds.

In-situ structural health monitoring is another important issue to keep a reliability of structural materials. AE (acoustic emission) method is widely applied in industry as one of the effective non-destructive inspection techniques for detecting damage with high sensitivity. However, it is difficult to analyze quantitatively because the wave propagation behavior is greatly affected by the shape of the structure due to the unique reflection characteristics of ultrasonic waves. The authors have been working on the detection of microscopic fractures occurring in various materials by AE analysis for many years. Recently AE data analysis based on data-driven approach has been developed to directly combine the physical quantities and AE measurement results. Analysis of fatigue behavior of various alloys and methodology as structural health monitoring will be presented

Manabu Enoki is Professor of the Department of Materials Engineering at The University of Tokyo. He received a Bachelor of Engineering degree at the Department of Metallurgy and Materials Science, School of Engineering, The University of Tokyo in 1984, and graduated with a Doctor of Engineering in 1989. He started his career as a Research Associate at Research Center for Advanced Science and Technology, The University of Tokyo. He moved to the Department of Materials Engineering in 2000. His research interest concerns the analysis of microfracture in various materials using non-destructive evaluation method, especially acoustic emission technique. He has continued the research on the integrity of structural materials, such as steels, Mg alloys, Ti alloys etc. using various experimental techniques and numerical simulations using physical based model and data-driven approach.

Invited Talk S1-3

Understanding the Brittle-to-ductile Transition Based on Shielding Theory

Masaki Tanaka

Professor, Department of Materials, Faculty of Engineering, Kyushu University, Japan

Abstract

The fracture toughness of crystalline materials is enhanced by plastic deformation at the crack tip. This phenomenon is known as the brittle-to-ductile transition (BDT). This BDT behavior is strain-rate dependent, and the transition temperature increases as the deformation rate increases. Several ideas have been proposed for a mechanism behind this toughness enhancement. The value of activation energy obtained from the strain rate dependence of BDT temperature is almost equal to the value of activation energy of dislocation motion, which leads to the understanding that BDT is controlled by a dislocation migration rate. The applied stress intensity factor during crack propagation, or in other words, the macroscopic fracture toughness K_{IC}, is given by the following equation.

$$K_{IC} = \sqrt{\frac{4\mu\gamma}{1-\nu}} - \Sigma k_d,$$

where μ, ν, and γ are shear modulus, Poisson's ratio, and surface energy for fracture, respectively.

The pioneering studies on BDT based on the dislocation theory were mainly conducted using model materials such as silicon single crystals. The presenter has extended the stress shielding theory to steels and investigated their BDT based on the stress shielding theory. It was demonstrated that the addition of nickel to interstitial free (IF) steels lowers the BDT temperature, which can be explained by considering that the addition of nickel increases the dislocation mobility at low temperatures. The addition of Mn to IF steels also increases dislocation mobility. This leads one to expect that the addition of Mn also causes a decrease in BDT temperature, however, the BDT temperature increases for adding Mn in steels instead. In the fracture surface after brittle fracture, the initial fracture in the Ni-added steels was transgranular, whereas that in the Mn-added steels was intergranular. From these results, it can be concluded that the addition of Mn has a stronger effect of deteriorating toughness by lowering the fracture surface energy than improving low-temperature toughness by increasing dislocation mobility, and that Mn addition acts to increase the transition temperature.

Prof. Masaki Tanaka completed PhD at Kyushu University in 2005. He was appointed as a professor to the Department of Materials, the Faculty of Engineering at Kyushu University after working as a postdoctoral research fellow at the Department of Materials, University of Oxford in UK, Post-doctoral researcher, Assistant Professor, and Associate Professor at the Department of Materials Science and Engineering, Kyushu University. His current research interest is mechanical properties (mainly deformation and fracture) of crystalline materials such as steels, silicon, titanium alloys and so on, based on dislocation theory.

Invited Talk S1-4

Interactions among Hydrogen-transformation-crack in Metastable Austenitic Steels

Motomichi Koyama
Associate Professor, Tohoku University, Japan

Abstract

Hydrogen embrittlement issue has been regarded as a bottleneck for developing hydrogen-energy-related infrastructures. In this regard, austenitic steels, which are composed of a face-centered cubic (FCC) phase, show significant resistance to hydrogen embrittlement. However, the austenitic steels can also be susceptible to hydrogen embrittlement when the FCC phase is metastable against other phases such as body-centered cubic (BCC) phases. More specifically, when deformation-induced martensitic transformation occurs, hydrogen-related failure occurs. In this talk, we present hydrogen-assisted cracking and subsequent failure behaviors in metastable austenitic stainless steels toward understanding and controlling the hydrogen-related cracking behavior associated with martensitic transformation.

The representative metastable stainless steel is SUS304. The martensitic transformation sequence during plastic deformation in SUS304 is FCC → HCP → BCC. Because the BCC martensite is the most susceptible to hydrogen embrittlement in steels, it is generally known that hydrogen-related cracking occurs at a region where BCC martensite formation preferentially occurs. In this context, to control the hydrogen-related cracking, the hydrogen-transformation-cracking relationship must be understood. The BCC martensite-related cracking behavior was clarified by in situ deformation experiments with scanning electron microscopy. According to our analyses, hydrogen promotes FCC-HCP martensitic transformation, but the effect of hydrogen on HCP-BCC transformation depends on deformation temperature. Specifically, hydrogen promotes the formation of BCC martensite at ambient temperature, however, suppresses at cryogenic temperature. This implies that the hydrogen effect suppressing BCC martensite formation requires hydrogen diffusion from HCP/BCC phase interface to the BCC martensite region. To support this interpretation, we will present some experimental results in this talk, in terms of microstructure distribution and hydrogen desorption during deformation.

Motomichi Koyama obtained a PhD in Materials Science and Engineering (2012) at University of Tsukuba, Japan. In 2012, he received a postdoctoral fellowship (JSPS Research fellowship for young scientist PD). During his postdoc, he spent about 1 year and 3 months in the Max-Planck Institute for Iron Research in Düsseldorf, Germany and was visiting scientist in that institute (2012-2013) in the group of Prof. D. Raabe. In 2013, he became full time assistant professor at Kyushu University, Japan. In 2020, he moved to Tohoku University as associate professor. He joined Institute for Materials Research and attempted to establish alloy deign of hydrogen-resistant steels. In addition, he has developed crack-specific microstructure characterization methodologies towards mechanics-metallurgy-based understanding of hydrogen-assisted damage evolution.

NIMS Talk S1-5

Hydrogen-related Fracture in high-strength Martensitic Steels

Akinobu Shibata
Distinguished Group Leader, Research Center for Structural Materials (RCSM)
National Institute for Materials Science (NIMS)

Abstract

To achieve the goal of reducing greenhouse gas emissions and transitioning to a carbon-neutral society, the transportation sector must focus on reducing the weight of vehicle bodies and improving fuel efficiency through the use of high-strength steels. Advanced high-strength steels are being developed worldwide to improve fuel economy. However, overcoming hydrogen embrittlement remains challenging. Hydrogen embrittlement is a phenomenon in which hydrogen is absorbed by materials, making them brittle and prone to sudden failure. Research on hydrogen embrittlement has traditionally focused on materials used in harsh hydrogen environments. However, as the material strength increases (tensile strength becomes higher than 1.2 GPa), the risk of hydrogen embrittlement increases even in natural atmospheric environments. It is therefore necessary to improve the hydrogen embrittlement properties of high-strength steels to enable their widespread use in commercial products. Understanding the relationship between the fracture behavior and microstructure is the key to retarding hydrogen-related premature fracture and improving the resistance to hydrogen embrittlement.

Crack morphology is an important characteristic; the crack surface area, crack discontinuity, and crack arrestability are closely related to the macroscopic mechanical properties. Although conventional 2D surface observation using SEM is appropriate for statistical analysis, it has some inevitable limitations for analyzing the crack propagation behavior. On the other hand, non-destructive X-ray computed tomography using transmitted images is a useful method for analyzing the macroscopic 3D crack morphology and distribution of defects (scale: μm^3–mm^3). The combination of serial sectioning and EBSD analysis allows for 3D microstructural / crystallographic characterization on a microscopic scale (scale: nm^3–μm^3). The local crack-arrestability and microstructural / crystallographic features of hydrogen-related fracture in high-strength as-quenched martensitic steel investigated by 3D multiscale analysis will be presented in the lecture.

Akinobu Shibata is Distinguished Group Leader in Research Center for Structural Materials, National Institute for Materials Science (NIMS), Japan and Professor in Subprogram in Materials Science, Graduate School of Science and Technology, University of Tsukuba, Japan. He received his Ph.D from Department of Materials Science and Engineering at Kyoto University in 2007. He worked at Tokyo Institute of Technology (Assistant Professor (2007-2010)), Kyoto University (Assistant Professor (2010-2014) and Associate Professor (2014-2020), and then joined Research Center for Structural Materials at National Institute for Materials Science since 2020. He also stayed at Mines ParisTech (France) as visiting researcher (2017-2018). His main research topics are microstructure evolution through phase transformation, correlation between fracture behavior and microstructure, etc., in metallic materials, and he currently focuses the study on hydrogen-related fracture of high strength steels.

Session 2:
High-temperature Materials

Invited Talk S2-1

Multi-material Designed Satellite Thruster through Ceramics/metal Dissimilar Joining

Eiichi Sato
Professor, Institute of Space and Astronautical Science, JAXA, Japan

Abstract

A thruster functions as a small engine for orbit maneuver and attitude control of a satellite. While conventional bipropellant thrusters are mainly made of Nb alloy, a Si_3N_4–ceramics thruster was successfully developed and used in Venus explorer AKATSUKI by ISAS/JAXA. Now, for further size enlargement targeting future interplanetary missions, ISAS/JAXA is currently developing a metal/ceramics hybrid thruster: heat-resistant Si_3N_4 is used only in the high-temperature sections (combustion chamber and throat), whereas light-weight Ti-6Al-4V alloy sheet is used in the low-temperature section (nozzle skirt) of the thruster.

Robust dissimilar joining of active metal of Ti-6Al-4V alloy to ceramics of Si_3N_4 is the key technology for the hybrid thruster, and it requires promoting residual-stress relaxation and suppressing brittle intermetallic compounds formation by insertion of Nb-interlayer. It has been achieved through transient-liquid-phase bonding (TLPB) of Ti-6Al-4V/Nb side with Cu and Ni laminated filler prior to active-metal brazing of Nb/ Si_3N_4 side with Ti-added Ag-Cu based CUSIL-ABA filler or Ti-added Ag-based SILVER-ABA filler. This two-step bonding brought about joints fractured from inside of Si_3N_4 and achieved higher average strength.

The effectiveness of stress-accommodation via Nb interlayer and filler's plastic flow was quantitatively verified with reasonable fidelity by finite-element analysis incorporating temperature-dependent elasto-plastic properties.

After graduating the University of Tokyo in 1985, Eiichi Sato has been working for ISAS/JAXA, specializing high temperature deformation and superplasticity, in addition to structural materials and reliability for space engineering. He is now serving Program Director of ISAS space science projects.

Invited Talk S2-2

Digital Twin Science of Powder Bed Fusion Metal Additive Manufacturing

Yuichiro Koizumi[1], Masayuki Okugawa[2], Yuheng Liu[3], Takayoshi Nakano[1]
[1]Professor, [2]Assistant Professor, [3]Specially-appointed Professor, Osaka University, Japan

Abstract

Metal additive manufacturing (AM), Powder Bed Fusion (PBF), can control not only the geometry but also microstructures from single crystal-like structure to fine grains by the control of solidification conditions. Solidification conditions can be tuned by the process parameters, such as beam power, scanning speeds, etc. There have been various interesting phenomena related to crystal growth as in PBF. They are quite different from those in conventional solidification process. Since the phenomenon occurs very rapidly in a narrow space, it is challenging to observe experimentally and elucidate their details despite the extensive experimental studies. Thus, computer simulations are commonly used. Computational fluid dynamics simulations elucidated that the cooling rate can be as high as 10^6 K/s. Even with such a high cooling rate, PBF can form single-crystal-like columnar grains. This is attributed to the extremely high temperature gradient of around 10^7 K/m at solidification front. On the other hand, the possibility of absolute stability needs to be taken into account for a very fast solidification rate over approximately 1 m/s. On the other hand, recently, cyberspace replicas of a system are called digital twin (DT). In general, a DT is utilized to predict phenomena occurring in the system and optimize control parameters. We propose to use a DT to elucidate the unique solidification mechanisms occurring in PBF, and we propose to define the applications of DT for obtaining scientific knowledge as "digital twin science (DTS)." In this presentation we introduce our recent studies on computer simulations and process monitoring relevant to PBF process with a special focus on the relationship between the extreme condition characteristic of the PBF process and solidification microstructures. For instance, we have elucidated the unique relationship between solidification conditions and the tendency of equiaxed grains and epitaxially grown columnar grains in the microstructures formed by electron beam irradiation on stainless steel, and laser irradiation on eutectic Al-Si alloy. Moreover, we demonstrated the repetition of epitaxial growth in laser-PBF with narrow pitch results in the formation of single crystals. Lastly, we present our recent challenges to extract information of melt-pool from the data obtained via the monitoring system consisting of on-axis and off-axis dual photodiodes, paving the way for real-time in-process examination of crystal orientation and microstructure. Accumulation of the data and knowledges DTS approach will open up a new horizon for the future technologies to create materials with desired properties with confidence, advancing the frontier of metal AM.

Yuichiro Koizumi earned his Ph.D. in 1999 from the Department of Materials Science at Osaka University. He subsequently joined the Department of Adaptive Machine Systems at Osaka University as an Assistant Professor. Later, he spent a year as a visiting scientist in the Department of Materials Science and Engineering at the Massachusetts Institute of Technology (MIT). In 2010, he became an Associate Professor at the Institute for Materials Research, Tohoku University, Sendai, Japan. By 2018, he was appointed as a professor in the Division of Materials and Manufacturing Science, Graduate School of Engineering at Osaka University, where he oversees research in Materials Design and Processing. To date, he has published approximately 200 papers.

Invited Talk S2-3

Grain Boundary Segregation and Creep Pupture Strength of High-Temperature Materials

Yuhki Tsukada
Associate Professor, Department of Materials Science and Engineering,
Nagoya University, Japan

Abstract

Solute segregation at grain boundaries (GBs) changes mechanical properties of high-temperature materials. For example, it is known that a trace amount of boron added to nickel-based superalloys segregates at GBs and improves the creep rupture strength of the alloys, although its strengthening effect has not yet been quantified. Recently, it has been demonstrated that the computational method combining the Hillert's grain-boundary phase model and CALPHAD (calculation of phase diagram) database is effective for predicting GB chemistry (equilibrium composition of random high-angle GBs) in multicomponent alloys. It has been shown that this method can predict the GB segregation of molybdenum and boron in nickel-based superalloys, the GB segregation of boron and phosphorous in an austenitic stainless steel, and GB segregation of nickel and manganese in a high-entropy alloy. By using this method, the GB chemistry of commercial polycrystalline nickel-based superalloys was computed, and its correlation with the creep rupture strength of the alloys was examined. A weak positive correlation was confirmed between the GB concentration of boron and the creep rupture strength. Furthermore, a linear prediction model of the creep rupture strength of nickel-based superalloys was proposed, where the computed GB concentrations of solute elements were used as explanatory variables. The trained model has a sufficient degree of prediction accuracy and clearly shows the importance of regulating the GB concentration of boron for improving the creep rupture strength of nickel-based superalloys.

Yuhki Tsukada is an associate professor at Department of Materials Science and Engineering, Nagoya University, Japan. He received Bachelor's, Master's and Doctoral degrees in Engineering from Nagoya University, Japan in 2007, 2009 and 2011, respectively. He joined Nagoya Institute of Technology, Japan as an assistant professor in 2011. He moved to Nagoya University, Japan as an assistant professor in 2015, and was promoted to an associate professor in 2016. His main research area is the phase-field modeling of microstructure evolution during solid-state phase transformations. He is also interested in data assimilation methods that combine experimental data with a microstructure simulation model. He is serving as a subject editor of Science and Technology of Advanced Materials, and an associate editor of Science and Technology of Advanced Materials: Methods.

NIMS Talk S2-4

Development of Ni-based Superalloys for Jet Engine Applications

Toshio Osada

Principal Researcher, High Temperature Materials Group, Research Center for Structural Materials (RCSM), National Institute for Materials Science (NIMS)

Abstract

Ni-based superalloys are alloys with high heat resistance and are one of the important energy-related structural materials that are widely used as high-temperature components in aircraft engines, gas turbines for power generation, and even automobile engines. Increasing the turbine inlet temperature is extremely important for increasing the efficiency of gas turbine engines and reducing CO_2 emissions, so the development of Ni-based superalloys with excellent heat resistance has been actively carried out around the world.

In particular, high-pressure turbine blades and disks in aircraft engine are rotating bodies that require a high degree of safety, and the Ni-based superalloy used has been required various properties, such as excellent creep properties, low-cycle fatigue properties, high-cycle fatigue properties, high-temperature crack growth resistance and fracture toughness, as well as high-temperature oxidation and corrosion resistance. In this way, Ni-based superalloys for high-pressure turbines are one of the "extreme environment materials" that are extremely difficult to design and put into practical use among structural materials that require advanced performance under extremely harsh operating environments.

