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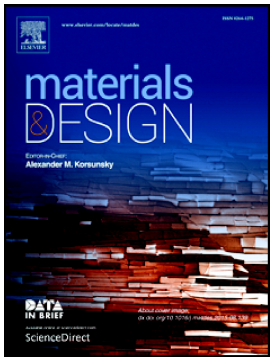

Hard-sphere displacive model of extension twinning in magnesium

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Hard-sphere displacive model of extension twinning in magnesium.

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Abstract

A crystallographic displacive model is proposed for the extension twins in magnesium. The atomic displacements are established, and the homogeneous lattice distortion is analytically expressed as a continuous angular-distortive matrix that becomes a shear when the distortion is complete. The calculations prove that a volume change of 3% occurs for the intermediate states. The twinning plane, even if untilted and restored when the distortion is complete, is not fully invariant during the transient states. The crystallographic calculations also show that the (90°, **a**) twins observed in nano-pillars and the (86°, **a**) twins observed in bulk samples differ only by a slight obliquity angle (± 3.4°). Continuous features in the pole figures between the low-misoriented (86°, **a**) twin variants are expected; they are confirmed by EBSD maps acquired on a single crystal of magnesium. As the continuous mechanism of extension twinning is not a simple shear, a "virtual work" criterion using the value of the intermediate distortion matrix at the maximum volume change is proposed in place of the usual Schmid's law. It allows predicting the formation of extension twins for crystal orientations associated with negative Schmid factors.

Keywords : Extension twins; hexagonal close-packed; magnesium; Schmid factor; angular-distortive matrix; hard sphere.

1. Introduction

1.1. The choice of paradigm

It seems important to make clear the paradigm used in this work. Indeed, the manuscript in its first formulation, i.e. without the sections 1.1, 5, 6.2 and 6.3 [1], was rejected twice from other journals mainly because it does not imply "disconnections" and because it is an "oversimplification". We hope that this preamble will help the reader to understand why we think that the mechanism of deformation twinning is not compatible with the "disconnection" theory, and why the "displacive" paradigm has been chosen. We admit that the electronic structure of the crystal is ignored in first approximation, but a simple model is not a false model; it is just a first step toward a more accurate model.

Deformation twins appear in the face centered cubic (fcc) and body centered cubic (bcc) metals deformed at high speeds or low temperatures. They are more commonly formed in hexagonal close-packed (hcp) metals because of the lowest number of slip systems. Deformation twinning share many characteristics with martensitic transformations; they are formed at very high speed (close to the speed of sound) and they take the shape of lenticular plates that become highly intricate at high deformation rates: both deformation twinning and martensitic transformations belong to the wide class of displacive transformations [2]. Deformation twinning has been mathematically treated as a *homogeneous* shear for more than one century [1]-[9]. Bevis and Crocker [7] adopted the definition "*twinning shear is any shear which restores a lattice in a new orientation*" and used it to build a generalized theory that predicts the possible twinning matrices. The more realistic ones were chosen among those with the minimum shearing magnitude. The use of shear matrices relies on the observations of planar interfaces between the parent and its twins. As explained by Christian and Mahajan [2]: "*Since a parent crystal and its twin remain in contact at the interface plane during the formation of the twin, the relation between the structures must be such that this plane is invariant in any*