



ICAMS Special Seminar

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Room IC 02-718

Prof. Dr. Yunzhi Wang

Department of Materials Science and Engineering
The Ohio State University
Columbus, USA

Form of Critical Nuclei at Homo-Phase Boundaries

Even though more than six decades have passed since the first theory on heterogeneous nucleation (HN) at grain boundaries (GBs) was established in the 1950s, the concurrent shape variation (co-deformation) of both the nucleus and the GB was not captured by existing models. By using a fully variational approach, where orientation relationships between the product and parent crystals and interaction between low-energy interface facets on the nucleus and the GB plane are considered simultaneously, we demonstrate for the first time the effect of interface co-deformation on the fundamental properties of a critical nucleus. Without any a priori constraints on the shapes of the critical nucleus and the GB surface, our calculations show that a nucleus is highly deformable in response to its interaction with the GB along the triple junction line. Consequently, its energy of formation can be reduced by orders of magnitude relative to predictions by previous methods.