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Detwinning of face-centered cubic deformation twins via the correspondence matrix approach

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ABSTRACT

Transformation of dislocations during detwinning of face-centered cubic materials is shown. The analysis is based on the correspondence matrix method and the results are additionally presented on the stereographic projection of a double twin/matrix lattice. The results show the existence of three different detwinning modes. One associated with reverse twinning mode and two others associated with pseudo-reverse twinning modes. It was found that only the reverse twinning mode is eventually able to cancel physical consequences of face-centered cubic deformation twinning (change of crystal shape and crystal orientation) including the effect of dislocation hardening (glissile to sessile dislocation transition). The other two detwinning modes lead to further dislocation hardening of a de-twinned crystal by instead producing very sessile dislocation configurations. The differences in physical consequences between the different detwinning modes will be effectively enhanced during further deformation processes involving higher order detwinning, except for the effect of crystal orientation. The obtained results and the elaborated analytical methods may serve as a proper geometrical basis for further experimental procedures involving transmission electron microscopy techniques to study de-twinned structures of dislocated face-centered cubic materials.

1. Introduction

Deformation twinning and its reverse mode (i.e. detwinning) are properly described using the concept of the correspondence matrix [C] and the reciprocal $[C]^{-1}$, respectively [1,2]. Already, well over half a century has elapsed from the time of the discovery of the [C] twinning mode in face-centered cubic (FCC) materials [3]. This mode was found by Blewitt and colleagues in deformed copper single crystals that were tested by tension at liquid helium temperature. However, the existence of the reverse twinning (i.e. $[C]^{-1}$ detwinning mode) was only recently proven by Szczerba and colleagues in copper–aluminum alloy single crystals that were pre-twinned at room temperature by primary tension and then subjected to secondary plastic deformation by compression [4]. Direct evidence performed by transmission electron microscopy (TEM) observations of the mutually reversible FCC twinning modes was very recently reported by Lee and colleagues in gold nanowires subjected to plastic tensile/compression straining [5]. It is to note that finding the $[C]^{-1}$ FCC detwinning was preceded by the discovery of a similar detwinning mode in hexagonal materials [6]. The correspondence matrix [C], as a product of the twin shear matrix [S] and the twin orientation matrix [R] (i.e. $[C] = [R][S]$), integrates the two well-known effects of deformation twinning i.e. change of crystal shape and crystal orientation. Therefore, during the reverse twinning the change of a twinned crystal back to the parent crystal shape and the restoration of its orientation must simultaneously take place. The consequences of the reverse twinning can be properly described by the reciprocal correspondence matrix $[C]^{-1}$ (i.e. $[C]^{-1} = [S]^{-1}[R]^{-1}$).

However, another important physical aspect, which deals with twin transformation of dislocations, should be taken into account during the $[C]^{-1}$ detwinning mode. As was experimentally proved by Basinski and colleagues [7] and Szczerba and colleagues [8], deformation twinning leads to important physical changes of pre-existing dislocations as well as to significant increase of strengthening of a twinned material. The changes result from the twin transformation of slip dislocations (glissile type, G) to cube dislocations (sessile type, S) making the dislocation substructure of a

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twin much stronger than that of an un-twinned crystal. The effect of glissile to sessile transition (G → S) is especially significant in FCC structures, because they usually twin after an appreciable amount of plastic deformation by slip is already accumulated in a deformed material and thus, it may contain very large density of dislocations [9,10]. Another useful geometrical analysis regarding transformation of dislocations during twinning was given by Basinski and colleagues [11] and re-discussed in terms of the dislocation node conversion process by Christian and Mahajan [9]. It was shown that formation of cube dislocations during FCC twinning is inevitable, even when the initial dislocation configuration forms a twin anti-generating node. Therefore, a deformation twin differs from the un-twinned crystal region not only by shape and orientation but also by changes made to the internal dislocation substructure. These changes are directly related to the property of deformation twinning, which is an affine and non-isometric transformation. By changing the interatomic distances, deformation twinning leads to physical changes of pre-existing dislocations (e.g. the change of the length of Burgers vectors). Such an effect is properly described using the twin shear matrix [S].

One can conclude that the reverse twinning must be recognized as a process of detwinning, which cancels all of the physical consequences induced by primary twinning (e.g. the G → S transition of dislocations). However, the term "detwinning" is often used in recent literature studying twin deformation induced phenomena in various metallic structures. Detwinning was reported, for instance, in pre-twinned polycrystalline magnesium alloy [6], in polycrystalline copper–aluminum alloy pre-twinned by dynamic plastic deformation [12], in structures of growth twins of copper and silver obtained by electrochemical deposition or magnetron sputtering methods [13–16], or in twinned structures of martensites generated due to temperature induced phase transformations [17–19]. The detwinning is considered here as a deformation process that changes a region of a lamellar twinned structure as to become a single orientation one (the $[R]^{-1}$ approach), and much less attention is paid in these cases to the $[S]^{-1}$ approach.