NIMS has carried out continuous research activities on the design, development, and prediction technology of Ni-based superalloys for gas turbine applications for more than 40 years. As a result, we have successfully proposed various superalloys, including single-crystal superalloys (TMS alloys) for turbine blades and Ni-Co-based superalloys (TMW and TMP alloys) for disks. Especially, a single crystal superalloy has been successfully applied to Rolls-Royce Trent 1000 engines. In this presentation, in addition to past efforts of development of superalloys, we will introduce the latest activities regarding to design, manufacturing, prediction of Ni-based superalloys for future applications.

Toshio Osada is a principal researcher at High Temperature Materials Group in National Institute for Materials Science (NIMS), Japan. He received his Ph.D. from Yokohama National University, Japan, in 2009. From 2009 to 2012, he was a postdoctoral researcher at High Temperature Materials Center in NIMS. From 2012-2013, he worked as specially appointed assistant professor in Yokohama National University. From 2013-present, he worked in NIMS. From 2016-2018, he also worked as a guest researcher at Delft University of Technology, the Netherlands. Further, from 2022-present, he also worked as Professor at Department of Mechanical Engineering, Materials Science, and Ocean Engineering, Yokohama National University. His research interests include superalloys, self-healing ceramics, strength prediction, and gas turbine materials.

NIMS Talk S2-5

On the Role of Atom Probe Tomography in Understanding of Microstructural Origin of High Strength in Metallic Alloys

Taisuke Sasaki

Group leader, Nanostructure analysis group, Research Center for Magnetic and Spintronic Materials (CMSM), National Institute for Materials Science (NIMS)

Abstract

Atom probe tomography (APT) provides direct 3D mappings of constituent elements with near-atomic spatial resolution and is useful for characterizing solute clusters, nano-sized precipitates, solute segregation to dislocation cores, *etc*. This presentation introduces examples where APT has played a critical role in understanding the microstructural origins of high strength in some metallic alloys in which nanostructure control is critical, *e.g.*, Ni-Co-based superalloys, Mg alloys, and pearlitic steel.

Strain aging is widely used to strengthen the steel and aluminum alloy sheets used in automotive body applications, and elucidation of the strengthening mechanism requires direct observation of the solute-dislocation interaction, which is difficult with TEM. Fig. 1 shows the 3D atom map of Ca superimposed on the BF-TEM image of an originally developed Mg-Al-Zn-Ca-Mn alloy showing a strength increase of 40 MPa by 2% straining and subsequent artificial aging. The correlative TEM/APT analysis convincingly shows that the strength increase is due to dislocation locking by Ca, Al, and Zn segregation and dispersion of a high density of solute clusters.

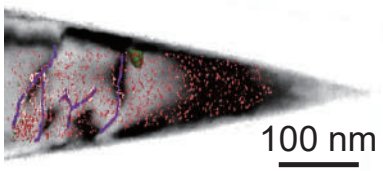

Fig. 1. 3D atom map of Ca overlaid BF-TEM image obtained from a strain aged Al-Zn-Ca-Mn alloy

APT also has significant value over analytical TEM in the analysis of light elements, including hydrogen (H). An example is the identification of hydrogen trap sites in pearlitic steel in which the cold deformation simultaneously results in high strength and excellent resistance to hydrogen embrittlement. As shown in Fig. 2, APT analysis of a deformed pearlite charged with deuterium (D), a natural isotope of H, showed D segregation at the cementite/matrix interface, whereas there is no D trapping at the cementite/matrix interface in the undeformed pearlite. This allows us to understand that H trapping delays H accumulation at the crack initiation sites, resulting in excellent resistance to hydrogen embrittlement.

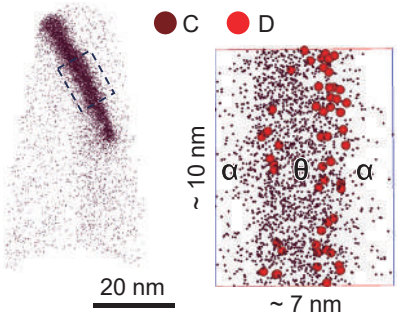

Fig. 2. 3D atom map of C and D distribution obtained from a deformed pearlitic steel

Taisuke Sasaki is a group leader of the Nanostructure Analysis Group in the Research Center for Magnetic and Spintronic Materials at the National Institute for Materials Science (NIMS), Japan. He received his Ph.D. degree in engineering from the University of Tsukuba, Japan, in 2008. His research interests include understanding the structure-property relationship in various metallic materials using scanning electron microscope (SEM), transmission electron microscope (TEM), and three-dimensional atom probe (3DAP). Taisuke Sasaki can be reached by e-mail at Sasaki.Taisuke@nims.go.jp.

Abstracts of Poster Presentations

P1 **Process**

P2 **Characterization**

P3 **Evaluation**

P4 **Modeling**

P1-01

New Microstructure Design of Heat-resistant Titanium Alloys with Property Improvements Using Super Thermal Field

Y. Toda [1], R. Ozasa [2], T. Matsunaga [3], Y. Yamabe-Mitarai [4] and T. Nakano [2]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Graduate School of Engineering, Osaka University
[3] Institute of Space and Astronautical Science, Japan Aerospace Exploration Agency
[4] Graduate School of Frontier Sciences, The University of Tokyo

The poster will introduce the activities of "Science for Creation of Super-Titanium by Super-Thermal Field", which is one of the Planed Researches of "Creating Materials in Super-Thermal Fields: Neo-3D Printed by Manipulating Atomic Arrangements through Giant Potential Gradients (Director: Prof. Y. Koizumi at Osaka University)" accepted for a Grant-in-Aid for Transformative Research Areas (A) by the Ministry of Education, Culture, Sports, Science and Technology in FY2021.

It is necessary to further expand the application temperature range of heat-resistant titanium alloys in order to improve the energy efficiencies of jet engines. However, the limits of microstructural control and improvement of high-temperature properties in these alloys by conventional forge and/or cast processing have been reached.

This study will apply a steep temperature gradient and a fast-cooling rate in the super thermal field of additive manufacturing to retaining a supersaturated solid solution of β phase at room temperature and to controlling a crystal orientation of the β matrix and the precipitation of α phase. This trial will lead to a new microstructure and an improvement of high-temperature properties which has never been achieved before.

P1-02

Introduction of Millefeuille-like α/β Layered Structure into Ti-Mo Alloy through Thermomechanical Treatment

S. Emura
Research Center for Structural Materials, National Institute for Materials Science (NIMS)

To control the microstructure and to enhance the mechanical properties of titanium alloys, various types of thermomechanical treatment (combination of deformation (forging, rolling, etc.) and heat treatment) have been performed. For β titanium alloys, mainly consist of bcc β phase, α phase precipitation on deformed structure such as dislocation is favorable way to obtain fine and homogeneous microstructure, and many efforts have been done to optimize this thermomechanical treatment process. In this study, we use another thermomechanical treatment, α phase precipitation on {332}<113> deformed twins (typical twinning system in β titanium alloys), to realize millefeuille-like layered α/b structure in Ti-12 mass% Mo alloys. We performed slight cold rolling on β single phase Ti-12Mo plates followed by α precipitation aging treatment. During aging treatment, film-like α phases were precipitated and grew on the twin boundaries and finally made an alternately stacked α/b layered structure.

P1-03

Compositionally Graded Titanium to Aluminum Processed by Laser Powder Bed Fusion Process: Microstructure Evolution and Mechanical Properties

P. Daram[1], A. Singh[2] and M. Watanabe[1]
[1]Research Center for Structural Materials, National Institute for Materials Science (NIMS).
[2]Research Network and Facility Services Division, National Institute for Materials Science (NIMS).

A compositionally graded Ti-Al alloy with a designed composition range from pure Ti to pure Al could be successfully produced by a laser powder bed fusion (L-PBF) system equipped with two powder feeders. The compositionally graded Ti-Al profile is confirmed by scanning electron microscopy (SEM), X-ray diffraction analysis (XRD), electron backscatter diffraction microscopy (EBSD) and transmission microscopy (TEM). The graded material is free of macro-horizontal crack, but micro-cracks appeared at the center of the sample. With changing Ti and Al ratio through build direction, the sample exhibits a microstructural and phase changes consisting of α+β-Ti $\rightarrow$ solid solution + intermetallics (Ti and Al)$\rightarrow$ Al phase together with different morphology of each phase. Moreover, the effect of Ti-Ai ratio on the formation of microstructure and phase evolution lead to the different mechanical properties of each layer in the graded material. The results demonstrate that the L-PBF process is able to produce continuously compositionally graded Ti-Al material in one time. Moreover, this work has the potential to design and create a large set of compositional variants for high entropy alloy to study microstructural evolution, phase transformation, physical and mechanical properties in the future.

P1-04

Development of Apatite and LDH Coatings of Mg alloys Depending on the Application

S. Hiromoto [1,2]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[2] Department of Materials Science, Waseda University

Mg alloys are expected to be used as lightweight materials for vehicles like Al alloys and as biodegradable metallic materials for bone plates and screws and so on. In both cases, the poor corrosion resistance limits their practical application. Surface modification, such as coatings, is one approach to improve the corrosion resistance.

For Mg and Al alloys as lightweight materials, we are developing layered double hydroxide (LDH) coatings loaded with corrosion inhibitors as self-healing coatings. Inhibitor-loaded LDH (LDH-inh) is prepared and then coated on metal surfaces by co-electrodeposition with metal hydroxides. It has been demonstrated that the LDH-inh particles can be fixed to metal surface with metal hydroxide gel which partly transitions to LDH with NO_3^- at the interlayer. The LDH-inh-coated Mg alloy showed higher corrosion resistance than the alloy coated with LDH with CO_3^{2-} at the interlayer.

For biodegradable Mg alloys, we have been developed hydroxyapatite (HAp) and carbonate apatite (CAp) coatings since apatite is a main component of bone. HAp is stable in physiological environments, whereas CAp can be absorbed by osteoclast cells and replaced by bone. The HAp and CAp coatings showed comparable corrosion suppression ability for Mg alloys in cell culture medium, and the CAp coating showed osteoclastic resorption under culturing osteoclast cells. Then, the CAp- and HAp-coated Mg alloys are implanted in rabbit femur, and the degradation of CAp coating was shown in the area where new bone adheres.

P1-05

Improvement of Corrosion Resistance of Type 420J2 Martensitic Stainless Steel by Laser thermal Processing

Y. Tsutsumi [1], T. Manaka [2] M. Goto[3], M. Kadowaki[1], T. Ishimoto[2] and H. Katayama[1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[2] Aluminum Research Center, University of Toyama
[3] Fuji High-Frequency Co., Ltd.

The laser thermal processing was utilized to improve the corrosion resistance of martensitic stainless steel. Type 420J2 stainless steel plate was prepared and the steel surface was subjected by laser irradiation to form partially-remelted and recrystallized layer. The top surface showed roughened and dull-colored morphology due to thermal oxidation just after the processing. Newly-formed inner remelted and recrystallized layers was found under the outermost oxidized film. The depth of the two layers was about several hundred micrometers and they showed excellent corrosion resistance in chloride containing testing solution. In addition, the Vickers hardness of both layers were much higher than that of untreated steel. Therefore, laser thermal processing was found to realize both hardening and corrosion resistance improvement for martensitic stainless steels.

P1-06

Low-Temperature and Non-vacuum Surface Modification for Anti-Hydrolysis Hybrid Bonding

A. Shigetou [1] and N. Hosoda [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

For the social implementation of automatic traffic control using the mobile IoT (Internet of things), the use of terahertz-band electromagnetic waves, which are tolerant to the ambient environment, is expected to increase. For this purpose, device substrates and structural materials must be assembled (bonded) individually all at once. Such hybrid bonding should be obtained without high temperature and a vacuum atmosphere, and the method must be industrially simple. Particularly for the use of organic materials, anti-hydrolysable reliability is required. Given heat-resistant resin such as polyimide (PI) and metals such as Cu and Ti as typical materials for forming such hybrid bodies, the key issue is achieving a pseudo-hydrophobic interfacial bridge layer. For organic materials, the surface had to be hydrophilized to form an adhesion layer. However, hydrophilic surfaces degrade the interfacial reliability by hydrolysis reactions. One of the most promising candidate structures is the alkyl chain carrying hydroxyl- (or amine-) only at the ends. For this, we developed a vapor-assisted vacuum ultraviolet (V-VUV) surface modification method. This method uses VUV irradiation in a nitrogen atmosphere, including vapor of chemical solvent's vapor. The radical species, obtained by dissociating vapor molecules, help generate ultrathin bridge layers. In this study, the growth conditions of the bridge layer were optimized using Xray photoelectron spectroscopy (XPS). Then bonding experiments were performed in various combinations of materials. For the bonded interfaces, transmission electron microscopy (TEM) and electron energy loss spectroscopy (EELS) analyses were carried out.

P1-07

Observation and Numerical Prediction of Concentration Distribution at Cast Coating Interface of Solid Pt, Ir, Re Using Liquid Ni-based Alloys

Machiko Ode, Hisao Esaka, Akira Ishida, Susumu Takamori and Hideyuki Murakami
Research Center for Structural Materials (RCSM), National Institute for Materials Science (NIMS)

The applicability of a cast-coating process for improving the oxidation resistance of cast Ni-based superalloys was evaluated. Specifically, metallic plates of Pr, Ir, and Re expected to improve oxidation resistance when they are enriched on the cast alloys were placed in a mold and cast coating using Ni-10at%Al alloy was performed in order to investigate the formation of the Pt, Ir, or Re-enriched layer on the casting surface. Then the microstructure of the Ni-based alloy/specimen interface was observed. To analyze the concentration profile in the interdiffusion region, solidification and diffusion simulations were performed. It was found that Pt easily dissolves into the molten Ni-based alloy, and Re cannot expected to modify cast metal surfaces due to its low solubility into the Ni-10at%Al alloy. On the other hand, Ir forms smooth interdiffusion layer, and numerical calculations predicted that Ir can maintain the modification ability even in a process time of 1 hour, which is equivalent to the casting time of Ni-based turbine blades.

P1-08

Delayed Fracture of Ultra-high Strength Steel Processed by Warm Tempforming

Y. Kimura [1] and T. Inoue [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Warm tempforming is a thermomechanical treatment that deforms tempered martensite at elevated temperatures. Warm tempforming using multi-pass caliber rolling on medium-carbon low-alloy steel can create an ultrafine elongated grain (UFEG) structure with a strong <110>// rolling direction (RD) fiber texture. In this presentation, delayed fracture properties of the warm tempformed steel with UFEG structure will be presented. 0.4%C-2%Si-1%Cr-1%Mo steel was quenched and tempered at 500°C and then subjected to warm tempforming using multi-pass caliber rolling to create the UFEG structure. Delayed fracture properties were evaluated using slow-strain-rate-test and hydrogen immersion test. The results showed that at ultra-high tensile strength of 1.8 GPa, the warm tempformed (TF) samples with UFEG structure exhibited much higher delayed fracture resistance than the quenched and tempered (QT) samples. Delayed fracture behavior in long-term outdoor exposure tests is also presented for ultra-high strength bolts fabricated from TF and QT samples.

P1-09

Microstructures and Mechanical Properties of Fe–15Mn–10Cr–8Ni–4Si Seismic Damper Cast Alloy

S. Takamori, F. Yoshinaka and T. Sawaguchi
Research Center for Structural Materials, National Institute for Materials Science (NIMS)

A seismic damper alloy with the composition of Fe–15Mn–10Cr–8Ni–4Si that exhibits excellent plastic fatigue properties has been developed. This material was designed for thermo-mechanical processing, and its properties as a casting material have not been investigated. In this study, sand castings and permanent mold castings were made from this alloy to investigate the microstructures and material properties. The cast alloy was heat-treated at 1000°C for up to 24 hours, and the changes in microstructure and tensile and fatigue properties were examined. The results showed that both sand castings and permanent mold castings exhibited good tensile properties. Permanent mold castings showed good plastic fatigue properties at heat treatment times of 2 to 8 hours, and the number of failure cycles exceeded 10,000 cycles with a strain amplitude of ±1%. Transformation from γ-austenite to ε-martensite was observed during plastic deformation, suggesting that this transformation contributed to the good plastic fatigue properties. In the cast microstructure, Mn, Ni, and Si were observed to segregate clearly in the interdendritic region, suggesting that the remaining segregation also contributes to the good fatigue properties.

P1-10

Evaluation of Laser Absorptivity of Titanium Powder by Using Ray Tracing

H. Honda and M. Watanabe
Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Additive manufacturing is expected to be new production methods due to its capability to make complex shaped products rapidly. In laser metal-based powder-bed fusion additive manufacturing, metal powder is spread in a sheet and melted by laser, and the solidified parts are piled up. Laser absorptivity is one of the parameters influencing the additive manufacturing process, and it is necessary to evaluate laser absorptivity of metal powder in order to understand the process. In this study, the laser absorptivity of titanium powder was evaluated by using a ray-tracing simulation program assuming the powder consists of spheres of a single size.

