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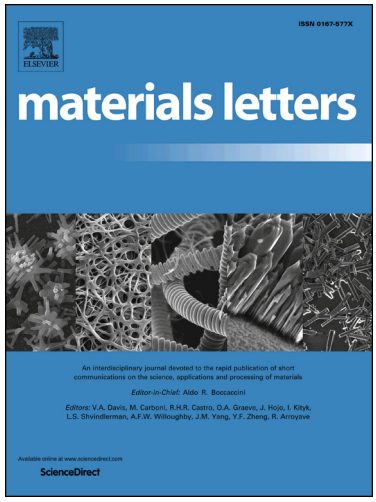

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Statistical analysis of grain boundary mobility in Al simulated using a modified synthetic driving force molecular dynamics method

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Abstract

The intrinsic mobilities of a series of symmetrical tilt grain boundaries (GBs) in Al were simulated using a modified synthetic driving force method. Statistical analysis of the mobility data reveals that low-angle GBs are on average more mobile and show larger spread in their mobilities than high-angle GBs. GBs with axes broadly near ⟨111⟩ or boundary planes close to {110} have relatively high mobility. No visible correlation is found between GB mobility and energy.

Keywords: grain boundary mobility; driving force; misorientation; boundary plane; molecular dynamics

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1. Introduction

Grain boundary (GB) mobility is known to play a key role in recrystallization and grain growth. Up to now, reduced or intrinsic mobility results of a considerable number of distinct GBs have been determined through experimental [1–5] or computational [6–11] approaches. The GB mobility is found to vary significantly with the GB crystallography, which is defined by five macroscopic degrees of freedom [12,13].

In addition to scattered mobility data obtained in various studies, attempts have been made to seek for general trends in the influence of each macroscopic parameter through statistical analysis of large datasets of GB mobility [10,14]. Notably, Olmsted et al. [10] conducted the most comprehensive simulation-based evaluation of the correlation between GB mobility and common scalar parameters, based on the mobilities of 388 GBs in Ni calculated using a synthetic driving force (SDF) molecular dynamic method. This study revealed some new insights and suggested that GB mobility could not be