The effect of transformation of dislocations described by the $[S]^{-1}$ matrix seems not so important for the structures of growth twins and those induced by phase transformations [13–19]. In such twinned materials the twin and matrix regions are fairly indistinguishable from each other; therefore, they can be somewhat arbitrarily chosen to suffer a detwinning deformation. Moreover, both the twin and the matrix regions are of very low dislocation density. However, the $[S]^{-1}$ approach is critically important for structures induced by primary deformation twinning [4,6,12]. This is because the region where detwinning can take place – a deformation twin – is strictly distinguishable from the un-twinned matrix region and it can be physically determined by deformation history. It should be emphasized that FCC deformation twins are usually recognized as regions of high density of dislocations. Thus, the answer to the question of what will happen to dislocations of a pre-twinned FCC structure during the detwinning process is of great interest. This is especially important within the FCC materials, where because of symmetry reasons, two other detwinning modes may exist and also change a twin/matrix structure to a single orientation one. These modes are characterized by different de-twin shear vectors (different de-twin shear matrices) in comparison with that of the reverse twinning mode; therefore, they must be described by the correspondence matrices that will differ from the $[C]^{-1}$ matrix of the reverse twinning mode.

The main aim of the present paper is to introduce new detwinning modes able to exist within the FCC materials and further emphasize their different physical consequences. In particular, it will be shown that FCC materials may be deformed plastically using three different detwinning modes, each being able to restore the crystal orientation. However, only one of them, the reverse twinning, may lead to a detwinning process that cancels all of the effects induced by primary twinning. Since the other two are unable to bring back the crystal shape and to inverse, for instance, the G → S dislocation transition, they will be recognized as the pseudo-reverse modes of deformation twinning.

2. Detwinning of FCC structures via the correspondence matrix method

As was experimentally proven for the case of FCC materials [7,8], physical changes made by deformation twinning to a crystal shape and orientation as well as to its internal dislocation substructure are predictable by the correspondence matrix method. This method will also be suitable for predicting the changes induced by deformation detwinning, since detwinning must be treated as another deformation twinning process but occurring within a lattice of already twinned crystal. An attempt at such predictions was recently reported for the twinned martensite structures of Ni–Mn–Ga Heusler alloy subjected to cyclic detwinning process [20]. On the atomistic level, it is convenient to discuss the changes made by deformation twinning and/or detwinning modes considering what will happen to a representative piece of a crystal lattice when a specific twin shear mode is applied. In the case of FCC structures, such a piece is composed from the tetrahedron ABCD and its adjacent configuration BCDE (Fig. 1). A specific twin shear of FCC lattice is fully represented by the movement of atom C to the position C_T along the vector η_1 parallel to the twin shear plane K_1. As a result, the tetrahedron ABCD transforms into its twin shear distorted configuration ABC_TD (operation of matrix [S]), the latter being congruent to configuration BCDE. This can be immediately seen rotating the twin shear distorted tetrahedron ABC_TD (operation of matrix [R]) by 180° around normal to the twinning plane K_1. The lattice piece BCDE is in turn sheared to the tetrahedron BC_TDE of crystallographic equivalence to the tetrahedron ABCD. Thus, the FCC lattice is immediately restored in the twin crystal position. All the crystallographic consequences of twin shear referred to the crystal axes of the twin lattice are finally described by correspondence matrix [C] following the relation: $[{}_TC_M] = [{}_TR_M][{}_MS_M]$. The extended notation with the subscript letters is used here after Christian [2] to emphasize the consecutive change from the base of the matrix to the base of the twin crystal lattice. Eqs. (1) and (2) express the well-known mathematical forms of the matrix operators [S] and [R], respectively, in terms of the unit vectors K_1 and η_1. Here, [I] is a three dimensional unit matrix and $[\eta_1][K_1]^T$ is a

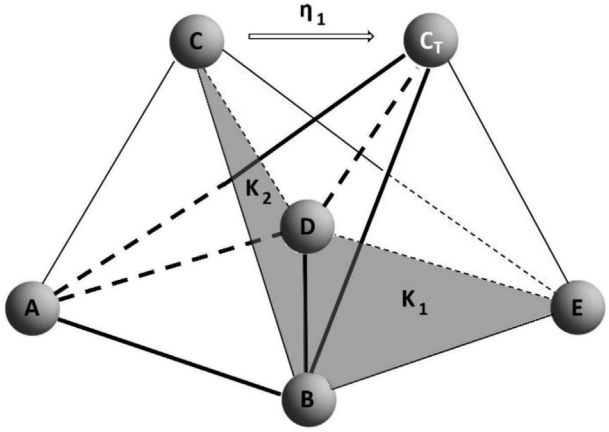

Fig. 1. The twin shear in the FCC lattice.