金属材料談話会

日本金属学会東海支部 日本鉄鋼協会東海支部

韓国・Kookmin University (国民大学校)の教授4名が名古屋大学に来訪されます。それぞれのご専門を 活かし「計算・データ科学」「複合材料・積層造形」の2部構成のセミナーを企画しましたので、奮っ てご聴講下さいますようご案内申し上げます(聴講無料)。

記

日時:2024年1月26日(金) 13:00~16:50/ 意見交換会:17:30~19:00 場所:名古屋大学ES総合館1階(名古屋市千種区不老町)/ 意見交換会:ES総合館内 シェジロー アクセス <u>https://www.nagoya-u.ac.jp/access/index.html</u> キャンパスマップ <u>https://www.nagoya-u.ac.jp/access-map/index.html</u> 談話会参加費:無料 意見交換会費:無料

13:00~13:10 Opening Remark

Toshiyuki Koyama, Nagoya University

 $13:10 \sim 13:50$ Development Endeavors of Microstructure Prediction Models at the ICAPE (Integrated Computer-Aided Process Engineering) Center for Structural Materials

Pil-Ryung Cha, Kookmin University

[Abstract] With the explosive development of computational power and artificial intelligence (AI) algorithms, efforts are being made worldwide to accelerate the process from materials design to commercialization based on new research methodologies such as integrated computer-aided engineering (ICME) and AI. The representative examples of the efforts include the PRISMS and CHiMaD in US, Sweden's hero-m program, and Japan's SIP program. In line with this global trend, the Ministry of Science and ICT (MSIT) recently launched a new program called 'Integrated Computer-Aided Process Engineering (ICAPE)'. The purpose of this program is to develop a platform that accelerates the development of a scale-up process for mass production of materials design to commercialization, by combining ICME and AI. In this presentation, a brief introduction to the ICAPE program and its recent achievements in the field of structural materials will be presented. Especially, the endeavors to develop a phase model for predicting the microstructure evolution in structural materials will be highlighted in more detail.

13:50~14:30 Active Learning Approach in Designing Entropy Alloy Nanocatalyst

YongJoo Kim, Kookmin University

[Abstract] Design of bifunctional multimetallic alloy catalysts, which are one of the most promising candidates for water splitting, is a significant issue for the efficient production of renewable energy. Owing to large dimensions of the components and composition of multimetallic alloys, as well as the trade-off behavior in terms of the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) overpotentials for bifunctional catalysts, it is difficult to search for high-performance bifunctional catalysts with multimetallic alloys using conventional trial-and-error experiments. Here, an optimal bifunctional catalyst for water splitting is obtained by combining Pareto active learning and experiments, where 110 experimental data points out of 77946 possible points lead to effective model development. The as-obtained bifunctional catalysts for HER and OER exhibit high performance, which is revealed by model development using Pareto active learning; among the catalysts, an optimal catalyst (Pt0.15Pd0.30Ru0.30Cu0.25) exhibits a water splitting behavior of 1.56 V at a current density of 10 mA cm-2. This study opens avenues for the efficient exploration of multimetallic alloys, which can be applied in multifunctional catalysts as well as in other applications.

14:50~15:30 Strengthening of Aluminum by Non-Metallic Elements

Hyunjoo Choi, Kookmin University

[Abstract] The relative abundance and high specific strength of aluminum have contributed to its prominence as a structural material for use in the aerospace and automotive industries. However, usage of aluminum as an engineering material has been limited by its low-specific strength compared to other engineering metals such as steel or titanium. One possible way to enhance the mechanical properties of aluminum is to reinforce it with strong materials, producing aluminum-based composites. Herein, we select the nano-carbon materials (e.g., fullerenes, carbon nanotubes, and graphene) as reinforcing agents, try to uniformly disperse them in the aluminum matrix via powder metallurgy, and investigate their strengthening efficiency in the composites. Furthermore, we also propose a new idea for the development of nano-network structures in Al/C60 composites by the self-assembly of Al-C phases. Carbon atoms, dissembled from the individually dispersed C60-fullerenes, are intercalated into the interstitials of aluminum, producing Al-C phases with artificially moderated lattice structures. The isolated Al-C phases grow with a strong anisotropy derived from lattice mismatch, meet neighbor Al-C phases, and then self-assemble into network structures. The novel nano-structures, extremely stable at high temperatures, offer significant potential for the development of thermally-stable high-strength structural aluminum. The controlled lattice provides a new paradigm for atomic level design of crystalline materials.

15:30~16:10 Anomalous Mechanical Behavior of Aluminum Alloys Produced by Additive Manufacturing

Naoki Takata, Nagoya University

[Abstract] Laser powder bed fusion (L-PBF) process can produce aluminum (Al) alloy parts with a melt-pool structure (formed by a repetition of selective melting and subsequent rapid solidification by scanning laser irradiation) containing supersaturated solid solutions, which contributes to their unique mechanical behaviors. One of the unique behaviors is a negative strain rate sensitivity of flow stress (harder in slower deformation, softer in faster deformation) at an early stage of tensile deformation. The heat-treated Al-Si binary alloy specimens exhibited a positive strain-rate sensitivity and none of these specimens exhibited a serrated stress-strain curve, indicating a mechanism different from *Portevin–LeChatelier* effect. The dynamically precipitated Si phase interacted with the introduced dislocations, enhancing the flow stress during the early stages of plastic deformation. The dynamic precipitation could contribute to the negative strain-rate sensitivity of the flow stress at an early stage of tensile deformation. Another unique behavior is an anisotropic tensile ductility depending on the loading direction with respect to the building direction. The digital image correlation (DIC) strain analyses for in-situ observed SEM images of the identified area in the melt-pool structure revealed that high strain was localized around the melt-pool boundaries. The localized strain could play a significant role in crack initiation and propagation to failure.

16:10~16:50 Additive Manufacturing Design for Bone Cancer Implants

Hyokyung Sung, Kookmin University

[Abstract] Additive manufacturing, particularly electron beam melting, has been extensively researched for producing bone replacement implants to treat tumors. In this talk, we will discuss implants that combine solid and lattice designs to ensure a strong bond between bone and soft tissues. It's crucial for these hybrid-design implants to possess the mechanical resilience required to withstand continuous weight-bearing throughout a patient's life. Considering the unique requirements of each clinical case, a range of implant shapes and configurations, both solid and lattice, require evaluation to inform the design process. Our research focused on the mechanical integrity of the hybrid lattice, analyzing two implant shapes, comparing solid to lattice proportions, and evaluating their microstructure, durability, and computational attributes. The results highlight the advantages of tailor-made implants with optimal lattice ratios, offering improved mechanical performance and promoting bone cell growth.

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