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Atomic displacements accompanying deformation twinning: shears and shuffles

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ABSTRACT

Deformation twins grow by the motion of disconnections along their interfaces, thereby coupling shear with migration. Atomic-scale simulations of this mechanism have advanced to the point where the trajectory of each atom can be followed as it transits from a site in the shrinking grain, through the interface, and onwards to a site in the growing twin. Historically, such trajectories have been factorised into shear and shuffle components according to some defined convention. In the present article, we introduce a method of factorisation consistent with disconnection motion. This procedure is illustrated for the case of $(10\bar{1}2)\langle 1011 \rangle$ twinning in hexagonal close-packed materials, and shown to agree with simulated atomic trajectories for Zr.

Impact Statement: Shear and shuffle displacements accompanying $(10\bar{1}2)$ twinning are quantified consistently with growth by the observed mechanism of disconnection motion. This advance will facilitate the understanding of twinning kinetics.

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Twin growth; disconnections; atomic-scale simulation; shear and shuffle; displacements

Twinning is a ubiquitous mechanism of deformation and has been studied for many decades. Developments have been reported in an extensive literature, and the most recent comprehensive review was published in 1995 by Christian and Mahajan.[1] The objective of the present authors is to discuss progress over the two decades since Christian and Mahajan's review regarding a key aspect of twinning, namely the division of atomic displacements accompanying twinning into shear and shuffle components. Such displacements are factors relevant to the active mode of twinning and growth kinetics.

In the pioneering treatments, twin formation is described phenomenologically as a homogeneous simple shear, but subsequent experimental investigations demonstrated that twin growth actually proceeds by motion of twinning dislocations along the twin interface, that is, by an inhomogeneous deformation mechanism.[1] Figure 1(a) is a schematic representation of the twinning elements for homogeneous twin formation: the invariant plane, K_1 , the shear direction, η_1 , and their conjugate quantities, K_2 and η_2 . The line PQ in the parent crystal represents a fiducial marker parallel to the trace of K_2 in the plane of shear. Following the twinning shear, γ , this is rotated, but not distorted, becoming parallel to QR, that is, the trace of K'_2 . By contrast, Figure 1(b) schematically depicts twin formation through

motion of twinning dislocations. Here, we refer to such defects as 'disconnections', represented by the parameters, (b, h) , signifying their Burgers vector and step height, respectively.[2] These defects move sequentially along consecutive K_1 planes. During the passage of each individual disconnection leftwards, the twin crystal (designated white, and represented by the symbol λ) is displaced rigidly by $-b$ with respect to the parent (black, μ) material, and, concomitantly, the K_1 plane steps downwards by $-h$. Observed macroscopically, the fiducial line QR would appear as a continuous line, like Figure 1(a). However, at the microscopic scale, such shearing would cause discrete shear offsets, as represented schematically in Figure 1(b). Moreover, these shears may not be sufficient to create the correct twinned crystal structure, in which case additional local atomic shuffles must occur simultaneously with the shear.[1,3,4]

For a complete elucidation of atomic displacements during twin growth, it is necessary to continuously track the position of each atom during its motion from an initial position in a perfect μ crystal site, through the advancing interface, and into to a perfect λ site. Such atom tracking has not yet been followed in detail experimentally. However, atomic-scale simulations of twin growth have advanced to the point where atomic displacements can be tracked. Below, as an example, we