P1-11

Effect of Cooling Rate from Sub-Solvus Solution Treatment Temperature on Hardness in Powder Metallurgy Ni-Co-base Superalloy

T. Saito[1], T. Shibayama[2], T. Osada[1], M. Okuno[3], D. Nagahama[3] and T.T. Sasaki[1]
[1] National Institute for Materials Science (NIMS), [2] Mitsubishi Heavy Industry, Ltd, [3] Honda R&D Co., Ltd

Powder metallurgy (P/M) processed TMP5002 (HGN200) has been developed by mixing conventional Ni-based and Co-based superalloys with γ-γ' two-phase microstructure and is known as a Ni-Co-based superalloy with the highest temperature capability of 740 °C among P/M Ni-based superalloys[1)]. Sinc the excellent high-temperature capability, *i.e.*, high strength, is due to the dispersion of γ' precipitates, the ideal microstructure must be developed during the solution treatment and subsequent artificial aging, which is carried out within a practically acceptable time, and the precipitation of γ' must be utilized during cooling process. The cooling rate from the solution treatment temperature is crucial for the cooling γ' precipitation. This work investigated the effect of the cooling rate from the solution treatment temperature on the room temperature properties in P/M TMP5002 alloys.

The samples were solution-treated at a sub-solvus temperature of 1110 °C for 4 h and then cooled at different cooling rates. The samples were then subjected to standard two-step aging at 650 °C for 24 h and at 760 °C for 16 h. The highest room temperature hardness of the aged sample is achieved in the sample cooled at 100 °C/min, but further increase in cooling rate tends to decrease the hardness. Atom probe tomography and SEM analysis revealed that the composition of the γ' reached the equilibrium composition at 760 °C, and the volume fraction of γ' precipitates in the two-step aged sample is similar regardless of the cooling rate. Therefore, we can conclude that the dispersion of a high volume fraction of nanoscale γ' with approximately 30 nm diameter is important to maximize the strength.

Reference: [1)] Y. F. Gu, *et al.*, Proc. 13th Int. Conf. on Superalloys, (2016), 210.

P1-12

Three-Dimensional Cellular Automaton for Grain Growth of Inconel 738LC in Laser Powder Bed Fusion

M. Kusano [1] and M. Watanabe [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Laser powder bed fusion (L-PBF), one of additive manufacturing techniques, can fabricate a near-net shape product by repeating powder spreading on the platform and selective scanning of the focused laser. The fabricated part undergoes a cyclic thermal history involving melting and solidification through the process. Consequently, epitaxial and competitive growth in such thermal cycles results in the formation of complex solidification microstructures. The objective of the current study was to predict such microstructure so that a three-dimensional cellular automaton (3D-CA) model was developed by coupling with a finite element thermal analysis for a nickel superalloy Inconel 738LC in the process. The 3D-CA results showed that columnar crystal grains along the building direction, which were strongly influenced by laser scanning conditions. Validation by comparison with microscopic observations of the fabricated samples confirmed that the developed 3D-CA model was effective in predicting solidification microstructures in L-PBF.

P1-13

Fabrication of Single Crystals in Laser Powder Bed Fusion Using a Flat-Top Laser

T. Kitashima [1, 2] and M. Watanabe [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[2] Department of Materials, Kyushu University

The fabrication of single crystals of Ni-base superalloys using powder bed fusion has gained attention for high-temperature applications. We successfully fabricated a pure-Ni single crystal using a flat-top laser beam in the laser powder bed fusion process. In this study, we investigated the formation mechanism of the single-crystal structure in LPBF. The bidirectional laser scanning promoted the growth of <001>-oriented solidification cells in the build direction, resulting in a uniform <001>-texture formation. Simultaneously, a <001>-epitaxial growth occurred in a direction deviated by 45° to the scan direction (SD) near the melt pool tail. The 90° rotation of hatching direction (HD) at every layer caused the formation of the <101> textures parallel to both SD and HD. Thus, a single-crystal structure was formed via both the bidirectional laser scanning and the 90° hatching rotation.

P1-14

Materials Integration for Laser Powder Bed Fusion Process

M. Watanabe[1], Tomonori Kitashima[1], Masahiro Kusano[1], Houichi Kitano[1], Kiata Ito[1], Sukeharu Nomoto[1], Dmitry S. Bulgarevich[1] and Jun Katagiri[1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Laser Powder Bed Fusion (LPBF) is a process that directly builds three-dimensional structures by layering materials according to computer-aided design by utilizing laser beam. It enables the production of components with complex shapes that are difficult to produce using conventional technologies, as well as reducing the number of parts by manufacturing them as a single component. It is expected to be used increasingly in the aerospace and energy industries, where high quality products are required in small quantities. When applying this process to the production of high-performance heat resistant alloy components, it is important to control the occurrence of defects during the process, optimize the microstructure and mechanical properties, and develop new alloys suitable for AM. In our research, we have developed various multi-physics simulation and data science techniques (called as materials integration) for the LPBF process and developed in-situ monitoring techniques to validate these predictions and to inspect metal components fabricated by LPBF. A comprehensive overview of these achievements will be presented.

P1-15

Anisotropy of Uniaxial Yield Stress of Pearlitic Steel Caused by Compressive Deformation

R. Ueji [1], H. Somekawa [1], S. Emura [1] and T. Inoue [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Pearlite, which is a layered structure of ferrite and cementite in steel, is a fundamental microstructure in high-strength wire drawing materials and is important in industry. The deformed pearlite exhibits various types of heterogeneous deformation microstructures that many researchers have studied to find the relation between these and mechanical properties. One of the possible reasons for these heterogeneity lies on the lamellar structure as well as the hierarchical structure in pearlite consisting of nodules and colonies. This microstructural complexity prevents the understanding of the formation mechanism of the heterogeneous deformation in pearlite, and thus it can be expected that the systematical examination with the pearlitic steel deformed into various strains bring key knowledge to clarify the relation between the plastic anisotropy and the deformation microstructure. In this study, we used a double compression test method on pearlite steel (JIS-SUP12, Fe -0.55C -0.7Mn -0.76Cr -1.48Si [wt%]), and the anisotropy of the yield stress was investigated in detail by systematically varying the strain and the axis of the second compression A slight first compression of about 10% causes plastic anisotropy in which the larger the interaxial angle with the first compression axis, the smaller the yield stress during the second compression. It was found that the internal stress field exhibiting strong plastic anisotropy was evolved mainly by the larger plastic strain locally in ferrite.

P1-16

High-throughput Search for High-performance Materials Using Composition-graded Bulk Specimens

R. Yurishima [1], A. Ikeda [2] and T. Ikeda [1]
[1] Graduate School of Science and Engineering, University of Ibaraki
[2] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

In recent years, there has been a growing interest in integrating information science, including machine learning, into materials development within the field of materials science. However, the effectiveness of these methods depends on the availability of a substantial amount of experimental data. To meet this data requirement, the development of high-throughput experimental methods using composition-graded bulk samples is in progress. These samples are prepared through both the multiple diffusion method and the Bridgman method, resulting in compositional gradients at various scales. These specimens facilitate the exploration of phase diagrams and the optimization of material characteristics based on chemical composition. The multiple diffusion method involves sintering or welding various elemental powders or masses, followed by heat treatment to promote interdiffusion at the interface. Mapping measurements are carried out within the compositional gradient. This technique offers an overview of multi-component phase diagrams. An example is provided for the Fe-Co-Ni phase diagram determined using the multiple diffusion method. The process involved mixing and sintering elemental powders of Fe, Co, and Ni, followed by annealing and water cooling. EPMA mapping analysis estimated the compositional range of phases. Subsequently, alloys were prepared based on these results, and diffusion couples were created. Phase boundary compositions were determined through point analyses, resulting in phase boundaries within the Fe-Co-Ni system.

P1-17

Biomimetic Reversible Interconnection

N. Hosoda[1]

[1]Smart Interface Group, Research Center for Structural Materials, National Institute for Materials Science (NIMS)

The mass production and consumption-oriented manufacturing of the past has caused problems of resource depletion and environmental destruction due to mass disposal, and has become an obstacle to sustainable development. Now that there is a demand for manufacturing based on recycling and re-use, separation and dismantling technology is a core technology for a sustainable society. Conventional joining and bonding technologies are often developed for strong joint strength, making disassembly difficult during dismantling. On the other hand, there are quick adhesion and detachment mechanisms in nature that excel in recycling-oriented manufacturing.

This research aims to elucidate the principles of adhesion and detachment developed by living organisms and to develop new adhesion and detachment techniques based on developmental biology biomimetics that incorporate the formation processes of living organisms. A new reversible adhesion was developed using the Drosophila pupa as a model.

P2-01

Nano-mechanical Characterization for Multi-scale Modeling in Mechanical Behavior of Metallic Materials

T. Ohmura
Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Plastic deformation behavior is characterized through nano-mechanical testing in a small scale associated with microstructures including inter-phase and grain boundary. Plasticity initiation behavior was characterized for ferrite-cementite interface with different coherency in a pearlitic steel[1]. Transmission Electron Microscope (TEM) in-situ straining was applied to reveal dislocation-grain boundary interactions[2,3]. The mechanism of the slip transfer can be modeled in a simple dislocation reaction in the vicinity of grain boundary. Deformation mechanisms of plasticity initiation and subsequent behavior were modeled through stochastic analysis based on a pop-in phenomenon on a loading segment obtained from nanoindentation measurement[4]. The critical stress for the plasticity initiation shows Gaussian like distribution function, indicating a thermally-activated process including a nucleation of shear loop dislocation at defect-free region. In the subsequent stage, the loading curve shows intermittent plasticity, and the probability function for the event magnitude shows power-law type, suggesting a catastrophic phenomenon with a fractal dimension such as dislocation avalanche.

References
1) Y. Wang, Y. Tomota, T. Ohmura, W. Gong, S. Harjo, M. Tanaka, Acta Mater., **196**, (2020) 565-575.
2) H. Li, S. Gao, Y. Tomota, S. Ii, N. Tsuji, T. Ohmura, Acta Mater., **206**, (2021) 116621.
3) H. Li, S. Ii, N. Tsuji, T. Ohmura, Scripta Mater., **207**, (2022) 114275.
4) Y. Sato, S. Shinzato, T. Ohmura, T. Hatano, S. Ogata, Nature Comm., **11**, (2020) 4177.

P2-02

Microstructure of Modified 9Cr-1Mo Steel Manufactured by Laser Powder Bed Fusion

T. Hatakeyama [1], K. Sawada [1], M. Suzuki [1] and M. Watanabe [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Modified 9Cr-1Mo steel (9Cr-1Mo-V-Nb steel) is a creep strength enhanced ferritic steel widely employed in boiler tubes and pipes in ultra-supercritical plants and as structural components in the nuclear industry. Laser powder bed fusion (LPBF) is recognized as a promising manufacturing process for producing the complex geometries. Additionally, improved performance is expected because of the unique microstructure formed through the extremely rapid solidification process.

In this study, the microstructures of modified 9Cr-1Mo steels manufactured under various LPBF conditions were meticulously investigated [1]. The as-built samples exhibit a duplex structure composed of δ-ferrite and martensite. δ-ferrite was formed due to the extremely rapid cooling, on the order of 10^6 K/s, provided by the LPBF process. Conversely, martensite was derived from the austenite transformed from the δ-ferrite during reheating in the heat affected zone of subsequent laser scans. A higher energy density and random scan strategy result in a greater volume fraction of martensite, leading to a higher Vickers hardness at room temperature. In other words, it was suggested that the volume fraction and distribution behavior of δ-ferrite and martensite can be controlled by optimizing the LPBF parameters to achieve the desired mechanical properties.

[1] T. Hatakeyama et al., Additive Manufacturing, 61 (2023) 103350.

P2-03

Hierarchical Fatigue Damage Mechanism and Development of Fatigue-resistant Alloy

F. Yoshinaka [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Fatigue is a major cause of failure in mechanical structures, and prevention of fatigue is crucial to ensure their safety. Fatigue failure results from fatigue crack initiation and propagation on a macroscopic level, but plastic deformation at the crack initiation site or crack tip region drives the crack initiation and propagation on a microscopic level. In other words, metallic fatigue is a phenomenon that spans dislocations, plastic deformation, and cracks, and necessitates comprehension at all level of the hierarchy. Thus, we are undertaking research to clarify the fatigue mechanism by examining the factors affecting fatigue properties on a multi-scale using various types of microscopes and synchrotron radiation techniques, mainly for alloys characterized by variety of plastic deformation mechanisms. Based on the findings of multi-scale characterization of fatigue deformation and fracture, we are developing new fatigue-resistant alloys. The research indicated that the fatigue durability can be improved by increasing the deformation reversibility, and bidirectional martensitic transformation could be an effective deformation mechanism to achieve high reversibility. The bidirectional transformation-induced plasticity (B-TRIP) steel developed showed a fatigue life 20 times longer than general steels.

P2-04

On the Three-dimensional Atomic Scale Characterisation of Nano-Scale B2 Phase in Ni-Alloyed Fe-Mn-Al-C Low-density Steel

Mainak Saha [1], M.B. Ponnuchamy [1], M. Sadhasivam[1] and K.G. Pradeep [1,2]
[1] Correlative Microscopy Laboratory, Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai, 600036, India.
[2] National Facility for Atom Probe Tomography, Indian Institute of Technology Madras, Chennai, 600036, India.

The enhanced mechanical properties of Al-alloyed Fe-Mn-C based multi-component steels are primarily derived from the different phases present in them in addition to their size, distribution, morphology, volume fraction and stability. Here we report on the thermal stability and the associated phase evolution sequence especially that of nanoscale precipitates in a hot-rolled 5Ni-alloyed Fe-16Mn-9Al-0.9C (wt.%) low-density steel. Systematic heat treatment studies were performed in the temperature range of 600-1200 $^{\circ}$C. Bulk phase analysis using X-ray diffraction indicates the presence of three phases, namely FCC structured γ, $L1_2'$ structured κ and BCC phases in as-rolled condition which is in good agreement with the thermodynamic phase stability estimates. Combined microscopic analysis involving three-dimensional atom probe tomography reveals the presence of nano-scale κ and B2 precipitates, highly localized within the majority γ and banded BCC phase regions respectively. This presentation, therefore will focus on the temporal evolution of B2 nanoprecipitates and their localisation within the banded BCC phase regions along with their stability as a function of varied thermal treatments.

P2-05

Effect of Grain Boundary Segregation On Mechanical Properties in Mg Alloys

H. Somekawa and Alok Singh
Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Magnesium (Mg) and its alloys have attracted immense attention, because of being the lightest among common metallic materials. However, the magnitude of application of these alloys is still very limited due to low ductility and poor formability at ambient temperature, associated with the hexagonal crystal structure. As in case of other metallic materials, control of microstructure and alloying are the well-known strategy to overcome such intrinsic issues. Particularly, grain refinement is one of the effective methods for improving mechanical properties, e.g., ductility and toughness, and secondary formability. Thermomechanical process is generally used to control the microstructure in metallic materials. It is noted that alloying elements are segregated at grain boundaries during these processes, which affect mechanical properties and deformation mechanisms. Nevertheless, there are no systematic studies on this aspect on Mg alloys. Therefore, in this study, we have examined the impact of solute atoms segregation at grain boundaries on mechanical properties using fine-grained Mg binary alloys. Alloying elements are confirmed to be segregated at grain boundaries, irrespective of the type of solute element. The mechanical properties are changed by grain boundary segregation; especially, segregation of Mn to grain boundaries leads to enhancing ductility due to grain boundary sliding.

P2-06

Effect of Yttrium Addition on the Nanoindentation Behavior at Mg–Y Alloy Grain Boundaries

V. Paul [1], H. Somekawa [1] and T. Ohmura [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

The effect of Y addition in Mg–Y alloy on the local mechanical behavior was investigated via the nanoindentation technique to reveal diffusive and displacive phenomena near the grain boundary. Both creep and constant strain rate tests were performed on the Mg–Y alloy, and the data points on the flow stress vs. effective strain rate plot align linearly across a significantly wide range spanning six orders of magnitude in strain rate. Additionally, the strain-rate sensitivities of the grain interior and boundary in the Mg–Y alloy were similar, suggesting a consistent plasticity even at the grain boundary. Physical hardness (α), which is derived from the slope of the P/h–h curve (P and h represent load and displacement, respectively), was analyzed to determine the plastic deformation resistance at the grain boundary. According to the results, there is no remarkable plasticity resistance by the grain boundary. Based on these findings, it is presumed that the addition of Y stabilized the grain boundary to reduce the diffusivity and enhance the activation of the non-basal slip system in a displacive behavior, leading to suppression of the grain boundary effect in the Mg alloy.

P2-07

Application of Friction Stir Welding for Fe-Mn-Si Alloy

T. Nagira [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

The Fe-15Mn-10Cr-8Ni-4Si (FMS) alloy was recently developed to utilize as a seismic steel damper owing to its excellent plastic fatigue life. However, the alloy is highly susceptible to solidification cracking. In this study, friction stir welding (FSW), which is one of the promising solid-state joining techniques, was applied to the 10 mm thick plate for the FMS alloy using a polycrystalline cubic born nitride (pcBN) tool. Because it has several advantages over the conventional fusion welding. For example, FSW enable us to suppress the solidification cracking and improve the mechanical properties including the strength and toughness induced by the grain refinement of weld zone.

