Plastic deformation and phase transition in chalcogenides: insights from atomistic computer simulations

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Abstract

Chalcogenides have enabled many important electronic and optical applications, including flexible electronics. Previously, it is necessary to sputter chalcogenide thin films onto flexible substrates, because most chalcogenides are brittle. Recently, exceedingly large plasticity was discovered in a semiconducting chalcogenide bulk crystal, namely, hexagonal InSe. In this talk, I will provide atomic insights into the mechanical deformation mechanism in a couple of hexagonal III-VI bulk crystals, including hexagonal InSe / GaSe and monoclinic GaTe. In the second part of the talk, I will discuss the use of solid-state phase transition between the amorphous and crystalline phase of a group of chalcogenides, including GeTe and Ge-Sb-Te alloys, for non-volatile memory and neuromorphic computing applications. I will highlight how atomistic computer simulations can guide experimental research for better materials and devices in these fields.

Biography

Wei Zhang is a professor of materials science and the director of Center for Alloy Innovation and Design (CAID) at Xi'an Jiaotong University, China. He received his bachelor and master degrees both at Zhejiang University, China, and his Ph.D. degree with distinction at RWTH Aachen University, Germany. His current research interests include phase-change materials for non-volatile memory and neuro-inspired computing, first-principle materials design and deformable semiconductors.