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# The candidacy of shuffle and shear during compound twinning in hexagonal close-packed structures

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**Abstract**

This paper proposes a systematic generalized formulation for calculating both atomic shuffling and shear candidates for a given compound twinning mode in hexagonal closed-packed metals. Although shuffles play an important role in the mobility of twinning dislocations in non-symmorphic crystals, their analytical expressions have not been previously derived. The method is illustrated for both flat planes and corrugated planes which are exemplified by $\{1\,1\,\bar{2}\,2\}$ and $\{1\,0\,\bar{1}\,2\}$ twinning modes, respectively. The method distinguishes between shuffle displacements and net shuffles. While shuffle displacements correspond to movements between ideal atom positions in the parent and twin lattices, net shuffles comprise contributions from shear on overlying planes which can operate along opposite directions to those of shuffle displacements. Thus, net shuffles in the twinning direction can vanish in a limiting case, as is interestingly the case for those needed in the second plane by the $\mathbf{b_4}$ dislocation candidate in $\{1\,1\,\bar{2}\,2\}$ twinning. It is found that while shuffle displacement vectors can be irrational when $K_1$ is corrugated, net shuffle vectors are always rational.


*Keywords:* Crystallography; Shear; Shuffle; Hexagonal; Twinning; Slip

## 1. Introduction

Recent intense consideration of magnesium and titanium by the automotive and aerospace industries as the best metallic lightweight candidates for massive weight reductions have invigorated investigation of the anisotropy and asymmetry of hexagonal close-packed (hcp) structures. These anisotropy and asymmetry issues are mainly caused by the inability of any close-packed shear deformation mode to provide $\langle c\rangle$-axis deformation. Thus, in the absence of any observed highly glissile pyramidal slip mode, a more difficult non-basal slip direction is required to provide the minimum of five independent slip systems required for arbitrary deformation. The most widely accepted dislocation in the literature possessing a non-zero $\langle c\rangle$ component operates on the second-order pyramidal plane $\{1\,1\,\bar{2}\,2\}$ with a net Burgers vector equal to $\frac{1}{3}\langle 1\,1\,\bar{2}\,\bar{3}\rangle(\langle c+a\rangle)$ [1–4]. However, the critical resolved shear stress (CRSS) of this dislocation at low temperatures turned out to be higher than that of twinning on any of the pyramidal planes. Hence, various twin modes activate to accommodate either compression or tension of the $\langle c\rangle$ axis. Twinning has been correlated with early crack nucleation, and there is a consensus in the literature that it reduces the ductility of Mg at low temperatures. This limited ductility is currently the main barrier to broader application of Mg in vehicles [5–10]. Because of the diffusional nature of shuffles, some authors "tacitly" proposed that appropriate additions of impurities may be effective in hindering shuffles and, thus, reducing the propensity to twinning [11–13]. Furthermore, shuffles have also been found to play a critical role in the

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mobility of twinning dislocations by narrowing their core width [14]. Despite the importance of shuffles in twinning, their analytical expressions have not yet been derived.

If the Burgers vector of a compound twinning dislocation in an hcp structure acts on the first plane ($\mathbf{b_1}$) above the $K_1$ composition plane, i.e. the step height is a single interplanar spacing, then shuffles in the twinning direction may not be needed to achieve mirror symmetry. However, many active twin modes can lower their characteristic shear via growth by disconnections, which have a step height greater than or equal to two interplanar spacings. In fact, the only observed twin mode that "probably" has a $\mathbf{b_1}$ type dislocation is $\{11\bar{2}1\}$ extension twinning, which occurs in Ti and Zr. The reduction of the shear magnitude with a dislocation of higher step, however, comes at the expense of increasingly requiring atoms to shuffle along complex paths within the plane of shear [15]. Through atomistic simulations, Serra et al. [14] showed that the core width of active twinning dislocations is noticeably affected by the complexity of atomic shuffles during the passage of the disconnections along the twin boundary.

Bilby and Crocker [16] gave an analytical expression for the calculation of shuffles, which required several iterations with estimated values to solve. However, the solutions for particular twin modes have never been derived. Moreover, the only available method to derive crystallographically possible Burgers vectors of twinning dislocations is that corresponding to the seminal theoretical analyses by Pond and co-workers [17–20], which were based on broken translation symmetry and combinations of symmetry operations from each of the two adjacent crystals. Serra et al. [21] have used this theory to derive three possible Burgers vectors for $\{11\bar{2}2\}$ twinning. Although comprehensive, this theory has not been adapted yet for shuffles.