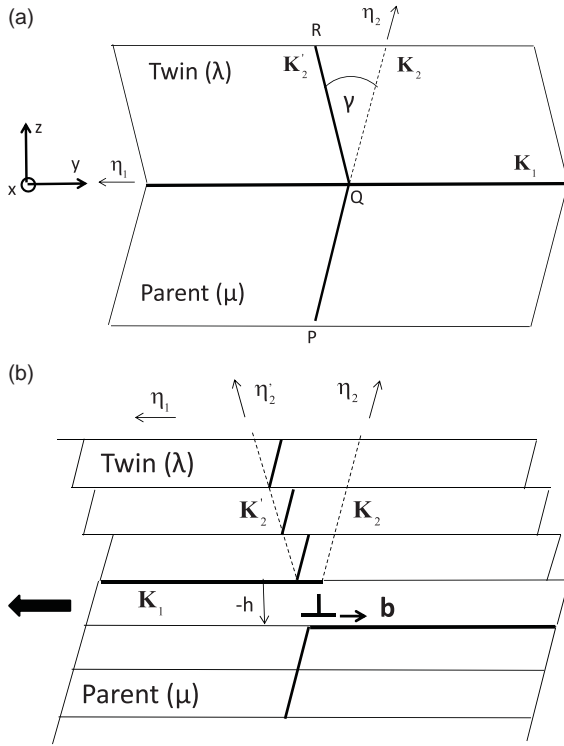


Figure 1. (a) Schematic representation of twinning by homogeneous simple shear, and (b) inhomogeneous deformation by motion of disconnections with Burgers vector, \mathbf{b} , and step height, $-h$. The bold black arrow in (b) denotes the direction of motion of successive disconnections, and their line-direction, ξ , is out of the paper.

summarise the atom tracking reported for simulated $(10\bar{1}2)\langle\bar{1}011\rangle$ twinning in Zr.[5] In earlier work,[3,4] a crystallographic method for identifying the overall displacement between the end points of an atomic track was introduced. Here, we refer to these as being ‘permanent’ since the ‘transient’ locations between the end points are not considered: permanent displacements can also be extracted from plots of simulated atomic tracks.

As discussed by Christian and Mahajan,[1] alternative prescriptions for the division of permanent displacements into shear and shuffle components are equally valid within the classical framework. Thus, in one visualisation, atoms are regarded as being embedded in a continuum which is sheared homogeneously to give the twin. In a second visualisation, atomic motif units are considered to be rigid, and each atom in a motif is assumed to undergo the same homogeneous displacement as its associated lattice point.[3,4] In their overview of twinning in superlattice structures, Christian and Laughlin [6] concluded that the selected prescription is a matter of mathematical convenience and does not imply kinetically separate processes. The present authors propose that a self-consistent, physically realistic, factorisation is feasible when the topological properties of disconnections

are considered explicitly. In this approach, atomic displacements associated with motion of the step and dislocation parts of a disconnection are considered separately. Thus, shuffles can be envisioned to be associated with the motion of the step part, and shear from the motion of the dislocation part.

Here, we illustrate the factorisation of permanent displacements for the particular case of $(10\bar{1}2)\langle\bar{1}011\rangle$ twinning in Zr. Consider leftward motion of disconnections along the \mathbf{K}_1 planes as depicted in Figure 1(b). Experimental observations show that $(\mathbf{b}_2, -h_2)$ disconnections are active in $(10\bar{1}2)$ twinning,[7,8] where $h_2 = 2d_{(10\bar{1}2)}$, that is, twice the spacing of $(10\bar{1}2)$ planes, and $\mathbf{b}_2 = q[10\bar{1}\bar{1}]$, where $q = \{3 - (c/a_0)^2\}/\{3 + (c/a_0)^2\}$, and a_0 is the hexagonal close-packed (hcp) lattice parameter.[1,7] A simulation of a $(\mathbf{b}_2, -h_2)$ disconnection, taken from Khater et al.,[5] is depicted in Figure 2, and corresponds very closely with experimental images.[7,8] In the theory of interfacial defect character,[9] \mathbf{b}_2 can also be expressed as, $\mathbf{b}_2 = \mathbf{t}(\lambda) - \mathbf{t}(\mu)$, where $\mathbf{t}(\lambda) = [10\bar{1}0]_\lambda$ and $\mathbf{t}(\mu) = [000\bar{1}]_\mu$, as indicated in the figure.

We consider λ and μ atomic lattice-complexes, that is, the interpenetrating arrangement of atomic sites in perfect crystals. Such configurations are referred to here as dichromatic complexes, or DCs,[10] and a section of that for $(10\bar{1}2)$ twins is depicted in Figure 3. It is necessary to specify a reference DC where the λ and μ atomic lattice-complexes have some chosen relative position: a convenient choice in the present case is where λ and μ centres of symmetry coincide, Figure 3. Other relative positions are defined by a rigid body displacement, \mathbf{p} , of the μ lattice-complex away from the chosen reference position, $\mathbf{p} = 0$, that is, a shift of μ with respect to λ . We define two cells within the DC, both delineated by the same interface translation vectors, $1/3[\bar{1}2\bar{1}0]_{\lambda,\mu}$ and $[\bar{1}011]_{\lambda,\mu}$, and where the third vectors are the aforementioned translation vectors, $\mathbf{t}(\lambda)$ and $\mathbf{t}(\mu)$, Figure 3. These