The sound FSW joint was obtained without the macro-defects. However, many small pores with diameters of 1-5 μm were formed throughout the stir zone under the high heat input condition. EDS analysis showed that the formation of pores was caused by the drop-off the BN particles induced by the wear of the pcBN tool. The decrease in the heat input remarkably suppressed the tool wear. The grain refinement occurred in the stir zone owing to the sever deformation during FSW. The FSW specimen under the low heat input condition showed the higher tensile strength of 759 MPa due to the grain refinement and the relatively high elongation of 50% compared to the base metal. In addition, the FSW specimen showed the excellent fatigue life of 9723 cycles.

P2-08

Elevated Temperature Exploration of Mechanical Behavior in Zr-based Bulk Metallic Glass through Nanoindentation Testing

S. Pomes [1,2], N. Adachi [3], M. Wakeda [1] and T. Ohmura [1,2]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[2] Department of Materials Science and Engineering, Kyushu University
[3] Department of Mechanical Engineering, Toyohashi University of Technology

Metallic glasses offer significant potential as structural materials, enabling the development of lightweight, durable, and energy-efficient transportation and infrastructure systems. Their utilization aligns with several sustainable development goals, including affordable and clean energy, sustainable infrastructure, and responsible consumption and production. However, their structural state and deformation behavior are significantly influenced by environmental temperature, particularly in the range of glass transition temperatures, further complicating their application in structural scenarios.
In our study, we investigate the mechanical response of a Zr-based bulk metallic glass in two distinct structural states: as-cast and as-relaxed. We employ elevated-temperature nanoindentation testing, conducting experiments at room temperature and both above and below the glass transition temperature, spanning a range of 100°C to 500°C with 100°C increments. Our extensive experimental dataset is analyzed to assess mechanical properties and explore potential creep deformation dynamics as a function of temperature. This analysis provides valuable insights into the material's response to applied stress under varying temperature conditions, shedding light on its deformation mechanisms.

P2-09

Thermoelectric Generation by Joining Interface Control of thermocouple Metals

S. Meguro [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Thermoelectric generation is one of promising technologies for actualization of carbon neutral society. However, it is still far from social implementation. Moreover, Seebeck coefficient of thermocouple metals is much lower than thermoelectric semiconductors. Nevertheless, we find that thermocouple metal joint with large area joining interface can generate current to some extent. In this study, we focused on combination of copper (Cu) and constantan (55Cu-45Ni) which are known as T type thermocouple. We investigated a thermoelectric generator module using 144-pair series connected copper-constantan laser welded joint. In this case, area of each joining interface is 0.4x12cm. In addition, thermoelectric generation of the module is available up to higher temperature than most of thermoelectric semiconductors. In this study, the large area joints are covered with oxidation-resistant coating and kept 1173K in a muffle furnace. As the result, the module generated 450mW thermoelectric power output in 800K over temperature gradient environment. On the other hand, result of microanalysis at joining interface shows steep distribution of each element. From the results, laser welding fabricates suitable joint for thermoelectric generation with steep joining interface. In the future, establishment of immobility high temperature waste heat collection system with the thermoelectric metal joint is expected.

P2-10

Unveiling the Transformation Pathways of Hierarchical γ_{90} – ε_{twin} – α' Triple Phase Structure Formation at ε-ε Martensite Intersection

D. Singh[1], W. Tasaki[2], F. Yoshinaka[1], S. Takamori[1], S. Emura[1], K. Tsuchiya[1,2] and T. Sawaguchi[1*]
[1] National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan
[2] University of Tsukuba, 1-1-1 Tennodai, Tsukuba 305–8577, Japan

Deformation-induced martensitic transformation (γ-austenite → ε/α'-martensite) in austenitic steels has garnered significant interest owing to its transformation-induced plasticity effect. To elucidate the orientation-dependent intricate γ/ε/α' phase microstructure at deformation induced ε – ε intersection, a single crystal of 316 austenitic stainless steel was compressed along the $[001]_\gamma$ axis at a cryogenic temperature (173 K). Electron backscattered diffraction analysis was employed to reveal the deformed microstructure on the $(110)_\gamma$ surface. A hierarchical triple phase structure was discovered at ε–ε intersection, where the γ rotated 90º from the matrix (γ_{90}), $\{10\bar{1}2\}$ ε-twin, and α' phases coexist. Depending on the operative shear angle with a common intersection axis, either 90º (Type I) or 30º (Type II), three distinct atomic rearrangements of the intersection volume were observed: γ_{90} was present at Type I intersection, and α'-phase was developed at Type II intersection, respectively. $\{10\bar{1}2\}$ ε-twin also occurred at Type I intersection, serving as an accommodation mechanism alongside the intersection γ_{90}. Transformation paths for three intersection products were visualized by the unified tetrahedron model, considering T/2 or T/3 γ-twinning shear as an intermediate state. Moreover, a novel scheme is proposed to index the α'-martensite crystallographic variants at ε–ε intersections by establishing a correlation between the Bain distortion and double shear process.

P2-11

Tensile Properties and Deformation Behavior at Low Temperatures in Ferrite and Austenite Duplex Stainless Steel with Various Grain Sizes

N. Koga [1], M. Noguchi [2] and C. Watanabe[1]
[1] Faculty of Mechanical Engineering, Institute of Science and Engineering, Kanazawa University
[2] Division of Mechanical Science and Engineering, Graduate School of Natural Science and Technology, Kanazawa University

Ferrite and austenite duplex stainless steels exhibit an excellent strength-ductility balance at low temperatures. On the other hand, it is well known that grain refinement improves not only the strength but also the toughness of metallic materials. In this study, the effects of grain size on the low-temperature tensile properties of ferrite and austenite duplex stainless steel having different grain sizes were revealed, and then, the improvement mechanisms of the properties by grain refinement were discussed based on the obtained deformation behavior. Three specimens of duplex stainless steel with identical chemical compositions in each phase and phase ratio but different grain sizes ranging from 2.0 to 7.4 μm were prepared. At room temperature, the strength increased, but the elongation decreased with refining the grain size. Whereas at 77 K, both strength and elongation were increased by grain refinement. The formation of deformation-induced martensites was detected in the fractured specimens at 77 K, and its volume fraction increased with the grain size refinement. Therefore, the transformation-induced plasticity effect should provide high elongation at 77 K in the fine-grained specimen. The increase in strength by grain refinement strengthening at 77 K was significantly larger than that at room temperature. These results strongly suggest that grain refinement effectively improves the low-temperature tensile properties of ferrite and austenite duplex stainless steel.

P2-12

Excellent Combination of Strength and Ductility of an Ultrafine-grained Stainless Steel at Cryogenic Temperatures Studied by in Situ Neutron Diffraction

Wenqi MAO[1], Si GAO[2], Wu GONG[1], Takuro KAWASAKI[1], Tatsuya ITO[1] and Stefanus HARJO[1]
[1] J-PARC Center, Japan Atomic Energy Agency
[2] Department of Materials Science and Engineering, Kyoto University

The yield strengths of traditional austenitic stainless steels (ASSs), such as 304 ASS, remain relatively low at cryogenic temperatures, due to the face-centered cubic crystal structure. Recent studies reveal that ultrafine-grain (UFG) refinement of 304 ASS can be easily achieved by heavy cold-rolling and subsequent annealing. Compared to conventional 304 ASS with coarse grains, at room temperature, the UFG 304 ASS has significantly higher yield strength owing to the grain refinement strengthening, while it still maintains good ductility. However, the low-temperature mechanical properties of UFG 304 ASS are still unclear. In this study, we systematically investigated the tensile deformation behavior of an UFG 304 ASS at different temperatures ranging from 77 to 295 K. The results showed that the optimal mechanical properties were achieved at 77 K, with extremely high yield strength and ultimate tensile strength as well as a relatively good elongation. The low-temperature deformation mechanism of UFG 304 ASS was discussed in light of in situ neutron diffraction and microstructure observation. The details will be presented in the poster. This study got partially support from MEXT with No. JPMXP1122684766.

P2-13

Static and Dynamic Characterization of Grain Boundary-dislocation Interaction

S. Ii and T. Hara[1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Grain boundaries, which inevitably exist in polycrystalline engineering materials, often govern their mechanical and functional properties. Among them, the relationship between the yield stress and the grain size is well known as the Hall-Petch relation. However, the unknown physical meaning of that relation remains as well. Recently, we have focused on the grain boundary-dislocation interaction, which is an elemental process of understanding the Hall-Petch relation, attempting to clarify from the standpoint of static, such as geometrical dislocation reaction at the grain boundary, and of dynamics of the microstructure evolution by the state-of-the-art in situ TEM straining experiment. It has directly observed the dislocation activated at the adjoining grain by in situ straining with the simultaneous measurement of the stress in Al bicrystal, including a single Σ3 grain boundary. The measured critical resolved shear stress was consistent with the estimated one from the past data obtained by the macroscopic tensile tests of the bulk materials.

The dislocation reaction at the grain boundary was also analyzed based on the slip system activated in both grains. That dislocation reaction process was discussed with a few models proposed so far. The most favorable slip system for the activation in the adjoining grain depended on the models. The model explaining our experiments was based on the geometrical viewpoint. Another model takes macroscopic continuity at the boundary into account. In our experiments, the grain boundary sliding was also observed at the middle and later stages of the in situ straining; that contradiction is the reason for the consistency of the models proposed so far and our experimental data.

P2-14

Microstructure Characterization through *in Situ* Neutron Diffraction with Diffractometer TAKUMI

W. Gong [1], T. Kawasaki [1], W. Mao [1], T. Ito [1] and S. Harjo [1]
[1] J-PARC Center, Japan Atomic Energy Agency

Neutron diffraction, as a powerful microstructure probe, is reliable for tracking globally averaged crystallographic information associated with microstructure evolution and deformation behavior in structural materials. TAKUMI [1], is a neutron diffractometer for engineering materials studies at MLF, J-PARC, covering a wide d-range with a good balance between high neutron flux and high resolution. Additionally, a variety of specific sample environments at TAKUMI enable the *in situ* studies under extreme conditions, such as cryogenic deformation (10K~), thermomechanical controlled processes (~1473K), fatigue, etc. Crystallographic information including phase fraction, lattice strain (stress), texture, dislocation density, stacking fault probability, etc., obtained by neutron diffraction can uniquely provide insights into microstructure evolution and deformation mechanisms in bulky materials. Various *in situ* studies on various metallic materials, as well as *ex situ* measurements, such as residual stress mapping and microstructure characterization for specific purposes, have been conducted. In the presentation, the specifications of the diffractometer TAKUMI and several recent studies on deformation mechanisms in metallic materials using *in situ* neutron diffraction will be introduced.

Reference:
[1] BL19 TAKUMI website: https://mlfinfo.jp/en/bl19/
This study got partially support from MEXT Program: Data Creation and Utilization Type Material Research and Development (JPMXP1122684766).

P2-15

Improvement of Resistance Against Hydrogen Embrittlement by Carbon Segregation at Prior Austenite Grain Boundary in As-Quenched Martensitic Steels

K. Okada [1], A. Shibata [1], T. Sasaki [2], H. Matsumiya [3], K. Hono [2] and N. Tsuji [3]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[2] Research Center for Magnetic and Spintronic Materials, National Institute for Materials Science (NIMS)
[3] Department of Materials Science and Engineering, Kyoto University

High-strength steels, such as martensitic steels, are highly susceptible to hydrogen embrittlement, so that it is desired to improve their resistance against hydrogen embrittlement for wide application of high-strength steels. The hydrogen-related intergranular fracture occurs mainly along prior austenite grain boundaries (PAGB). Recently, first-principles calculations have revealed that carbon (C) segregation in iron suppressed the reduction of GB cohesive energy by hydrogen. However, it has not yet been verified whether C segregation at PAGB is effective or not in reducing susceptibility to hydrogen embrittlement in martensitic steels. The present study experimentally demonstrated that the resistance against hydrogen embrittlement in martensitic steels can be improved by increasing C segregation at PAGB. Using an Fe-3Mn-0.2C (wt.%) alloy, we successfully increased the carbon segregation at PAGB without changing structural unit size and dislocation density (Non-seg specimen: lower C segregation, Seg specimen: higher C segregation). The ultimate tensile strengths of the uncharged specimens were almost the same (~ 1520 MPa). In contrast, in the hydrogen-charged specimens, the maximum tensile stress was higher in the Seg (1186 MPa) than that in the Non-seg (666 MPa) though the diffusible hydrogen content were similar values (~0.48 wt. ppm). In addition, the fraction of intergranular fracture surface was 11.3% in the Seg, which was significantly reduced from that in the Non-seg (55.5%).

P2-16

Development of Analysis Methods for SEM-based Techniques and X-Ray Contrast Tomography: Application to Strain Localization Phenomena and Hydrogen-induced Effects on Plasticity in High-strength Steels

I. Gutierrez-Urrutia[1] and A. Shibata [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

We present a summary of the analysis methods developed in the last years for the characterization of crystal defects (stacking faults, full and partial dislocations) in the SEM by the Electron Channeling Contrast Imaging (ECCI) and Transmitted-forescattered Imaging (t-FSEI) techniques, and the reconstruction of 3D Diffraction Contrast Tomography datasets. The developed methods comprise the establishment of novel technical, methodological and theoretical insights for the understanding of 2D/3D Steel Science. Specific examples applied to the investigation of strain localization phenomena and hydrogen-induced effects on plasticity of high-strength FeMnAlC low-density steels will be given.

P2-17

In Situ Neutron Diffraction Study on Deformation Behavior of Hydrogen-charged SUS310S Austenitic Steel

T. Ito [1], Y. Ogawa [2], W. Gong [1], W. Mao [1], T. Kawasaki [1], K. Okada [2], A. Shibata [2] and S. Harjo [1]
[1] J-PARC Center, Japan Atomic Energy Agency (JAEA)
[2] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Hydrogen is being considered as an alternative energy carrier to fossil fuels to achieve the goal of "Carbon Neutrality". While hydrogen has historically been associated with causing steel embrittlement, Ogawa *et al.* reported that the introduction of hydrogen to SUS310S (Fe-24Cr-19Ni (mass%)) enhances both strength and ductility, thus counteracts the embrittlement effect [1]. Although this phenomenon was qualitatively explained by the hydrogen-induced solid-solution strengthening and the promotion of deformation twinning, the influence of hydrogen on the development of dislocations and stacking fault (*i.e.*, twin nuclei) during deformation remains less understood. The aim of this work is to investigate the effects of hydrogen on the evolution of these crystal defects by using in situ neutron diffraction measurements. A SUS310S specimen was exposed to a hydrogen gas environment at 100 MPa and 270 ˚C for 200 hours, with a uniformly pre-charged hydrogen concentration of 140 mass ppm. In situ neutron diffraction measurements at room temperature were conducted by the engineering neutron diffractometer TAKUMI at MLF of J-PARC. When comparing the analysis results of neutron diffraction patterns for hydrogen-charged and non-charged samples, the difference of stacking fault probability was hardly observed although hydrogen is generally considered to reduce the stacking fault energy [2]. The dislocation density was determined through CMWP analysis, and the increase of dislocation density due to hydrogen under a given strain was verified. This study got support from MEXT Program (JPMXP1122684766) and Grant-in-Aid for Research Activity Start-up (JP23K19189).

[1] Y. Ogawa *et al.*, *Acta Mater.,* **199** (2020) 181 [2] M. B. Whiteman *et al.*, *Phys. Status Solidi*, **7** (1964) 109

P2-18

Advanced FIB-SEM Serial-Sectioning Techniques Dedicated for 3D-EBSD Analysis

T. Hara, A. Shibata and H. Nishikawa
Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Recently, higher spatial resolution and larger observation volume have been required for FIB-SEM serial sectioning observation. For the former purpose, higher resolution, we have developed and applied an orthogonal arranged FIB-SEM. Since this arrangement is ideal for the serial-sectioning, higher resolution, contrast, and stability are simultaneously realized. For the latter requirement, larger volume, we introduced the Plasma FIB(PFIB)-SEM-femtosecond Laser tri-beam system.
Several results applying these FIB-SEMs will be introduced in this poster:
1. 3D-EBSD by the orthogonal FIB-SEM: Orthogonal FIB-SEM has an advantage in obtaining 3D-EBSD. This equipment realizes a ‘pure’ static arrangement for the serial sectioning EBSD. Since there is no need to move the sample stage during observation, high stability measurement in a shorter time can be achieved. We applied this feature for the 3D-EBSD analysis around a crack tip in high-strength steel to understand the relationship between the crack propagation and the microstructure.
2. PFIB-SEM for more extensive volume observation: We often need a larger volume 3D observation, which the standard Ga-FIB cannot reach. Xe PFIB is utilized in such cases. We performed 3D-EBSD, SIM, and SEM microstructural observations of whole micro fatigue cracks in Ni-Co base superalloy over 200um widths. From this observation, we can analyze the crack propagation mechanism in detail. In the poster presentation, we would like to present such measurement techniques, including these applications.