In this paper, we fill this current gap by introducing a simple method which allows derivation of shuffles associated with each compound twinning dislocation candidate on any pyramidal plane in hcp metals. This method can also be used to derive the Burgers vectors of these twinning disconnection candidates and corresponding lattice rotations. We illustrate the method for both flat and corrugated pyramidal planes by applying it to $\{1\bar{1}22\}$ and $\{10\bar{1}2\}$ twins in Ti and Mg, respectively.

## 2. The general formulation for shuffles and Burgers vectors

It should be noted from the outset that the current theory was constructed under the hypothesis of compound twinning, which satisfies both Type I and Type II twinning characteristics. It may be valid or extended otherwise, but we have not verified the applicability of the theory for all twins due to the complexity of the problem. However, one must bear in mind that all observed twinning modes in hcp structures that are relevant to current engineering problems are in fact compound twins.

The notation and variables for the general formulation in the present work are described in the next several paragraphs and are accompanied by the schematic in Fig. 1. To be consistent with the notation introduced by Christian and Mahajan [22], the orthogonal unit vectors in the direction of shear, normal to the composition (twin) plane and normal to the plane of the shear ($S$) are denoted by $\mathbf{l} = \mathbf{x} = \boldsymbol{\eta_1}/\eta_1$, $\mathbf{y} = \mathbf{m}$ and $\mathbf{z} = \mathbf{m} \times \mathbf{l}$, respectively. A given compound twin mode is defined by the composition plane or simply the twinning plane $K_1$ and corresponding shear vector $\boldsymbol{\eta}_1$, a secondary undistorted, but rotated plane $K_2$ and corresponding vector $\boldsymbol{\eta}_2$, and the shear plane $S$ whose normal is a direction common to both $K_1$ and $K_2$ with no rotation ($\mathbf{z}$ direction). By this definition, note that the shear plane $S$ also contains both $\boldsymbol{\eta}_1$ and $\boldsymbol{\eta}_2$.

For a given twin mode, several twinning dislocation candidates may exist. Each candidate will operate on a certain $n$th plane above the final position of the twin boundary and has its own Burgers vector $\mathbf{b}_n$ and accompanying shuffles vectors $\mathbf{d}_p$ ($p \leqslant n$) which can be systematically and formally expressed. Formally expressing the shuffle vectors is critical since for twinning dislocations with $n > 1$, the shear alone may not be able to exactly bring atoms of planes lying between the twinning dislocation plane and the composition plane to their exact twinned lattice positions (sometimes, shuffles in the $z$ direction are required even for $n = 1$ as in the case of $\{11\bar{2}1\}$ twinning [23]). Hence, in many cases, shuffles in the $\mathbf{x}$ and/or $\mathbf{z}$ directions may be required in these intermediate planes. The shuffle in the $\mathbf{x}$ direction on the $n$th plane may also be a candidate for a Burgers vector, but a twinning dislocation may not be favored for a few reasons: (i) if the required $\mathbf{b}_n$ is too large for atoms to move in the same sense,[1] or (ii) if the direction of the Burgers vector $\mathbf{b}_n$ opposes the shear direction $\boldsymbol{\eta}_1$. Also, shuffles in the $\mathbf{x}$ direction might be easier when cooperating with the affine shear of an overlying twinning dislocation. Therefore, shuffles are often a necessary component in hcp metals if a dislocation candidate is to operate on an overlying $t$th plane where $t > n$. Therefore, a criterion must be specified to predict for each $n$th plane above the $K_1$ plane those planes that can undergo shear from those that cannot (except by shuffles). A sound theoretical criterion must also simultaneously lead to the magnitude of each corresponding Burgers vector candidate and that of each shuffle vector candidate. Such a theoretical framework has not yet been developed.

For a given twin mode, such a criterion must first recognize that there are multiple crystallographically admissible $\boldsymbol{\eta_2}$ vectors for which a shear on the $n$th plane is able to bring atoms of that plane to the twin positions. Furthermore, for every $n$th plane above the final position of the twin boundary, there is an infinite number of mathematically possible Burgers vectors, but our choice herein is restricted to the two smallest Burgers vectors in the shear plane $S$. Without loss of generality, the criterion must be

[1] See, for example, in Section 3 the cases of $\mathbf{b}_2$, $\mathbf{b}_5$ and $\mathbf{b}_6$ for $\{11\bar{2}2\}$ twinning.