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Invited Paper

Atomistic simulations of martensitic phase transformation and deformation behaviors of metallic materials

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ABSTRACT

A diffusionless martensitic transformation has received great interest owing to its broad academic and technological relevance. A representative class of materials utilizing the martensitic transformation is shape-memory alloys (SMAs). SMAs are widely used in many applications by virtue of their shape-memory and superelasticity behavior, which can be controlled by reversible temperature- and stress-induced martensitic transformations, respectively. As applications of SMAs recently entered the arena of smart materials for micro- and nano-electromechanical systems and nano-composite materials with exceptional mechanical properties, distinctive characteristics of martensitic phase transformations at the nanoscale have attracted particular attention. Moreover, there is a recent advance in the development of light-weight Mg-based SMAs, but there is a lot of room for improving the properties of alloys.

In this study, a detailed mechanism of phase transformation and plastic deformation at the nanoscale is investigated using atomistic simulation techniques such as the molecular dynamics. For this purpose, an interatomic potential capable of reproducing the martensitic phase transformation was developed based on the second nearest-neighbor modified embedded-atom method (2NN MEAM) model. As a fitting method of potential parameters, the force-matching method based on purely density functional theory (DFT) calculation was used instead of using the existing experimental data and DFT results simultaneously. The resulting interatomic potentials reproduce accurately the temperature- and stress-induced martensitic phase transformations of an equiatomic NiTi alloy and deformation process of pure Mg, as well as various fundamental physical properties. Subsequent molecular dynamics simulations verified that developed potentials can be successfully applied to provide insights into the atomic details of the phase transformation and plastic deformation.

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