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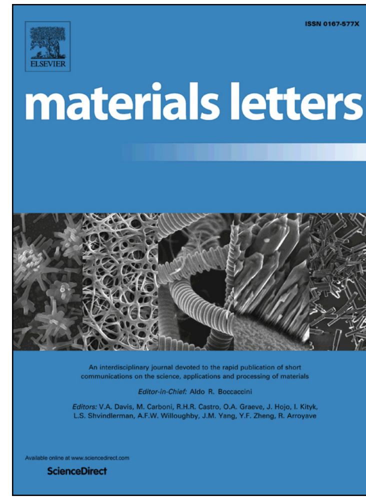

The balance between the energies of the symmetric (1012) twin boundaries and asymmetric basal/prismatic interfaces in hcp metals

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The balance between the energies of the symmetric $(10\bar{1}2)$ twin boundaries and asymmetric basal/prismatic interfaces in hcp metals

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Abstract

The energies of grain boundaries with different inclination of the boundary plane for a misorintation close to 90° about the $[1\bar{2}10]$ axis in hexagonal close packed metals are discussed. On the basis of large scale computer simulations with an empirical potential for magnesium, it can be illustrated that the basal/prismatic interfaces possess special properties.

Introduction

Deformation twinning is frequent in metals with hexagonal close packed (hcp) structure such as magnesium [1]. Particularly, twinning makes significant contribution to plastic deformation and accommodates the deformation about <c> axis. The room for twinning activity occurs due to relative hardness of non-basal slip [2, 3]. There are several twinning modes observed, however, the most frequent one is so-called "tension" twinning on twinning plane $(10\bar{1}2)$.

Despite a great effort to understand deformation twinning, some details of its mechanism are subject of discussion. For example, the presence of basal–prismatic (BP) interfaces. As a consequence, the twin boundaries can consist of the symmetrical $(10\bar{1}2)$ and non-symmetrical $(0001)/(10\bar{1}0)$ facets, the later represent a termination of one grain by the basal plane and on the other side by the prismatic plane. The BP interfaces have low formation energies that are comparable to the energy of a twin boundary [4-6] and therefore it is expected that the occurrence of this interface can affect the kinetics of twin boundary migration.

The objective of this paper is to study the relationship between the symmetric twin boundary facets and asymmetric facets formed by the BP interfaces in twin embryo.

Equilibrium shape of the $(10\bar{1}2)$ twin embryo

It was observed in computer simulations that the growing twin embryo is delimited by the conjugate $(10\bar{1}2)$ and $(10\overline{12})$ twin boundaries that are almost perpendicular one to the other [5, 7, 8]. For the ideal *c*/*a* ratio, the angle between them is about 86.6°. Presence of conjugate $\{10\bar{1}2\}$ facets was also observed experimentally in Zn in $(10\bar{1}2)$ twin tips [9, 10]. At the