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Atomistic Simulations of Grain Boundary Mediated Plastic Deformation Mechanisms in Nanostructured Metals

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ABSTRACT

Nanostructured metals contain vast amount of grain boundaries which are crucial to their mechanical behaviors. The plastic deformation mechanisms mediated by grain boundaries have been attracted increasing attentions in recent years. Our recent studies have been focused on using atomistic simulations to understand the grain boundary mediated plastic deformation mechanisms including deformation twinning initiated by dislocation nucleation from grain boundaries [1], cyclic plastic deformability governed by reversible slip of grain boundary dislocations [2], and extreme shear deformation of nanocrystals induced by twin boundary sliding [3]. We have also proposed a misorientation-dependent model to explain the transition between grain boundary migration and sliding mechanisms [4]. Our works provide insights into the prediction and controlling of grain boundary behaviors in nanostructured metals.

KEYWORDS

Atomistic simulation; grain boundary; nanostructured metals; plastic deformation mechanism

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