CHiMaD Center for Hierarchical Materials Design

SPECIAL SEMINAR

Computational Materials Design for High Plastic Formability of Mg Alloys

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August 21, 2014 [Thursday]

COOK Hall, Room 2058 | 3:00pm - 4.00pm

ABSTRACT

The materials properties are strongly related to their microstructure, which is affected their processing. It is difficult for first-principles calculations to apply directly to materials design because the scale of the calculations is only about a hundred atoms. However, the first-principles calculations can approach to mechanism of materials properties using suitable modeling based on experimental results. The first-principles study of Mg–Zn–Ca alloys exhibiting high-stretch formability is an example. It is demonstrated experimentally that Mg–Zn–Ca alloy sheets show high-stretch formability although Mg–Zn and Mg–Ca alloy sheets do not show such formability. The calculation study focuses on improved plastic anisotropy of Mg–Zn–Ca alloys, and the improved plastic anisotropy gives rise to the reduced basal plane texture, resulting in the high formability of Mg–Zn–Ca alloys.

BIO Motohiro Yuasa is the Researcher at National Institute of Advanced Industrial Science and Technology – AIST in Japan. His study focuses on mechanical properties of metals and alloys using molecular dynamics simulations and first-principles density functional theory calculations. Yuasa investigated the deformation and fracture mechanisms related to grain boundaries in metals and alloys, and received his PhD degree from Kyoto University from 2009 to 2012. In AIST, Yuasa dedicates to computational and experimental works concerning of the mechanical properties of Mg alloys, such as plastic formability. One of his main research

projects is evaluation of the highly formable Mg alloys, which are developed in his research group. He also interested in twinning of Mg.