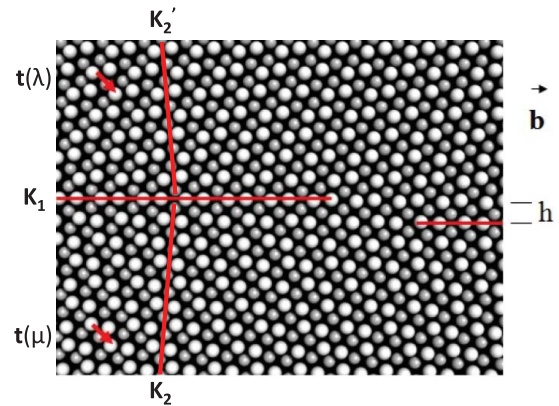


Figure 2. Projection of a simulated $(\mathbf{b}_2, -h_2)$ disconnection in a $(10\bar{1}2)$ twin in Zr [5] viewed along $-x$, which is parallel to $[\bar{1}2\bar{1}0]$.

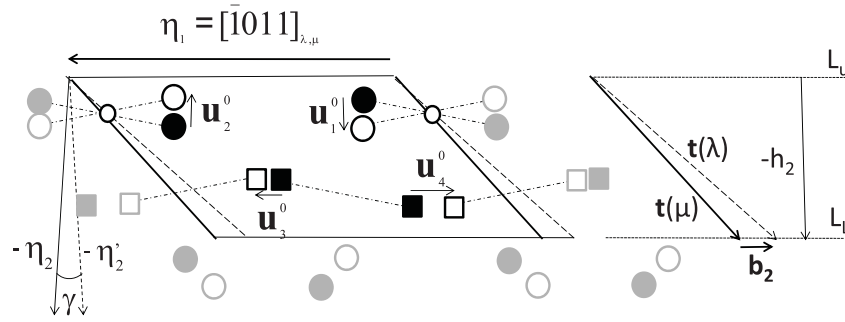


Figure 3. A section of the reference dichromatic complex for $(10\bar{1}2)$ twinning where $\mathbf{p} = 0$: λ and μ exchange cells are depicted for leftwards motion of a $(\mathbf{b}_2, -h_2)$ disconnection. Centres of symmetry are represented by small open circles. The four representative sites are depicted by bold circles and squares, corresponding to different levels along $[\bar{1}2\bar{1}0]$, and equivalent sites are shown as fainter symbols. The upper and lower interface levels are L_U and L_L , respectively.

cells extend from the upper to the lower interface levels in an ideal bicrystal, $[10] L_U$ and L_L , respectively, and are designated *exchange cells* because shuffles (for leftward motion of disconnections in this case) correspond to displacements from sites in the μ cell to sites in the λ cell. For conservative disconnection motion, there are equal numbers of sites in each cell, and these are designated *representative* atomic sites. In the present case, there are four representative λ and μ sites: these comprise two λ and two μ basis-pair sites, as indicated by the dash-dot lines in Figure 3. When exchange cells contain more than one site, as in the present case, a multiplicity of $\mu \rightarrow \lambda$ shuffles is possible. Those with the smallest magnitudes are indicated by arrows between the bold symbols in Figure 3. For comparison with Figure 1, the vectors $-\eta_2$ and $-\eta'_2$, are also outlined in Figure 3.

We now formulate the permanent displacements. These are relative motions, and in this case the μ lattice-complex is fixed (in agreement with the simulations described below, where the lowest surface of the μ crystal is fixed). Motion of the step part leftwards would produce the shuffle displacements designated, \mathbf{u}_i^0 , in Figure 3, where the superscript signifies that $\mathbf{p} = 0$, and the subscript refers to the representative atom in question, that is, $i = 1$ to 4. If a finite rigid body displacement is

present, these displacements are supplemented by $-\mathbf{p}$, so the permanent shuffles, $\mathbf{s}_i^{\mu \rightarrow \lambda}$, are given by

$$\mathbf{s}_i^{\mu \rightarrow \lambda} = \{\mathbf{u}_i^0 - \mathbf{p}\}. \quad (1)$$