References
1. T. Hara, K. Tsuchiya, K. Tsuzaki, X. Man, T. Asahata, A. Uemoto, J. Alloys and Compounds, 577, S717-721, (2013)
2. A. Shibata, I. Gutierrez-Urrutia, A. Nakamura, G. Miyamoto, Y. Madi, J. Besson, T. Hara, K. Tsuzaki, Acta Mater., 234, 118053 (2022)
3. H. Nishikawa, Y. Furuya, T. Osada, K. Kawagishi, T. Hara, Scripta Mater., 222, 115026 (2023)

P2-19

High Thermal Stability for Boron-Doped Diamond Field-effect Transistors

Jiangwei Liu,[1] Tokuyuki Teraji,[1] Bo Da[2] and Yasuo Koide[1]
[1] □
, National Institute for Materials Science (NIMS)
[2] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

Wide-bandgap semiconductor diamond has excellent intrinsic properties over other semiconductors, such as high critical breakdown field, large thermal conductivity, and high hole mobility. Diamond-based electronic devices are considered promising as they operate well with low power loss, high power-frequency, and high thermal limitation. Recently, *p*-type hydrogen-terminated diamond (H-diamond) and boron-doped diamond (B-diamond) field-effect transistors (FETs) have been developed greatly. However, with increase of annealing temperature, the H-diamond surface channel was damaged gradually and electrical properties of the H-diamond FETs were degraded greatly.

The B-diamond-based FETs are considered to be operating well at high temperature. However, due to the high activation energy for boron dopants (370 meV) at room temperature, hole density in the B-diamond was quite low and the B-diamond-based FETs operated with low output current and extrinsic transconductance. In this work, we will demonstrate our recent studies for the B-diamond-based FETs with high output current and good thermal stablity at high-temperature [1-4].

References
[1] J. Liu, T. Teraji, B. Da, and Y. Koide, IEEE Electron Dev. Lett. **40**, 1748–1751 (2019).
[2] J. Liu, T. Teraji, B. Da, H. Oosato, and Y. Koide, IEEE Tran. Electron Dev. **67**, 1680-1685 (2020).
[3] J. Liu, T. Teraji, B. Da and Y. Koide, IEEE Tran. Electron Dev. **68**, 3963–3967 (2021).
[4] J. Liu, T. Teraji, B. Da and Y. Koide, IEEE Tran. Electron Dev. **70**, 2199–2203 (2023).

P2-20

Effects of Temperature and Strain Rate on Mechanical Properties in FeMnNiCoCr High Entropy Alloy

R. Harada[1], N. Tsuchida[2], R. Ueji[3] and H. Somekawa[3]
[1] Graduate Student, Department of Materials and Synchrotron Radiation Engineering, University of Hyogo
[2] Department of Materials and Synchrotron Radiation Engineering, Graduate School of Engineering, University of Hyogo
[3] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

High entropy alloys (HEA) consist of five or more elements with equal or nearly equal atomic weight. Although it has been reported that combinations of elements exhibit excellent mechanical properties at cryogenic and high temperatures, there are few reports on the strain rate dependence. Thus, this study investigated the effects of strain rate and temperature on the mechanical properties of FeMnNiCoCr HEA. Tensile tests were conducted at deformation temperatures between 77 and 673 K and strain rates between 10^{3} and 10^{-4} s^{-1}. In the mechanical properties obtained from static tensile tests, 0.2% proof stress and tensile strength increased, and uniform elongation improved significantly below 296 K. Deformation twins are responsible for improving mechanical properties at low temperatures from SEM observations. The tensile test results at strain rates above 10^{1} s^{-1} showed that the temperature increase due to adiabatic heating and the stress increase due to strain rate canceled each other out, resulting in little change in uniform elongation. The volume fraction of the deformation twin is expected to decrease due to the adiabatic heating at high strain rates above 10^{1} s^{-1}.

P2-21

Deformation Behavior and Microstructure of Dual-phase CoCuNi Alloy Processed by High-pressure Torsion and Subsequent Annealing

S. LEE [1] and K. Tsuchiya [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Our research group has reported the fabrication of an equiatomic CuCoNi medium-entropy alloy and phase separation behavior after severe plastic deformation by high-pressure torsion (HPT) and subsequent annealing. After the annealing, the dual-FCC phase with Cu-rich and Co-Ni formed due to the large miscibility gap of Cu-Co. In this study, deformation behavior and microstructure evolution of CoCuNi processed by HPT and subsequent annealing were investigated.

An equiatomic CoCuNi MEA was produced by high-frequency vacuum melting the processed into a cylindrical shape by high-temperature rolling and swaging. The HPT process was applied on disk samples with a thickness of 0.85 mm at room temperature with a pressure of 5 GPa and a rotation speed of 1 rpm to 10 rotations. After the HPT, the sample was annealed at 400 ℃ and 600 ℃ for 100 hrs, and at 800 ℃ for 1, 10, and 100 hrs. To investigate the microstructure and mechanical properties, XRD, SEM-EBSD, EDS, and tensile tests were conducted.

The as-homogenized specimen showed a tensile strength of 400 MPa with 10% elongation. After the HPT, both the strength and ductility increased to 1.5GPa and 15%, respectively. With increasing annealing temperature and time, the ductility improved with the expense of the strength. The tensile strength decreased to 520MPa with 37% elongation after the annealing at 800 ℃ for 100 hrs. In this case, the extended Luders band was observed until the true strain of 0.15. The grain refinement of the Co-Ni phase was dominantly observed in the Luders band.

P2-22

Development of a new Age-hardenable Magnesium Alloy Sheet with Excellent Room Temperature Formability and Corrosion-resistance

K. Kikuchi [1], T. Nakata [1], Z. Li [2], Y. Miyashita [1] T. Sasaki [2] and S. Kamado [1]
[1] Department of Mechanical Engineering, Nagaoka University of Technology
[2] Research Center for Magnetic and Spintronic Materials, National Institute for Materials Science (NIMS)

Mg-Zn-Ca-Al-Mn (ZXAM) alloy is a new type of Mg sheet alloy with large room temperature (RT) formability and strength. A high content of Mn is the key to forming a high density of Al-Mn precipitates, which results in grain refinement and thus high strength. However, the Al-Mn precipitates promote galvanic corrosion with the Mg matrix, deteriorating the corrosion resistance. Therefore, it is required to develop low Mn-containing ZXAM alloys without the loss of strength. In this work, we focused on age-hardening, and effects of Zn and Ca contents on the RT formability, tensile and corrosion properties in low Mn-containing ZXAM alloys were investigated.

The Zn content has a small influence on the mechanical properties, whereas the Ca content is crucial to improving the RT formability and strength. The age-hardening response was improved by the Ca addition of ≥ 0.5%, and the yield strength is increased by ~30 MPa after aging without the large loss of the corrosion-resistance. However, the 1%Ca addition of formed coarse particles and thus decrease the formability. As a result, an optimum composition was Mg-2Zn-0.5Ca-0.2Al-0.2Mn. The Index Erichsen value of the alloy reaches 8.7 mm after solution treatment, and artificial aging results in a high yield strength of 213 MPa along the rolling direction. Combined with a low corrosion rate is ~3 mm/y in NaCl solution, this alloy exhibits superior properties compared with recently designed wrought Mg alloys.

P2-23

Short Fatigue Crack Growth Mechanism in Ni-Co Based Superalloy at Elevated Temperatures and in Oxidative Atmospheres

H. Nishikawa [1], K. Habib [1], Y. Furuya [1], T. Hara [1], T. Osada [1] and K. Kawagishi [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

In this study, to elucidate the oxidation effect on the short fatigue crack growth (SFCG) characteristics of Ni-Co based TMW-4M3 superalloy, fatigue tests were conducted at room/elevated temperature in air/vacuum and three-dimensional microscopic observation of the SFCs using a plasma focused ion beam – scanning electron microscope (PFIB – SEM) system. Fatigue lives tested under vacuum at elevated temperature were comparable to those at room temperature while those tested at elevated temperatures in air showed shorter fatigue life in higher stress regions and longer fatigue life in lower stress regions than the others. In situ observation of SFCs at elevated temperatures in air revealed SFCG deceleration in the small ΔK regions and acceleration in large ΔK regions. SFCs opening/closing behaviors at elevated temperatures measured by digital image correlation (DIC) showed the crack opening stress to be higher at elevated temperature in air, possibly due to oxide-induced crack closure. However, the crack closure effect did not fully explain the difference in FCG rate between room and elevated temperatures in air. Three-dimensional investigations revealed SFCs to form at elevated temperatures in air, showing straight transgranular FCG to be insensitive to microstructure in slow growth regions, and intergranular FCG to precede that in the surrounding material in fast growth regions, in contrast to microstructural SFCs features at room temperature. It appears that slow and straight unique SFCG at elevated temperatures might occur due to intermittent brittle fracture of oxides formed at the crack tip.

P2-24

Estimation of Mechanical Properties of Alloys Using Neighboring Indentation Test

Dayuan Liu [1], Ta-Te Chen [2] and Ikumu Watanabe [1, 2]
[1] Graduate School of Science and Technology, University of Tsukuba
[2] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

Instrumented indentation test, also known as depth-sensing indentation test, is an extension of the hardness test, in which the applied load and penetration depth are measured. The elastic stiffness and hardness can be estimated based on the resulting relationship between load P and depth h (i.e., the P-h curve). An inhomogeneous stress state is produced in the instrumented indentation test compared with the uniaxial stress state. Nevertheless, various estimation approaches for the stress-strain relationship corresponding to the tensile test have been proposed based on the results of instrumented indentation tests. It is recognized that a unique stress-strain relationship cannot be estimated from the P-h curve of a single indentation using a standard sharp indenter. In this context, a dual-indenter approach and a spherical indenter approach using two sharp indenters with different apex angles enable us to determine a unique set of material parameters in a simple constitutive model. In this study, we focus on the interactions between the existing and subsequent indentation tests to extract the plastic properties from the result of two indentation tests performed at neighboring positions. With this view, finite element simulations are performed to design suitable indentation conditions and draw the response surfaces of the indentation results to determine the material constants of the plastic constitutive model. Eventually, the proposed approach is validated in applications to aluminum alloys and stainless steel in which the material constants are read from the response surfaces.

P2-25

Evidence Supporting Reversible Martensitic Transformation under Cyclic Loading on Fe–Mn–Si–Al Alloys Using in Situ Neutron Diffraction

T. Sawaguchi [1], Y. Tomota [2], F. Yoshinaka [1] and S. Harjo [3]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[2] National Institute of Advanced Industrial Science and Technology (AIST)
[3] J-PARC Center, Japan Atomic Energy Agency

Fe–Mn–Si-based alloys, such as Fe–30Mn–4Si–2Al and Fe–15Mn–10Cr–8Ni–4Si (in mass%), show superior resistance to plastic fatigue compared to the conventional steels, which is ascribed to the reversible back-and-forth movement of {111} ⟨11-2⟩ γ Shockley partial dislocations associated with a reversible martensitic transformation between the face-centered cubic γ-austenite and hexagonal close-packed ε-martensite. The purpose of this study was to gather evidence of the reversible martensitic transformation using *in situ* neutron diffraction under cyclic loading. Three Fe–30Mn–Si–Al alloys with different Gibbs free energy differences at 298 K: Fe–30Mn–6Si ($\Delta G_{\gamma\rightarrow\varepsilon}$ = −250 J/mol), Fe–30Mn–5Si–1Al ($\Delta G_{\gamma\rightarrow\varepsilon}$ = −128 J/mol), and Fe–30Mn–4Si–2Al ($\Delta G_{\gamma\rightarrow\varepsilon}$ = −8.5 J/mol), were studied to unravel the effect of phase stability on the degree of reversibility. The reversible martensitic transformation between γ-austenite and ε-martensite during tension–compression loading is demonstrated as bulk-averaged insights in the Fe–30Mn–4Si–2Al alloy. The forward γ→ε transformation was induced by tensile loading, and the formed ε plates were reversed to γ during unloading and subsequent compressive loading.

P2-26

Corrosion Behavior of $Gd_2Si_2O_7$/ $Sc_2Si_2O_7$ with CMAS Melts for Environmental Barrier Coatings

S.H. Kim [1], T. Osada [1] and B.K. Jang [2]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[2] Interdisciplinary Graduate School of Engineering Science, Kyushu University

This study presents the high-temperature corrosion behavior of dual RE-disilicate. The high-temperature corrosion behavior of dual rare-earth disilicate sintered $Gd_2Si_2O_7$ (70 vol%) + $Sc_2Si_2O_7$ (30 vol %) and CMAS melts applied as promising EBCs materials were evaluated for 0.5, 2, 12, and 48 h at 1400°C. The reaction layer was classified into two layers. $Ca_2Gd_8(SiO_4)_6O_2$ (apatite) grown vertically in the form of elongated morphology by reaction of single $Gd_2Si_2O_7$ with CMAS in the top part and $Ca_2Gd_8(SiO_4)_6O_2$ mixed with $Sc_2Si_2O_7$ were analyzed. When comparing the results of the previous study in $Gd_2Si_2O_7$, the high-temperature corrosion reaction layer of CMAS and single $Gd_2Si_2O_7$ (100%) is reduced by 20%.

P2-27

Mechanical Response of Pure Fe Having Different Grain Sizes under Tensile Stress

N. Adachi [1], K. Iwamoto [1] and Y. Todaka [1]
[1] Department of Mechanical Engineering, Toyohashi University of Technology

It has been reported that ultrafine grained (UFG) materials shows not only high strength but also relatively large elongation. We previously investigated mechanical property of pure Fe having different grain sizes prepared by the high-pressure torsion and annealing processes[1)]. We found that the UFG pure Fe shows noticeable uniform elongation. In order to understand the interesting mechanical behavior of UFG pure Fe, elementary process of dislocation motion in the UFG sample should be clarified. In this study, mechanical behavior of the UFG pure Fe samples with difference grain sizes was investigated. Then, strain rate jump test was performed under three different strain rates. From the magnitude of the difference of flow stress before and after a strain rate jump, activation volume for dislocation motion in each sample was evaluated. The obtained activation volumes were plotted as a function of true shear stress in a double logarithmic graph. The plot indicated that the activation volume varies in inverse proportion to the shear stress irrespective of initial grain size of the sample. This relation implies that the main obstacle for dislocation is forest dislocation, and dislocation density under tensile test became larger with decreasing grain size. It is interesting to note that the pure Fe having a grain size of the 1 μm or lower showed unique mechanical response at the timing of a strain jump; the overshoot and undershoot of stress. The cause of such mechanical response will be also discussed in this presentation.

1) N. Adachi, H. Sato, Y. Todaka, and T. Suzuki, *Proc. Manuf.* **15** (2018) 1495–1501.

P2-28

Construction of a Materials Database for Aeroengine Materials

K.Kawagishi [1] and T. Osada [1]
[1]Research Center for Structural Materials, National Institute for Materials Science (NIMS)

The Ni-base superalloys developed by NIMS have the excellent temperature capability and can reduce CO_2 emissions when applied to aircraft engines. However, practical application to aircraft engine materials requires collecting a lot of data and verifying safety.
In order to strengthen the competitiveness of domestically produced superalloys, we will work with major domestic engine manufacturers to obtain material property data with the aim of obtaining certification from aviation authorities, and build a database that can be used within an all-Japan framework.

P3-01

Anisotropic Properties of Polyacrylonitrile- and Pitch-based Carbon Fibers

K. Naito [1,2]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[2] Department of Aerospace Engineering, Tohoku University

Polyacrylonitrile (PAN)-based and pitch-based carbon fibers with high axial stiffness and strength have been used to reinforce polymer-matrix materials in advanced composites. The trends in the development of carbon fibers are characterized as follows; high tensile strength, a fairly high strain to failure (approximately 2%) and a high specific modulus with high thermal conductivity. Several high strength (exceeding 5 GPa) PAN-based and high modulus (more than 900 GPa) pitch-based carbon fibers are commercially available at present. However, these fibers exhibit large anisotropies in the radial and axial directions. In addition, limited data has been reported on the elastic properties of fibers in other directions than longitudinal and transversal directions, and on the relationship between anisotoropic properties and fiber structures. In this study, the anisotoropic, structural and mechanical properties of PAN- and pitch-based carbon fibers were clarified in order to use multiscale analysis and optimum design of composite materials.

P3-02

Examining the Cryogenic Elastocaloric Effect in a Cu-Al-Mn Alloy

Sheng Xu [1], Yuxin Song [1], Tatsuya Ito [2], Takuro Kawasaki [2], Stefanus Harjo [2], Wu Gong [2], Xiao Xu [1], Toshihiro Omori [1] and Ryosuke Kainuma [1]
[1] Department of Materials Science, Tohoku University
[2] J-PARC Center, Japan Atomic Energy Agency

In the quest to realize a hydrogen society, efficient cryogenic methods for handling liquid hydrogen are important. Though gas refrigeration is the practically used technique, its energy efficiency is less than ideal. The focus is now shifting towards solid refrigeration that exploits the elastocaloric or the magnetocaloric effects. Especially the elastocaloric effect using superelastic alloys is known for potentially superior cooling efficiency. However, there is a hitch: conventional superelastic alloys, such as Ni-Ti, lose their superelasticity at ultra-low temperatures [1]. In contrast, we have reported that Cu-Al-Mn alloy retains this property even at a temperature of 4.2 K, which highlights its potential in cryogenic elastocaloric applications [2]. This research aims to examine the elastocaloric effect and assess the alloy's durability. We synthesized Cu-17Al-14Mn (at%) single-crystalline alloys, which exhibited remarkable superelasticity ranging from roughly 6 K to 120 K. By gauging the near-adiabatic temperature shift of the sample during rapid unloading, it was validated that the cooling induced by the elastocaloric effect persists down to about 24 K. Below this temperature, dissipation heating prevails. This observation dovetails with our thermodynamic evaluation. Additionally, cyclic loading-unloading tests conducted at 21 K brought to light the alloy's enhanced fatigue resistance under cryogenic conditions.

