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Dr. Hiroshi Mizuseki

Principal Researcher
Korea Institute of Science and Technology (KIST)
Seoul, Republic of Korea

Title: Atomistic configurations in alloying materials: Group–III nitrides and high-entropy alloys

Registration link: https://tinyurl.com/msy84xuc
**Zoom details will be shared with the registered participants*

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Short biography

Dr. Hiroshi Mizuseki is a Principal Researcher at the Korea Institute of Science and Technology (KIST) in Seoul, Republic of Korea since July 2013. He specializes in computational materials science, with a focus on the design of materials through first-principles calculations. His research interests include functional nanoclusters, crystals, multilayer films, gas storage materials, energy storage materials, two-dimensional materials, carbon allotropes, III-V semiconductors, and high-entropy alloys.

Dr. Mizuseki completed his doctoral studies in the Department of Materials Science at Tohoku University in Japan in March 1995. After completing his doctorate, he held various positions at Tohoku University's Institute for Materials Research, including Assistant Professor and Associate Professor.

Abstract

Properties of mixed crystals and alloying materials can be fundamentally controlled by composition and atomistic configuration of constituent elements. In this talk, I will discuss a factor that determines atomistic configuration of constituent elements based on first-principles calculation results, using group-III nitrides and high-entropy alloys as examples. To investigate the ordered phases of mixed group–III nitride ternary alloys, a first-principles based lattice model is applied to survey the atomistic configurations with the lowest formation enthalpy for a wide range of compositions. We find novel ordered phases in wurtzite structures having specific compositions. The configurations of group–III atoms on cation sites in those phases consist of a characteristic fragment of the ordered phases of one-third and one-half ordered phases that are reported previously [1]. The simulation results indicate that group–III cations in ternary nitrides follow spatial positioning "atomistic distancing rules" that can be described by pairwise interaction energy of group–III cations to realize the stabilities of the ordered structures. To minimize formation enthalpy of mixed crystal, minor B, Al, Ga, In atoms on cation sites remain neither too close to nor too distant from each other, hence, those ordered phases can be realized. It has been thought that high-entropy alloys (HEAs) have a random configuration of constituent atoms, however, ordered HEA phases have been reported as semi-ordered $L1_2$ structure. In this work, we systematically considered equiatomic quaternary alloys consisting of four out of Cr, Mn, Fe, Co, Ni, and Cu as constituent elements. Our high-throughput first-principles simulations [2] sampled and evaluated a large number of atomic configurations of their semi-ordered $L1_2$ and $D0_{22}$ phases as well as random solid solution phases, thereby investigating their energetics dependence. We found that the valence electron concentration and temperature considering the configurational entropy term are the key factor to determine the phase stability of the HEAs at finite temperature. Since the configurational entropy term is as important as the enthalpy term, the DFT calculation results indicate that the ordered-disordered coexistence phase stability is realized by enthalpy- and entropy-driven cooperation.

*Refs: [1] H. Mizuseki et al., J. Appl. Phys., **130** (2021) 035704. [2] H. Mizuseki et al., Sci. Technol. Adv. Mater.: Methods, **3** (2023) 2153632.*

Panelist

Dr. Ryoji Sahara

Group leader
Computational Structural Materials Group
National Institute for Materials Science (NIMS), Japan

Convener:
Prof. Yoshiyuki Kawazoe
Head, ACCMS-GRC
SRMIST, KTR

Organizers:
Dr. V.J.Surya & Dr.S. Yuvaraj
ACCMS-GRC Center-in-Charges
Dept. of Physics and Nanotechnology, SRMIST, KTR

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