Motion of the dislocation part leftwards imparts a shear displacement, $-\mathbf{b}_2$, on all λ sites above L_L . Thus, in an actual bicrystal, the same interface structure can form at level L_L as at the initial level L_U irrespective of transient relaxations. Therefore, the overall permanent displacements of the representative sites are given by

$$\mathbf{u}_i^{\mu \rightarrow \lambda} = \mathbf{s}_i^{\mu \rightarrow \lambda} - \mathbf{b}_2. \quad (2)$$

Factorisation into shuffle, $\mathbf{s}_i^{\mu \rightarrow \lambda}$, and shear components, $-\mathbf{b}_2$, reflects an essential difference between these two types of displacement. Shuffle displacements apply *only* to representative sites in the exchange cells. On the other hand, shear displacements are experienced by *all* λ sites above L_L . Thus, shear displacements produced by repeated passages of $(\mathbf{b}_2, -h_2)$ defects along an interface are *cumulative*, leading to the macroscopic (engineering) shear strain, $\gamma = b_2/h_2$, as in Figure 1(b). In other words, macroscopic shape changes in real bicrystals are related to shearing, but are not affected by shuffles.

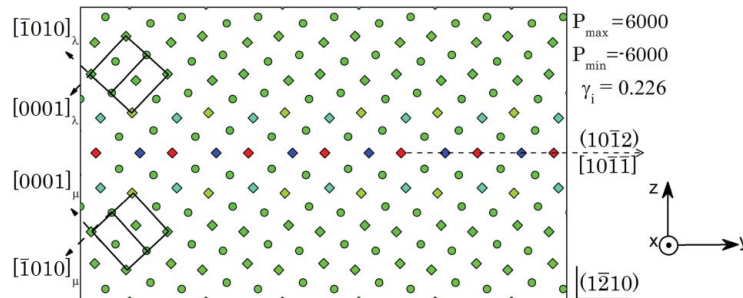


Figure 4. (Colour online) Projection along $[\bar{1}2\bar{1}0]$ of the simulated structure of a $(10\bar{1}2)$ twin in Zr.[5] Symbol colours represent hydrostatic pressure: atoms occupying blue and red sites in the composition plane experience positive and negative hydrostatic pressures, respectively.

Figure 4 shows the twin boundary structure obtained for Zr using atomic-scale simulation by Khater et al.[5] The puckered nature of $(10\bar{1}2)$ atomic planes is indicated in regions of the λ and μ crystals beyond the interfacial distortion field. We designate the distinct atomic sites of a basis-pair, A and B types, as is widely used to describe the stacking of (0002) atomic planes in hcp crystals. Then, we can represent the unequal separations of A- and B-type atoms along a $(10\bar{1}2)_\lambda$ plane by the repeating sequence, $\dots A - B - A \dots$, with a mirror related configuration in $(10\bar{1}2)_\mu$ planes. Along the composition plane, local relaxation has removed these puckers, forming a flat coalesced plane, where the atoms occupy positions intermediate between perfect λ and μ atomic sites. Relaxation also leads to a small rigid body displacement, $\mathbf{p} = [0, 0, p_z]$, where p_z is positive with magnitude ~ 0.01 nm for Zr corresponding to a small negative excess volume in the bicrystal. High-resolution transmission electron microscopy studies of $(10\bar{1}2)$ twins in Zn [7] and Ti [8] show similar structural features.

Khater et al. [5] recorded the atomic displacements of representative atoms during quasi-static simulations in which $(\mathbf{b}_2, -\mathbf{h}_2)$ twinning disconnections repeatedly pass leftwards along sequential $(10\bar{1}2)$ twin planes, Figure 5. The abscissa on each plot is the displacement of the λ

crystal leftwards relative to the μ crystal, calibrated in units of $|\mathbf{b}_2|$. The left-hand graph of Figure 5(a) shows the z coordinate changes for atoms 1 and 2. Their ‘rocking’ motion is evident from the reversal of z for each atom as they transit from μ to λ crystal sites. The coalesced plane at the interface is clearly indicated by the location where the z coordinates of atoms 1 and 2 become identical. The transient z displacements of atoms 1 and 2 during transit through the interfacial distortion field from μ to λ are evident, occurring over a distance equal to $z^e \approx 4d_{(10\bar{1}2)}$. In addition, the oscillations on the z curves correspond to elastic distortions experienced by these two atoms while in the μ crystal as disconnections pass along the interface above them, and, correspondingly, below them after entering the λ crystal.