[1] Niitsu K. et al. *Applied Physics Letters* **102**, 231915 (2013).
[2] Niitsu K. et al. *NPG Asia Materials* **10**, e457 (2018).

P3-03

Effect of Segregation of Alloying Elements on Creep Strength in Heat Resistant Steels

K. Sawada [1], T. Hatakeyama [1] and K. Kimura [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Effect of segregation on creep strength was investigated in heat resistant steels. For ASME T91 and T92 steels, the Cr segregation was observed along the longitudinal direction of the boiler tube. Heat-to-heat variation of Cr segregation was confirmed for the steels. The creep strength was lower when the Cr segregation was strong. The coarsening of $M_{23}C_6$ carbides and recovery of martensitic lath structure during creep exposure were promoted in the strongly segregated heat of the steels. The creep life of ASME T91 steel was improved by normalization at 1200°C because the normalization decreased the Cr segregation. The alloying elements such as V, Nb and Mo were also segregated along the longitudinal direction of the boiler tube in the same way as Cr. If the segregation of Nb is remained, prior austenite grain size becomes smaller in the segregation zone since undissolved NbC can pin grain boundaries in the segregation zone. The segregation should be reduced to obtain homogenous distribution of prior austenite grain size.

The segregation of Cr and Ni was also confirmed in austenitic stainless steels such as SUS304HTB, SUS316HTB, SUS321HTB and SUS347HTB. There was heat-to-heat variation of Cr and Ni segregation for the steels. However, no large effect of the segregation on creep strength and creep ductility was recognized for the steels.

P3-04

High-throughput Evaluation Methods for Ni Based Superalloys Using Composition and Process Temperature Graded Bulk Samples

A. Ikeda, T. Osada, T. Abe, K. Kawagishi and T. Ohmura
Research Center for Structural Materials, National Institute for Materials Science (NIMS)

A high quality database of mechanical properties and phase diagrams is key to the development of novel Ni-based superalloys. The compositional combinations of multi-component alloys increase exponentially with the number of constituents. Since Ni-based superalloys can consist of more than ten constituents, the construction of a database covering the compositional space using classical methods with homogeneous specimens requires a great deal of time and effort. In this study, a method has been developed to collect mechanical property and phase diagram data sets with remarkable efficiency by introducing a series of different compositions or process temperatures into a single sample and then performing micro-area tests (nanoindentation, oxidation tests, microstructural observations). A compositionally graded sample preparation technique with a spatial scale suitable for micro area testing has been developed using the diffusion couple and unidirectional solidification methods, as well as a method for heat treatment of single sample under a temperature gradient. These techniques have provided frameworks for the construction of isothermal quasi-quaternary state diagrams and the optimization of process temperatures, etc.

P3-05

Development of Prediction Technology for Corrosion Damage Risk of Infrastructures

H. Katayama
Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Many infrastructures were intensively constructed in Japan during the period of rapid economic growth, and in recent years, the damage and deterioration due to aging have become apparent. In order to ensure safe and continuous use in the future, it is expected that huge investments will have to be made in the repair and reconstruction of these infrastructures. As the countermeasure, it is important to equalize the maintenance costs by shifting from reactive maintenance to preventive maintenance.

In this research, we are focusing on infrastructure corrosion as one of the factors causing damage and developing two technologies. One is a corrosion damage risk prediction technology from meteorological and environmental data to identify in advance which infrastructures need to be repaired or reinforced, and the other is a simple inspection and evaluation technology for efficient diagnosis using hyperspectral cameras. The prediction map of corrosion damage risk can determine the priorities of repair and reinforcement for each infrastructure and can greatly contribute to leveling the maintenance cost. In addition, further advancement of hyperspectral analysis technology is expected to realize a simple and highly quantitative inspection technology for corrosion damage.

P3-06

Durable Biomass/Polypropylene Composites for Improving Sustainability in Structures

J. Tanks [1], K. Tamura [2] and K. Naito [1,3]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[2] Research Center for Electronic and Optical Materials, National Institute for Materials Science (NIMS)
[3] Department of Aerospace Engineering, Tohoku University

Lightweight plastics and their composites are being increasingly used in automobiles to reduce emissions and costs, but the market demand for fossil fuel-based plastics such as polypropylene (PP) creates several environmental problems such as pollution and waste. Although replacing PP with biomass such as lignin is not a new endeavor, the vast majority of past studies reported reduced mechanical properties as lignin content increases, which limits its application in industry. Herein, blends of PP and glycol-modified softwood-derived lignin biomass (GL) are successfully fabricated via a melt-mixing approach, which boast exceptional mechanical properties and thermal stability. Furthermore, GL protects the polymer from degradation by UV irradiation, leading to robust in-service performance and post-service recyclability. Synergistic performance enhancement is observed when combined with carbon fiber reinforcement, which is elucidated by nanoindentation of the fiber/polymer interface. This work contributes to the development of sustainable automotive structures by efficiently combining biomass and traditional materials.

P3-07

Gaseous Hydrogen Embrittlement of Pure Nickel and Copper Nickel Alloys

K. Wada [1] and J. Yamabe [2]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[2] Department of Mechanical Engineering, Fukuoka University

Pure nickel is one of the materials whose ductility is severely degraded by high-pressure hydrogen gas. For triggering the hydrogen embrittlement of pure nickel, hydrogen accumulation along grain boundaries is required. To achieve the accumulation, two mechanisms have mainly been suggested: (1) hydrogen trapping at the grain boundaries and (2) hydrogen transportation by moving dislocations. In the present study, the contribution of the above mechanisms on the hydrogen embrittlement of pure nickel is firstly discussed based on the experimental results at a cryogenic temperature. Then, the effects of copper addition on the dominant mechanism are evaluated. It was revealed that the alloy is embrittled mainly by the trapped hydrogen when the nickel fraction is more than 80%. However, when the nickel fraction decreased to be less than 80%, the hydrogen transportation by moving dislocation started contributing to the hydrogen embrittlement. The reason was discussed in terms of the nickel fraction dependence on the ability of hydrogen trapping along the grain boundaries.

P3-08

Magnetic Order and Phase Transformation in Fe-Mn-C Alloy at Cryogenic Temperature

S. Morooka [1,2], M. Koyama [3], T. Kawasaki [2] and S. Harjo [2]
[1] Materials Science Research Center, Japan Atomic Energy Agency (JAEA)
[2] J-PARC Center, Japan Atomic Energy Agency (JAEA)
[3] Institute for Materials Research, Tohoku University

Medium Mn steels have been actively investigated due to their excellent balance between material cost and mechanical properties. In particular, medium Mn steel with a nominal chemical composition of Fe-5.0Mn-0.1C (mass%) fabricated by intercritical annealing 923 K for 1.8 ks after cold-rolling, was the high-strength mechanical properties at low temperature. This strengthening mechanism evaluated by means of *in-situ* neutron diffraction under low temperature (engineering materials diffractometer (TAKUMI) at Japan Proton Accelerator Research Complex (J-PARC)), electron back scatter diffraction (EBSD), low temperature differential scanning calorimetry (DSC) and low temperature magnetic susceptibility measurement. We found that as the sample temperature decreases, face-centered cubic (FCC) structure transferred face-centered tetragonal (FCT) structure. Namely, it suggests that austenite transformed martensite like Fe-Pd or Fe-Pt alloy. Therefore, the origin of the high-strength mechanical properties at low temperature was in the presence of FCT martensite.

This study got partially support from MEXT Program: Data Creation and Utilization Type Material Research and Development (JPMXP1122684766).

P3-09

Activation of Non <*a*> Type Dislocations and Damping Capacity Improvement by Deformation Induced Martensitic Transformation in Mg-Sc Alloy

E. Chandiran [1], Y. Ogawa [1], R. Ueji [1], A. Singh [1], H. Somekawa[1] and T. Ohmura[1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Excellent strength-to-weight ratio of magnesium (Mg) alloys makes them desirable for structural applications. However, the room-temperature formability of wrought Mg alloys should be improved for wider applicability. Addition of rare earth elements such as Sc results in a better combination of strength and ductility, likely due to enhancement of non-basal dislocation slip. Nonetheless, it is unclear how Sc addition affects the deformation mechanisms of Mg, particularly in the early stages of deformation. As a result, effect of Sc addition on deformation behavior of a near-<0001> oriented Mg-alloy grain during micropillar compression has been investigated in this study. It was found that the addition of Sc increases yield stress and also promoted formation of <*c*+*a*> type dislocation slip while the formation of <*a*> type dislocation slip is inhibited. This demonstrates that alloying Mg with Sc enhances ductility by increasing activation of non-<*a*> type dislocations.
In addition to the above study, the effect of grain orientation on damping capacity (tanδ) is investigated in a Mg-Sc alloy with a hexagonal close-packed structure (HCP Mg-Sc) and a body-centered cubic structure (BCC Mg-Sc), using nano-dynamic mechanical analysis. The damping capacity of HCP Mg-Sc was found to be less dependent on grain orientation, whereas it was significantly dependent on grain orientation in BCC Mg-Sc. The deformation-induced transformation of BCC to orthorhombic martensite in grain aligned close to <111> contributed to improved damping capacity compared to other two orientations <001> and <101>.

P3-10

3D Visualization of Hydrogen Trapping Sites in Al-Zn-Mg Alloys

R. Abe [1], K. Shimizu [1], T.T. Sasaki[2], H. Toda[3] and Y. Kamada [1]
[1] Department of Physical Science and Materials Engineering, Iwate University
[2] Research Center for Magnetic and Spintronic Materials, National Institute for Materials Science (NIMS)
[3] Department of Mechanical Engineering, Kyushu University

A critical issue with high-strength wrought Al-Zn-Mg alloys is their low resistance to hydrogen embrittlement, which hinders the application of Al-Zn-Mg alloys with higher strength classes than commercial ones. A recent ab-initio study revealed that this could be due to hydrogen trapping at the precipitate/matrix interfaces, which semi-spontaneous debonding at these interfaces [1]. Imaging of hydrogen trapping sites would validate this hypothesis or elucidate an alternative mechanism for hydrogen embrittlement in Al-Mg-Zn alloys, thus providing a detailed design strategy with excellent resistance to hydrogen embrittlement. In this study, we attempted to visualize the hydrogen trapping site in an artificially aged Al-Zn-Mg alloy using a three-dimensional atom probe (3DAP).

The sample was charged with deuterium (D) to distinguish from residual hydrogen in the 3DAP analysis chamber, followed by 3DAP analysis. The obtained 3D atom map showed the enrichment of D around the η precipitates within the grain and those along the grain boundaries. Line composition profiles across the η precipitates show the depletion of D within the precipitate and the enrichment of D at a specific η/matrix interface, suggesting that hydrogen trapped at the semi-coherent η/matrix interface facilitated interface decohesion could lead to the low resistance to hydrogen embrittlement.

[1] T. Tsuru, *et al*., *Scientific Reports,* 10:1998, 1-8(2020).

P3-11

Evaluation of the Mechanical Response of Functional Lattice Structures

C. Mercer [1], T. Speck[2,3], M. Thielen[3], J. Lee[4] and D. S. Balint[4]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS), Japan
[2] Cluster of Excellence, Freiburg Center for Interactive Materials and Bioinspired Technologies, Germany
[3] Plant Biomechanics Group, University of Freiburg, Germany
[4] Department of Mechanical Engineering, Imperial College London, United Kingdom

Functional lattice structures are designed to exhibit interesting properties not typically found in bulk single materials. Furthermore, despite often complex geometries, such structures can be successfully fabricated via modern additive manufacturing methods. Two types of functional lattice are presented. The first is designed to exhibit low thermal expansion behavior to mitigate the effects of thermal strains in applications such as hypersonic vehicles and space mirrors. The second type of structure is an auxetic (negative Poisson's ratio) metamaterial which possesses excellent energy dissipation characteristics during impact. In both cases, the mechanical response of the structures is evaluated experimentally. Following this, analytical modeling tools are employed to optimize the performance of the structures. An optimized low thermal expansion structure can exhibit mechanical performance superior to that of the bulk material. Additionally, an optimized auxetic lattice structure can theoretically absorb over 90% of the energy of an impact.

P3-12

Measurements of Interfacial Strength between Sulfur-segregated Al_2O_3 and Ni-Al Single Crystal Alloy Using Nanoindentation

C. Tabata [1,2], T. Osada [1], T. Ohmura[1], T. Yokokawa[1], K. Kawagishi[1] and S. Suzuki [2]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[2] Department of Materials Science, Waseda University

Ni-base single-crystal superalloys have excellent oxidation resistance at high temperatures. However, impurity S are known to be detrimental especially for oxidation. This is most likely due to the decrease in the adhesion of the interface between the Al_2O_3 oxide layer and the Ni-base alloy by the segregation of S. Yet, determining the differences in interfacial strength caused by S segregation has been difficult to do experimentally. The purpose of this research was to propose a mechanical test method that clarifies the differences in interfacial strength between the Al_2O_3 oxide layer and the Ni-base alloy, depending on the S segregation level, using nanoindentation. Two types of Ni-9.8 wt.% Al alloys, alloy melted using an Al_2O_3 crucible (high S) and alloy melted using a CaO crucible (low S) were prepared, and nanoindentation was conducted using a diamond, 3-sided pyramid tip with the angle of 60 degrees. The initial indent position was at the Al_2O_3 oxide layer, 0.5 μm away from the interface, and the tests were conducted 17 times each, at 600 μN/s loading and unloading rate and 10 s holding time in between. The SEM images showed that the indentation moved towards the alloy during the test, helping initiate the crack at the interface. Alloy (high S), which has higher S segregation level at the Al_2O_3/alloy interface, showed that the first pop-in load was lower compared to alloy (low S). The Weibull distributions showed about 650 μN difference in the pop-in load due to the differences in S segregation level, and we were successful in terms of quantitatively comparing the interfacial strength of the two specimens.

P3-13

Elucidation of Fatigue Fracture Mechanism Focusing on the Environment and Interface in Materials

H. Oguma[1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

The use of high-strength materials, such as high-strength steels, titanium alloys, and fiber-reinforced plastics, is increasing in harsh environments as transportation equipment becomes faster, lighter, and more efficient. The study of fatigue fracture mechanisms has primarily focused on the impact of environmental conditions on cracks and material interfaces. The presentation summarizes ongoing research activities that aim to clarify fatigue features in real service conditions and use the ambient environment to explain fracture mechanisms and the dominant factors affecting strength properties. Systematic experimental data accumulation is being carried out, especially with regards to long-term reliability, to develop material and structural design methods. These efforts aim to facilitate the prompt implementation and utilization of innovative materials with high reliability under extreme environmental conditions.

P3-14

Beneficial Aspect of Hydrogen on the Mechanical Property of Fe-Cr-Ni Austenitic Steels

Yuhei Ogawa [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Hydrogen gas is an energy carrier attracting great attention toward realizing a carbon-neutral society. However, a critical problem in the robust design of structural metals for hydrogen gas-related devices is the degradation of strength and ductility caused by the dissolution of H atoms, *i.e.*, hydrogen embrittlement (HE). Nevertheless, while the negative aspect stands out, H can also beneficially impact the mechanical properties of metals. An example is the increase in yield stress associated with hydrogen occlusion, *i.e.*, solid-solution hardening; besides, notable improvement in the fracture elongation by solute hydrogen has sometimes been confirmed in stable austenitic alloys.

Note that any property changes in metals due to the presence of foreign elements are not limited to the case of hydrogen. Depending on the loading conditions and service environment, these changes potentially turn into either positive or negative. In this regard, HE can be viewed as a phenomenon in which only the negative aspects of hydrogen have been taken into account. If one can extract only the positive effects while suppressing all the embrittlement factors, it would be the strategy to develop innovative materials that could solve the long-standing HE problems in hydrogen-related industries.

We recently identified that solute hydrogen significantly improves the strength-ductility balance of some conventional Fe-Cr-Ni austenitic steels, wherein the above two notable outcomes: solid-solution hardening; enhanced elongation, simultaneously manifested. This newly discovered role of solute H will be reviewed, outlining central perspectives and phenomenological understanding.

P3-15

Small Ball Rebound Hardness Tester and Progress for Japanese Industrial Standards (JIS)

K. Miyahara [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

A small ball rebound hardness tester hits a specimen with a small (3 mm) alumina ball at 10 m/s. The velocity ratio before and after impact is called coefficient of restitution, often shown as *e,* and is a measure of specimen's hardness. Since the mass of the ball is only 0.056 g, the tester can be applied to small and lightweight specimens as well as large and heavy specimens.

