MRS-T 中國材料科學學會
Materials Research Society-Taiwan

Invited speaker's information form of IUMRS-ICA 2017

Presentation on Symposium F2:
Materials Design, Discovery, and Optimization Based on Computation

Presentation title: Strategies to Control Thermal Expansion of High Temperature Materials

Speaker's name and affiliation: Masato YOSHIYA, Osaka University

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Brief biography of Speaker:

He has obtained Ph.D. equivalent degree from Kyoto University, Japan, following Bachelor and Master degrees from Department of Materials Science and Engineering of the university. After working as a post-doc researcher at Materials Science Division of Lawrence Berkeley National Laboratory of US Department of Energy, he spent 3.5 years in Japan Fine Ceramics Center as a staff researcher before joining Osaka University in 2005. His expertise is not only in computational materials science including ab initio calculations, molecular dynamics and phase-field modeling, but also spectroscopies to identify wide spectrum of lattice defects and associated phenomena that controls materials' properties. In addition to duties in his university, he organizes a symposium of computational materials science at MRS-J almost every year since 2009. He serves as committee members of Japan Institute of Metals and Materials and Ceramics Society of Japan and as a division head in Physical Society of Japan.

Abstract:

Expansion of crystal lattice is inevitable and its mismatch between multiple materials leads to fatigue and fracture after thermal cycling, which is a serious problem for high-temperature materials used for jet-engines of aircrafts. From theoretical perspective, variation of coefficient of thermal expansion (CTE) can be attributed mostly to Grüneisen parameter, which does not facilitate understanding of the mechanism governing CTE. In this study, theoretical calculations of CTE for various high-temperature materials are conducted using ab initio lattice dynamics within quasi-harmonic approximation, in order to firstly obtain ideal values of CTE, and then to analyze identify factors governing CTE. Then, strategies to control thermal expansion is presented. If time allows, advantages and disadvantages of methods to calculate CTE whether ab initio calculations or classical force-field calculations are discussed.

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