In the right-hand graph of Figure 5(a), showing the y coordinate variations, the ‘swapping’ motions of atoms 3 and 4 are evident as they are displaced to λ sites, that is, where the puckered sequence $\dots A - B - A \dots$ in $(10\bar{1}2)_\mu$ planes changes to $\dots A - B - A \dots$ in $(10\bar{1}2)_\lambda$ planes. The difference between the y coordinate values for these atoms is larger in the μ crystal, corresponding to the separation $A - B$, than that after transit to the λ crystal, A-B: that is, atoms swap nearest neighbours within $(10\bar{1}2)$ planes. None of the

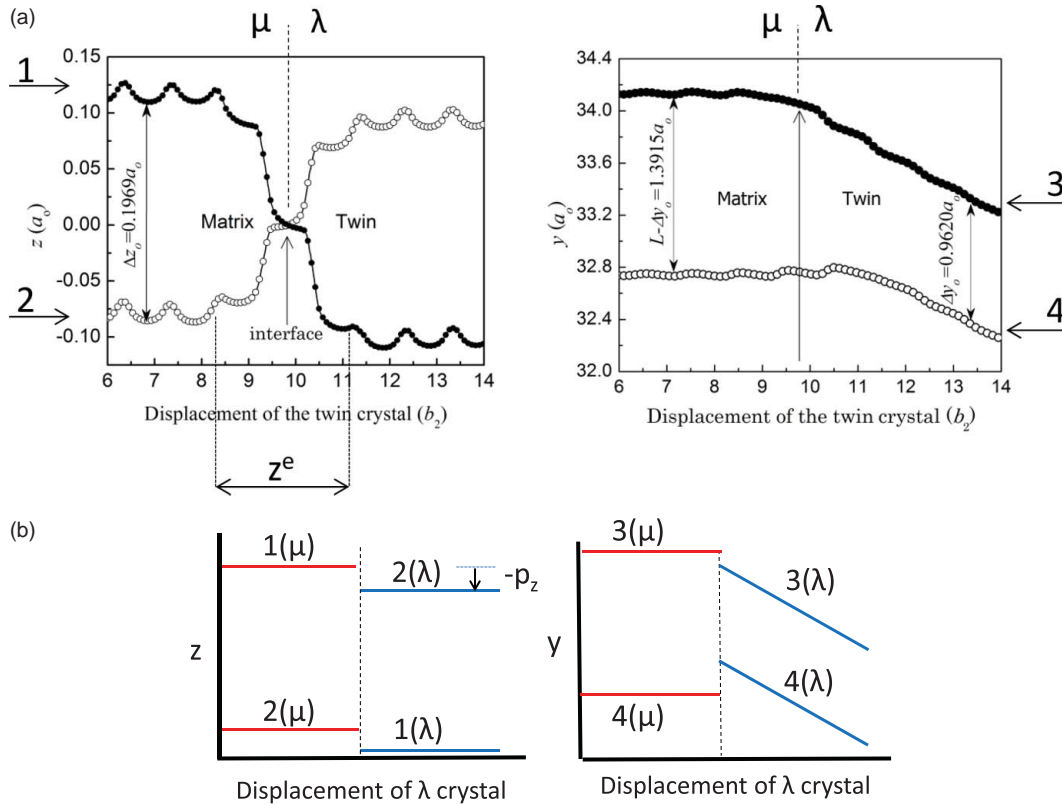


Figure 5. (Colour online) (a) atomic displacements for the four representative atoms associated with the motion of $(\mathbf{b}_2, -\mathbf{h}_2)$ disconnections moving leftwards in a $(10\bar{1}2)$ twin in Zr.[5] (b) permanent displacements deduced from (a) after suppression of the transient displacements.

Table 1. Shear and shuffle displacements for the four representative atoms when a $(\mathbf{b}_2, -h_2)$ disconnection moves leftwards in a $(10\bar{1}2)$ twin in Zr.[5]

Displacements	$x(a_0)$	$y(a_0)$	$z(a_0)$
\mathbf{b}_2	0	0.14	0
\mathbf{u}_1^0	0	0	-0.228
\mathbf{u}_2^0	0	0	0.228
\mathbf{u}_3^0	0	-0.117	0
\mathbf{u}_4^0	0	0.308	0
\mathbf{p}	0	0	0.031

representative atoms experienced displacements parallel to x .