The tester has been commercially available since 2017 through the collaborative efforts of several companies and NIMS. It can test hardness instantly and stably of various materials such as metals, foods, ceramics, rubbers, and woods, etc., some of which, ice lolly or dried bonito for example, are not suitable for conventional hardness testers. Due to its uniqueness and usefulness, work is currently in progress for Japanese Industrial Standards (JIS). In this poster presentation, several examples of interesting specimens, a model of elastic-plastic deformation and comparison with experimental results, and current progress on making a new JIS will be reviewed.

P3-16

Advancement of Welding Technology through the Use of AI Technology

H. Kitano [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Arc welding technology melts and unites weld metal and base metal by arc plasma, and is widely used as an inexpensive and fast joining method. However, arc welding technology has the problem that the temperature history during welding changes the material and mechanical state of the weld metal, possibly damaging structural properties. To solve the above problem, AI (Artificial Intelligence) and machine learning technologies are being developed to de-skill and improve the reliability of weld design and construction.

In this presentation, research on the development of a modeling method for predicting weld zone characteristics, a method for extracting microstructures from 3D metallographic images, and a method for determining heat input models for welding analysis will be presented.

P3-17

Review of Damage Evaluation and Remanufacturing for Material Sustainability

M. Hayakawa
Research Center for Structural Materials, National Institute for Materials Science (NIMS)

To investigate the microstructure and damage of friction-fatigued carburized martensitic steels for the reliability of remanufacturing - a key green innovation technology for achieving a carbon-neutral, circular economy. The retained austenite phase and residual stress were characterized by X-ray diffraction (XRD). We evaluated their changes before and after roller pitching tests, and before and after the operation of the gear parts.

Moreover, the development of functional recovery technology for surface treatments is crucial for remanufacturing. Laser hardening (LH), a type of surface treatment method, is known to be able to reform the partial surface of metals. This study focuses on the use of the laser hardening to allow the repair of friction-fatigue damage in used carburized martensite steel gears. As the surface of the fatigued specimen was rapidly heated by the laser and then cooled, the thin hardening layer quenched the surface layer. In addition, prior austenite grain refinement and restoration of the retained austenite phase in the laser hardening quenched layer were realized for the friction-fatigued specimen. Exploiting these characteristics, the friction-fatigued specimens were reheat-treated with the laser hardening; as a result, the number of cycles to failure increased by 3.8 times compared to that before the laser hardening treatment. For remanufacturing, the LH technique incurs lower environmental and processing costs than other surface treatments and is particularly beneficial when applied to gears and bearings, which are especially susceptible to wear and tear.

P3-18

Developing a Foundation for Material Evaluations to Support R & D on Liquefied Hydrogen-related Equipment

Y. Ono [1, 2], K. Wada [2], M. Hayakawa [2], M. Hibi [1], T. Shimizu [1] and H. Katayama [2]
[1] Research Network and Facility Services Division, National Institute for Materials Science (NIMS)
[2] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Hydrogen is expected to be an essential secondary energy source for achieving carbon neutrality. To implement hydrogen in society, Japan launched “the Green Innovation Fund projects”. One of them is the Large-scale Hydrogen Supply Chain Establishment project. To make the cost of supplying hydrogen competitive with fossil fuels, a group of companies is working on this project to commercialize a large-scale hydrogen supply chain.

On the other hand, to reduce the cost of liquefied hydrogen, it is important to establish cryogenic and hydrogen technologies for larger supply facilities. Therefore, in another project, NIMS is planning to install a materials evaluation facility to support the R&D activities of companies or newcomers to the hydrogen industry. The contents of NIMS project† will be presented in this presentation.

†The results in this presentation were obtained primarily as a result of work commissioned by New Energy and Industrial Technology Development Organization.

P3-19

Corrosion Resistance Evaluation of Structural Materials by Multimodal KFM-EBSD-EDS Analysis

Y. Murase [1] and H. Katayama [2]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Social implementation of high-strength steel materials is one of the important initiatives to promote energy conservation and environmental load reduction. The high strength of steel materials can be achieved by some precisely arranged heterogeneous interfacial structures. On the other hand, in general, corrosion susceptibility increases as the strength of steels becomes higher, hence the development of analysis techniques is urgently needed to evaluate the corrosion characteristics of heterogeneous interfacial structures at the nano/micrometer scales. Here, we introduce a multimodal KFM-EBSD-EDS analysis with the aim of obtaining design guidelines for high-strength steel materials with excellent corrosion resistance.

P3-20

High Temperature Fatigue Properties of SiC/SiC Composites via Novel Production Route Using Sandwich Prepreg Sheets

K. Shimoda and H. Kakisawa
Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Composites consisting of a SiC ceramic matrix and reinforced SiC fibers (i.e., SiC/SiC composites) are attractive materials for next-generation nuclear, aircraft, and aerospace components. This is because of their low specific gravity, ability to retain their essential thermo-mechanical properties at high neutron fluxes, and ability to withstand high temperatures with good fracture resistance. The characteristics of this material are, first, for the fiber coating, hexagonal boron nitride (BN) was adapted, which is more thermally stable than the previous generation pyrolytic carbon (PyC) interphase. The strength of SiC/SiC composites, especially in harsh environments, is mainly dependent on the integrity of the interphase between fiber and matrix. The interphase deflects the matrix-cracks, leads to debonding between the fiber/matrix interface, and then increases the toughness and prevents the sudden failure. However, the fiber/matrix interphase plays a critical role in determining the strength and fatigue properties of the SiC/SiC composites during oxidation at high temperatures. In general, two damage mechanisms should be involved in consideration when SiC/SiC composites are experiencing high-temperature fatigue. (i) Mechanical damage due to the external physical applied forces such as matrix-cracks; (ii) Chemical damage due to oxygen transportation through mechanical damage such as degradation of the interphase and/or matrix-cracking. The present study aimed to investigate the influence of oxidation during fatigue loading at 1200 °C under air atmosphere focused on the hex-BN interphase of the SiC/SiC composites. A tension-tension fatigue test under different fatigue load conditions was performed to investigate the fatigue deterioration of the SiC/SiC composites. The differences in strength and fracture morphology during the static and fatigue loading based on microstructural analysis were discussed, considering the effect of oxidation via matrix-cracks on BN interphase degradation.

P3-21

Electrochemical Measurement of Hydrogen Diffusion Coefficient for Mg-based Materials

K. Doi [1] and S. Hiromoto [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Hydrogen embrittlement of metallic materials has been reported mainly only for high-strength steels, and most hydrogen embrittlement studies have targeted steel materials; however, with the recent expansion of the use of Mg alloys, hydrogen embrittlement studies of these materials are accelerating. However, unlike steel materials, electrochemical hydrogen permeation testing of Mg alloys is difficult. One reason is that these materials are more corrosive than steel materials. In this study, we attempted electrochemical hydrogen permeation tests of Mg-based materials, which are particularly susceptible to corrosion, by devising test solutions for the hydrogen detection and introduction sides in the electrochemical hydrogen permeation test.

Thin sheets of pure Mg, AZ31 alloy, and WE43 alloy with 25 mm x 25 mm x 0.3 mm were used as specimens. A Devanathan-Stachurski cell was used for electrochemical hydrogen permeation tests. After the sample was set in the cell, the hydrogen detection side was filled with 2-propanol and the specimen was polarized at +200 mV (vs. SHE). The hydrogen introduction side was filled with saturated $Mg(OH)_2$ solution, and hydrogen was introduced into the specimen by applying a current. The hydrogen diffusing through the specimen was measured as hydrogen permeation current at the hydrogen detection side.

On the hydrogen detection side, the residual current was less than 0.1 $\mu A/cm^2$ immediately after the onset of polarization. For pure Mg, AZ31 alloy, and WE43 alloy, it took more than 10,000 s for the hydrogen permeation current to start increasing, suggesting that the hydrogen diffusion coefficient is much smaller for Mg-based materials than for steel materials.

P4-01

Computational Phase Diagrams and their Database Based on CALPHAD

T. Abe
[1] Research Center for Structural Materials National Institute for Materials Science (NIMS)

Through the assessment of the Gibbs energy functions of the phases in various alloy systems using the CALPHAD method, we are constructing a computational phase diagram database where users can download TDB (Thermodynamic database) files for calculations of thermodynamic quantities such as phase equilibria and Gibbs energies in unary to multicomponent systems. The CPDDB: Computational phase diagram database and its digitalized version, Digital-CPDDB, are available on MatNavi in the NIMS DICE system [1]. These databases cover more than 700 unary, binary, and ternary systems. We are also constructing databases for Ni-Base superalloys: Ni-Al-Co-Cr-Ti+α, Nd-based permanent magnets: Nd-Fe-B-Co-Cu-Dy-Al-Ga and Nd-Fe-B-Cu-O-C-Dy [2], Ag-based solder materials, high entropy alloys and MoSiBTiC alloys. These phase diagram databases enable the thermodynamic calculations for the actual processes of practical materials and provide effective knowledge for the optimization of process parameters. Since the Gibbs energy functions described in the TDB files are critically assessed by experts, they can be used as a high-quality data source for machine learning to estimate various properties.
References: [1] CPDDB, https://cpddb.nims.go.jp/cpddb/, [2] T.Abe, M.Morishita, Y.Chen, A.Saengdeejing, K.Hashimoto, Y.Kobayashi, I.Ohnuma, T.Koyama, S.Hirosawa, STAM, 22 [1] (2021) 557-570.

P4-02

Numerical Prediction of Strength Scatter in Ceramics Based on Microstructural Information

T. Maeda [1,2], T. Osada [2,3] and S. Ozaki [2,3]
[1] Graduate School of Engineering Science, Yokohama National University
[2] High Temperature Materials Group, Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[3] Division of System Research, Faculty of Engineering, Yokohama National University

Ceramics are used in a wide range of applications such as electric equipment components and medical products due to their light weight, high heat resistance, insulation, and biocompatibility. However, those use as a structural member is prevented because of scatter and size dependency of strength caused by their brittleness and microstructural heterogeneity. For overcoming the challenges and designing highly reliable ceramic members, it is necessary to predict the member strength by understanding the strength scatter, which is caused by the stochastic distribution of defects.
In this study, we proposed a numerical simulation method to predict the strength scatter of ceramics and its size dependency based on internal microstructural data obtained by using X-ray computed tomography and scanning electron microscopy with a fracture mechanics model. The microstructure information, such as pore size and grain size, was organized based on extreme value statistics, focusing only on fracture origin candidates. Prediction of the bending strengths was examined for the four types of bending tests with different effective volumes, of which the results were in good agreement with the experimental ones. It was also confirmed that the proposed method is applicable to analysis model discretized with arbitrary element size.

P4-03

Numerical Simulations to Analyze the Corrosion Behavior of Metallic Materials

M. Kadowaki [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

In automobile industry, lightweighting has become an important concept to reduce energy consumption. The weight of the vehicles can be reduced by utilizing lightweight materials, such as Al alloys, as an alternative of steels. It results in an inevitable increase in the percentage of Al alloy/steel coupled structures in automobile components. However, galvanic corrosion between Al alloys and steels is a fundamental problem. When Al alloy/steel coupled structures exist in corrosive environments, the Al alloys and steels typically act as anodic and cathodic sites, respectively, to cause galvanic corrosion. That is, corrosion damage preferentially occurs on Al alloys, while steels are basically protected from corrosion. In addition, it has been reported that when the anodic reaction on the Al alloys is insufficient, corrosion reactions (self-corrosion) also occur on the steels. However, it is difficult to simultaneously evaluate both the galvanic and self-corrosion rates based only on the experimental data. In this study, the corrosion behavior of Al alloy/steel couples was analyzed by using both finite element method (FEM) simulations and experiments. In particular, close attention was given to the balance between the galvanic corrosion and self-corrosion.

P4-04

Segregation Engineering of Structural Materials by CALPHAD Method

I. Ohnuma, Toru HARA and Takahito OHMURA
Research Center for Structural Materials, National Institute for Materials Science (NIMS)

It is well-known that alloying elements and impurities in polycrystalline materials segregate in the grain boundary (GB), which causes great influence on the microstructure formation, mechanical properties, *etc*. of structural materials. Recently, experimental studies on the GB segregation using atom probe tomography were performed and tremendous results of quantitative measurement of GB segregation were reported. However, precise thermodynamic calculation of the GB segregation in practical materials containing multiple alloying elements and impurities has not been carried out yet. In the present study, calculation method and calculated results of the GB segregation in structural materials by CALPHAD method will be presented.

The parallel tangent law proposed by Hillert was extended to the multicomponent system up to 10 alloying or impurity elements and applied to calculate the segregated compositions using the following conditions for the chemical potential of constituent elements:

$$\mu_M^{\mathrm{GB}} - \mu_M^{\mathrm{matrix}} = \mu_{X1}^{\mathrm{GB}} - \mu_{X1}^{\mathrm{matrix}} = \mu_{X2}^{\mathrm{GB}} - \mu_{X2}^{\mathrm{matrix}} = \cdots$$

where M represents solvent and $X1$, $X2$, $\cdots$ represent alloying or impurity elements. The GB phase was supposed to have random structure which has the free energy identical to that of the liquid phase. The Gibbs energy of the liquid and matrix phases was taken from Thermo-Calc using thermodynamic databases *via* TQ-Interface and used for the calculation. The effect of (1) grain size, (2) grain boundary energy, and (3) diffusion of alloying elements were also considered in the present calculation.

P4-05

Developing Thermodynamic Database from First-principles Calculations Data

A. Saengdeejing[1], R. Sahara[1] and Y. Toda[2]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[2] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

First-principles calculations have increasingly become essential tool to provide a thermodynamic data for assessing the thermodynamic database through the CALPHAD methodology. As the computational power becomes more powerful and easily accessible, first-principles calculations become a preferred method than the, time consuming and costly, experimental procedures used for determining the thermochemistry properties of the phases within the target system. This can help accelerating the alloys development process even in the complex multi-component system. First-principles calculations are performed to obtain the Gibbs free energy description of any structures that represented the end-members or disordered states in the binary and ternary systems. By using only first-principles calculations data for both end-members thermodynamic description and interaction parameters, the Al-Ni-Ti and Al-Nb-Ni ternary thermodynamic databases are constructed. Without relying on any experimental data, both Al-Ni-Ti and Al-Nb-Ni thermodynamic databases can reproduce the ternary phase diagram comparable to the published database from experimental data assessment.

P4-06

Kinetic Parameters for Strength Recovery in Self-healing Ceramics

M. Rahman [1], T. Osada [2,3] and S. Ozaki [2,3]
[1] Graduate School of Engineering Science, Yokohama National University
[2] High Temperature Materials Group, Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[3] Division of System Research, Faculty of Engineering, Yokohama National University

Self-healing ceramic materials are emerging candidates in various engineering components, including high-temperature structures, electronics devices, and even in biomedical implants. In the last couple of decades, numerous experimental investigations have been performed to examine the healing mechanisms, the factors affecting it, and the recovery of mechanical properties. Not only experimental, but also finite element (FE) modeling approaches have also become indispensable to study healing characteristics under arbitrary boundary conditions before applying them in sophisticated engineering applications. Kinetic parameters are reported to be necessary in FE analysis if universal damage-healing model is considered for matrices incorporated with healing-agents. Kinetic parameters can be approximately determined by inverse analysis in making comparison between experimental and theoretical strength recovery. Previously proposed volume-gain models such as bridging and tip-to-mouth filling models can be implemented in inverse analysis to determine kinetic parameters, healing-agent oxidation rate, and average strength recovery rate. Bridging model for short period of healing time and tip-to-mouth model for long period can be considered as remaining crack size is crucial factor to calculate theoretical strength recovery in nonlinear elastic fracture mechanics equation.

P4-07

Representative Volume Element Reconstruction and Crystal Plasticity Modeling of Stress-Strain Curves for Additively Manufactured Hastelloy X

D. S. Bulgarevich[1], M. Tsujii[1], M. Demura[2] and M. Watanabe[1]
[1] Research Center for Structural Materials (RCSM), National Institute for Materials Science (NIMS)
[2] Center for Basic Research on Materials (CBRM), National Institute for Materials Science (NIMS)

We had succeeded to reconstruct the statistical representative volume elements (RVEs) of Hastelloy X samples manufactured at different conditions by laser powder bed fusion (LPBF) process. Due to the complex history of the laser heat gradients and scanning patterns, the accurate and realistic representation of geometrical and spatial characteristics of corresponding microstructure constituents in RVEs for stress-strain curve (SSC) predictions was a serious challenge. So far, the published works had dealt with less demanding material textures or relied on one-to-one or just visual correspondence (not statistical one) of RVE with experimental data. This work addressed such issues. It is demonstrated that experimental/simulated SSC correspondence can be predicted with our reconstructed RVEs by fine tuning of parameters in phenomenological model for crystal plasticity with an internal deformation resistance and a power-law relation between driving force and deformation rate. It is revealed that fitted SSCs correspond to liner isotropic slip hardening process in all Hastelloy X samples. Simulated well-fitted SSCs for different RVEs vary by just two kinematic hardening parameter values: by critical resolved shear stress for onset of plastic deformations and by initial increase in the yield strength of the material due to dislocation interactions. Caused by discontinuous columnar or/and grain microstructures in RVEs, there is very little anisotropy between simulated SSCs with loads along X-, Y-, and Z-axes which reflects the inconsistency of experimental results in this respect.