When transient displacements are suppressed, the permanent displacements are more clearly revealed, Figure 5(b). Thus, the small displacement, $p_z \sim 0.01$ nm, is seen from the downward coordinate offset for both atoms after reaching the λ crystal, Figure 5(b) - left. In Figure 5(b) - right, the permanent swapping displacements are evinced by the difference between the y separations of atoms 3–4 when in the λ crystal compared with that in the μ crystal. Also, after transit into the λ crystal, these two atoms progressively accumulate a y displacement equal to $-\mathbf{b}_2$ for each disconnection that passes along the interface below them, as revealed in the graph by a gradient equal to minus unity. The factorised permanent displacement components extracted from Figure 5 concur with those predicted by Equation (2), and are listed in Table 1. Shuffles are equal to $\mathbf{s}_i^{\mu \rightarrow \lambda} = \{\mathbf{u}_i^0 - \mathbf{p}\}$: evidently, atoms 1 and 2 undergo equal and opposite z shuffles, \mathbf{u}_1^0 and \mathbf{u}_2^0 , that is, rocking, while, atoms 3 and 4 undergo swapping shuffles. The shear displacement of all four atoms is $-\mathbf{b}_2$ per disconnection.

We have described progress towards a fuller understanding of atomic displacements accompanying twinning, particularly atom tracking by quasi-static atomic-scale simulation of twin growth. Only two twinning modes have been studied using this promising technique so far, $(10\bar{1}2)\langle\bar{1}011\rangle$ and $(11\bar{2}1)\langle\bar{1}\bar{1}26\rangle$ in Zr,[5] and the former has been reviewed briefly here. In addition, we have related the atomic displacements so obtained to a simple mathematical expression describing permanent atomic displacements, that is, excluding transient contributions. Factorisation of permanent displacements into shear and shuffle components has been described for $(10\bar{1}2)$ twinning, the predominant mode in hcp materials.[1] Our method differs from earlier treatments,[3,4] wherein the shear displacements of lattice sites are homogeneous. Here, disconnection motion produces an inhomogeneous shear displacement equal to $|\mathbf{b}_2|$ across the interface level L_L . In consequence, the magnitudes of shuffles parallel to \mathbf{b}_2 are different in

the two approaches. A fuller account will be presented elsewhere.[11]

In a series of recent papers, it has been claimed that the $(10\bar{1}2)\langle\bar{1}011\rangle$ mode is ‘non-classical’ on the grounds that shuffling ‘dominates’ shear to such an extent that no shear strain is observed in microscopic specimens.[12–15] This contention has been criticised elsewhere,[16–18] and is clearly not supported by Table 1, where it is seen that the values of $|\mathbf{s}_i/\mathbf{b}_2|$ for atoms 1–4 in Zr are 1.41, 1.85, 0.86 and 2.21. Moreover, although the twinning shear strain for Zr is relatively small, $\gamma = |\mathbf{b}_2|/h_2 = 0.165$, active modes are known with smaller magnitudes than this in other materials.[1] Also, as pointed out by Yoo,[19] for hcp materials the magnitudes, $|\mathbf{b}_2|$ and h_2 , and hence γ , depend on c/a_0 : in particular, $|\mathbf{b}_2| \rightarrow 0$ as $c/a_0 \rightarrow \sqrt{3}$ because then, $\mathbf{t}(\lambda) = \mathbf{t}(\mu)$. However, in Cd–Mg alloys specially prepared with such lattice parameter ratios, the $(10\bar{1}2)\langle\bar{1}011\rangle$ mode is not activated.[1,p. 24] In twinning systems with this special crystallographic feature, that is, where the DC exhibits periodicity perpendicular to the \mathbf{K}_1 plane, pure steps could form, and hence could move by pure shuffling without accompanying shear.

Finally, there has also been confusion regarding the nucleation of $(10\bar{1}2)$ twins,[e.g. 14] as distinct from $(10\bar{1}2)$ twin growth. Wang et al.,[20] using atomic-scale simulation, showed that twin nuclei bounded by $\{10\bar{1}0\}_\lambda//\{0001\}_\mu$ and $\{0001\}_\lambda//\{10\bar{1}0\}_\mu$ facets form by pure shuffle. However, such nuclei formed in a constrained volume of the parent material, that is, without shape change, so no shearing took place during nucleation. This is typical of all types of solid-state nucleation where the initial nuclei are coherent to minimise surface energy, but growing crystals become semicoherent to minimise strain energy.

Disclosure statement

No potential conflict of interest was reported by the author.

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