P4-08

Design of High Temperature Materials Using a Multiscale Simulation without Empirical Parameter

R. Sahara[1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Most of conventional computer simulation techniques for designing high temperature materials introduce experimental data and empirical parameters. While, first-principles calculations based on density functional theory (DFT) is accurate but limited in their ability to characterize materials because of the very small time and spacial scales.

The purpose of the research is to renew conventional numerical simulation techniques which relied on experimental data and empirical parameters and to apply advanced computer simulation techniques, by combining first-principles calculations and our own coarse-grained calculation techniques to provide theoretical guideline to design wide range of high temperature materials.

P4-09

Reprogrammable Mechanical Metamaterials

Xiaoyang Zheng [a], Ikumu Watanabe [a] and Koichiro Uto [b]
[a] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[b] Research Center for Functional Materials, National Institute for Materials Science (NIMS)

Mechanical metamaterials are artificial structures with structure-dependent properties. They often harness zero-energy deformation modes, e.g., a single shape change that limits their applications, resulting in the need for changeable mechanical responses. We address this limitation by using a light-responsive shape-memory polydimethylsiloxane (SM-PDMS) to introduce reprogrammability into flexible mechanical metamaterials. The SM-PDMS is a rubber-like functional material with shape-memory and photothermal effects. In this study, we propose three different reprogrammable SM-PDMS metamaterials with different mechanical responses, namely, auxetic, chiral, and buckling-induced. Here, a buckling-induced SM-PDMS was harnessed to make a soft actuator with a reprogrammable preferred locomotion direction. Despite focusing on reprogramming flexible metamaterials using the light-induced SM effect, our strategy can be extended to other structures and smart materials. Also, our strategy paves the way to change the mechanical responses for similar architectures. Furthermore, our designed flexible metamaterials have the potential for different applications, such as soft robots, actuation, adaptive safety, and sports equipment.

Ref:
Zheng X, Uto K, Hu WH, Chen TT, Naito M, Watanabe I. Reprogrammable flexible mechanical metamaterials. Applied Materials Today. 2022 Dec 1;29:101662.

P4-10

Probing Chemical Reaction Dynamics through Excited-state Time-dependent *GW* Simulations

Aaditya Manjanath[1], Ryoji Sahara[1], Kaoru Ohno[2] and Yoshiyuki Kawazoe[3]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[2] Department of Physics, Yokohama National University
[3]New Industry Creation Hatchery Center, Tohoku University

Time-dependent density functional theory molecular dynamics has been the usual workhorse to probe the dynamics of such chemical reactions at a reasonable computational cost. However, the applicability of the adiabatic local density approximation exchange-correlation kernel to excited states is questionable as each one-electron level does not reflect the correct total energy of the corresponding Born-Oppenheimer surface. We emphasize that extended quasiparticle theory completely solves this problem and, contrary to conventional wisdom, guarantees applicability of the *GW* approximation to any excited eigenstate as the initial reference state. As it is a computationally formidable theory, its time-dependent (TD) extension, TD*GW*, has never been attempted before to obtain accurate dynamics. We have implemented an efficient algorithm of the same, in our home-grown code, Tohoku mixed basis orbitals (TOMBO) *ab initio* program and performed the TD*GW* simulation of a bond dissociation process in a simple system, the Methane (CH_4) molecule. I will demonstrate how TD*GW* accurately captures the bond dissociation dynamics in a reasonable walltime of the simulation.

P4-11

Computational Morphology Design of Duplex Structure Considering Interface Debonding

J. Zhou [1,2], I. Watanabe [1,2] and T. Yamada [1,3]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[2] Graduate School of Pure and Applied Sciences, University of Tsukuba
[3] Graduate School of Engineering, The University of Tokyo

A finite volume interface is an interface region with interface strength, and is most often generated during the fabrication (3D printing) of a duplex structure. However, it is often neglected in morphology design due to numerical complexity and computational difficulties. In addition, a sharp and perfect-bonding interface is usually assumed in literatures. However, such assumptions bring failure risks, thus limiting the industrial applicability of the morphology designs of duplex structures. This study aims to identify the optimal morphology design though a computational design method, considering the finite volume interface and debonding of a duplex structure. This method is based on topology optimization, which utilizes a level-set function for optimizing material distribution in the design space. To introduce finite volume interfaces in morphology design, a simple interface debonding model is integrated into implicit finite element analysis, based on the finite strain theory. Moreover, a distance function is employed to describe the interface region in addition to a level-set function for topology optimization. Further, a topological derivative based on an adjoint variable method is formulated for a debonding interface state in a nonlinear finite element analysis, which is incorporated in topology optimization to obtain the optimal duplex structures. The numerical demonstrations verified the applicability of the proposed approach.

P4-12

Atomistic Modeling of Nanoscale Interaction between Dislocation and Grain Boundary in BCC and FCC Metals

M. Wakeda [1] and T. Ohmura [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

Grain boundaries (GBs) are one of the dominant factors affecting the macroscopic mechanical properties of polycrystalline metallic materials. GBs disturb dislocation motion and also become nucleation sources of dislocations. We here investigated the dislocation-small angle GB interaction and the dislocation nucleation from GB. The molecular dynamics (MD) and free-end nudged elastic band (FENEB) simulations are useful methods to unveil the atomistic origin and dominant factors affecting dislocation-GB interactions. We systematically investigated the interaction between edge/screw dislocations and low-angle tilt/twist GBs in BCC Fe using MD techniques. The interaction is dominated by the structures of GB dislocations at low-angle GBs. In addition, the type of incident dislocations (such as edge or screw) also plays an important role in the interaction. Dislocation nucleation from the free surface was also investigated using FENEB method, which can evaluate the activation energy for the nucleation event at zero kelvin. From FENEB results, we can also evaluate activation energy, which is one of the important properties of the nucleation event. For BCC and FCC metals, we obtained activation energy and activation volume of the dislocation nucleation event from the free surface. The obtained result suggests that the normalized energy barrier for dislocation nucleation depends on the crystalline lattice structure as well as the element. These results should be fundamental knowledge of the GB-related strengthening mechanism in polycrystalline metals.

P4-13

Seamless Numerical Simulation for Laser Powder Bed Fusion Process by Lattice Boltzmann and Multi-Phase Field Methods

S. Nomoto [1], J. Katagiri [1], M. Kusano [1], T. Kitashima [1] and M. Watanabe [1]
[1] Research Center for Structural Materials, National Institute for Materials Science (NIMS)

A three dimensionally integrated numerical method using lattice Boltzmann method and multi-phase field method is proposed for simulating melting and solidification of metal alloy in laser powder bed additive manufacturing process. Modified lattice kinetic scheme that is a kind of lattice Boltzmann method is applied to simulate gas and fluid flows with free surface. Melting and solidification of metal alloy are modelled by multi-phase field method with consideration of grain anisotropy. Conserved Allen-Cahn equation, which is also transformed to the modified lattice kinetic scheme formulation, is adapted to track the liquid-solid free surface moving dynamics. Thermal equation with heat source of traveling laser beam is solved by coupling fluid flow, melting and solidification analyses. Highly parallelized computational program is developed by MPI and OpenMP hybrid methods. A three-dimensional single-track model for Ni alloy is built with consisting of atmosphere gas, multi-grain base plate, and powder regions. Ni alloy powder is modeled by Discreet Element Method. Simulations are performed in conditions of different beam power values. Simulated solidified microstructures are confirmed to be qualitatively agreement with experimental measurements.

P4-14

A Neural Network Accelerated Kinetic Monte Carlo Simulation of the Evolution of Chemical Order in CrCoNi Medium-entropy Alloy

Jun-Ping Du [1] and Shigenobu Ogata [1]
[1] Department of Mechanical Science and Bioengineering, Osaka University, Osaka 560-8531, Japan

The neural network potential (NNP) has been used to study the local structures of chemical order in the high-entropy alloys (HEAs) and the medium-entropy alloys (MEAs). However, little research has been conducted to reveal the kinetics of chemical ordering via vacancy diffusion by using NNP in kinetic Monte Carlo (KMC) simulations due to the heavy computation expense in estimating the vacancy diffusion energy barrier. Here, we developed an estimator of the vacancy diffusion energy barrier using the neural network method to accelerate the energy barrier computation in the KMC simulations. Using the neural network accelerated KMC simulations, the evolution of the chemical order in the CrCoNi MEA was simulated at various annealing temperatures. It was found that the short-range order was formed above 800 K, while below the temperature a chemical domain structure was displayed. The local structures of the chemical order obtained in the KMC simulations, such as the Cr/CoNi {100}, Cr/CoNi {110}, and Cr/CoNi {113} types of the superlattice, agree with those found by the density functional theory calculations and the experiments. With these simulations as a basis, time−temperature−chemical-order diagrams were drawn, which provide key information for controlling the chemical order through thermal processing.

P4-15

Artificial Intelligence and Expert Cooperative Design of Non-isothermal Aging Heat Treatment Schedules for Improving 0.2% Proof Stress in γ – γ' Binary Ni-Al Alloys

V. Nandal[1], S. Dieb[1], D. S. Bulgarevich[2], T. Osada[2], T. Koyama[3], S. Minamoto[1], M. Demura[1]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Research Center for Structural Materials, National Institute for Materials Science (NIMS)
[3] Department of Materials Design Innovation Engineering, Nagoya University

In this study, we devised a unique aging heat treatment method to increase the high-temperature strength by utilizing state-of-the-art Artificial Intelligence (AI) algorithms in binary Ni-Al alloys. We challenged ourselves to find a non-isothermal aging (NIA) pattern that surpasses isothermal aging from a huge combination of complex aging heat treatment patterns, including increasing temperature and lowering temperature (about 3.5 billion possible ways) while isothermal aging was used as a traditional method. As a result, we succeeded in finding 110 outperformed NIA heat treatment schedules from 1620 trials. In addition, through the analysis of the top 5 NIA patterns discovered by AI, we have derived the idea of a new two-stage aging system that combines high-temperature for a short time and low-temperature for a long time and confirmed that this surpasses the search results of AI. These results suggest that AI and experts can jointly develop new process methods.

Keywords: Machine learning, Artificial Intelligence, Monte Carlo Tree Search, Aging, Ni-based alloys.

P4-16

Highlier Efficient Neural Network Interatomic Potential of α-iron and Hydrogen System

Shihao Zhang [1], Fanshun Meng [1] and Shigenobu Ogata [1]
[1] Department of Mechanical Science and Bioengineering, Graduate School of Engineering Science, Osaka University, Osaka, 560-8531, Japan

Artificial neural network potential (NNP) provides an accurate tool to describe the atomic interactions toward atomic-scale understanding of hydrogen embrittlement in α-iron. However, the current NNP still suffers the high computational cost comparing with empirical potential, which much limits its application for many problems of practical interests in hydrogen embrittlement. In this work, following our previous work of iron-hydrogen NNP [Physical Review Materials 5, 113606 (2021)], a new NNP was developed and validated, which not only quantitatively describes the atomistic details of hydrogen behavior in the defective α-iron system with the accuracy of density functional theory, but also shows much higher efficiency (~40 times faster) than the previous NNP. Furthermore, the NNP was applied to study the hydrogen embrittlement using the polycrystalline model and sharp penny-shaped crack model of α-iron. We expect that this NNP would provide a high-efficiency tool for atomic-scale understanding of hydrogen embrittlement.

P4-17

Tandem Bayesian Model: Connection of Weld Joint Creep Performance and Welding Conditions Considering HAZ Shape Factor

Hitoshi Izuno[1], Masahiko Demura[1], Masayoshi Yamazaki[1], Satoshi Minamoto[1], Junya Sakurai[1], Kenji Nagata[2], Yoh-ichi Mototake[3], Daisuke Abe[4] and Keisuke Torigata[4]
[1] Research Network and Facility Services Division, National Institute for Materials Science (NIMS)
[2] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[3] Hitotsubashi University
[4] IHI Corporation

The creep rupture life of ferritic heat-resistant steel such as 2 1/4Cr-1Mo steel weld joints is dominated by Type IV cracking that occurs in the heat-affected zone (HAZ). The HAZ shape of a weld joint influences the rupture life through creep damage accumulation. We addressed the inverse problem of extending the creep rupture life of weld joints by controlling HAZ shape via welding conditions. Using the workflow that predicts creep rupture life from the predicted HAZ shape from welding conditions which have implemented in MInt system, we presented a tandem Bayesian model for predicting the welding condition for longer creep life via HAZ shape factors. The welding conditions and HAZ shape factors were connected by Gaussian process. A Bayesian linear regression that incorporates the concept of model selection was used to predict rupture life from HAZ shape factors. We connected these models probabilistically by Bayesian statistical mathematics and constructed a search algorithm based on the probabilistic model. Start from 49 initial HAZ shape factors and 22 creep rupture life data within the 5764801 welding conditions combination we performed forward calculations of 20 rupture lives to find welding conditions that can improve the creep rupture life by 12% over the initial data.

P4-18

Multiscale Finite Element Analysis of Yield Point Phenomenon in Ferrite-pearlite Duplex Steels

S. Yanagawa [1,2] and I. Watanabe [1,2]
[1] Degree Programs in Pure and Applied Sciences, Graduate School of Science and Technology, University of Tsukuba
[2] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

The yield point phenomenon is observed in a variety of materials and is particularly dominant in carbon steels. Mechanisms of the aforementioned behavior is believed to be the inhibition of dislocation motion by interstitial atoms such as carbon. The yield point phenomenon in which an abrupt stress drop and localized deformation occur is often neglected in numerical simulations such as finite element analysis because it is an unstable phenomenon and leads to the numerical instability. In this study, finite element analysis of Ferrite phase was performed using the constitutive model that takes into account the yield point phenomenon. The true stress–strain relationship of Ferrite phase was reproduced by minimizing residual error between a computational simulation and experiment of tensile test, where the yield point phenomenon in a tensile test of Ferrite steel was reproduced. Additionally, finite element models of ferrite-pearlite duplex microstructure with pearlite volume fractions of 21.5% and 40.3% were prepared and used to investigate the macroscopic response and microscopic deformation mechanisms. Furthermore, finite element simulations of uniaxial tensile tests were performed using the stress-strain relationship of ferrite-pearlite duplex microstructure to reproduce the yield point phenomenon in uniaxial tensile tests. The yield point phenomenon in Ferrite-Pearlite duplex steels was successfully reproduced.

P4-19

3D Microstructure Reconstruction of Metallic Materials Using Generative Adversarial Networks

K. Sugiura [1], T. T. Chen [1], F. Sun [1], T. Ogawa [1, 2], I. Watanabe [3] and Y. Adachi [1]
[1] Department of Materials Design Innovation Engineering, Nagoya University
[2] Department of Mechanical Engineering, Faculty of Engineering, Aichi Institute of Technology
[3] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)

For a more precise development of metallic materials, including steel, it is essential to analyze not just 2D microstructures, but also their 3D microstructures. Traditionally, experiments and simulations have been used to obtain 3D microstructures, but they require a significant amount of time and effort. To address this challenge, we attempted to reconstruct 3D microstructures using Generative Adversarial Networks (GANs). Specifically, we developed a program based on the GANs algorithm "SliceGAN" proposed by S. Kench et al.[1)], which generates 3D microstructures from only three orthogonal cross-sectional images.

GANs are a type of deep learning technique proficient in image generation. GANs consist of two types of AI models: the Generator, which creates fake images, and the Discriminator, which determines if images are real or fake. GANs autonomously learn the features of the given data and can generate synthesized data that closely resembles the original. With GANs, we can quickly obtain large quantities of 3D microstructures of any size, regardless of the material type or image scale. This offers the potential for obtaining 3D microstructures that were technically challenging with traditional methods and realizing 3D microstructure reconstruction in a shorter and simpler manner.

Reference: 1) S. Kench et al., Nat. Mach. Intell. **2021**, 3, 299.

NIMS Award Symposium 2023

Organizer: National Institute for Materials Science (NIMS)

Sponsor: Ministry of Education, Culture, Sports, Science and Technology (MEXT)

NIMS Award Committee

Chair: Takashi Taniguchi (NIMS)

Tadashi Furuhara (Tohoku University)

Hideharu Nakashima (Kyushu University)

Nobuhiro Tsuji (Kyoto University)

Eiichi Sato (JAXA)

Manabu Enoki (The University of Tokyo)

Kaneaki Tsuzaki (NIMS)

Takahito Ohmura (NIMS)

Masahiko Demura (NIMS)

Hideki Katayama (NIMS)

Makoto Watanabe (NIMS)

Kazuhiro Kimura (NIMS)

NIMS Award Symposium 2023 Action Committee (NIMS)

Chair: Takahito Ohmura

Hideki Katayama

Makoto Watanabe

Kota Sawada

Kyoko Kawagishi

Akinobu Shibata

Rintaro Ueji

Ryoji Sahara

Yuuji Kimura

Toshio Osada

Satoshi Kishimoto

Official Website

構造材料 × カーボンニュートラル

November 6th (Mon) - 7th (Tue), 2023

TSUKUBA International Congress Center