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Atomic-Scale Comparison Between $\{\bar{1}101\}$ and $\{\bar{1}102\}$ Twin Growth Mechanisms in Magnesium

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The two most frequently observed twins in hexagonal close-packed (HCP) Mg, $\{\bar{1}101\}$ and $\{\bar{1}102\}$ twins, have surprisingly different properties and morphologies, with $\{\bar{1}101\}$ twins appearing under higher stresses and being much thinner than $\{\bar{1}102\}$ twins. By considering the atomic-scale elementary properties of the twin interfaces and their disconnections, we show that (1) the transverse propagation of $\{\bar{1}101\}$ twins is hindered by the absence of low-energy mobile interfaces, whereas $\{\bar{1}102\}$ twins benefit from prismatic-basal interfaces and (2) the thickening of $\{\bar{1}101\}$ twins is slowed by higher energy barriers against both the nucleation and propagation of disconnections along their interfaces.

Keywords: Pure Magnesium, Twinning, Disconnections, Molecular Statics

1. Introduction Twinning is a deformation mechanism particularly important in hexagonal close-packed (hcp) crystals, providing together with pyramidal slip, a means to accommodate deformation along the *c*-axis. [1–3] A significant body of experimental and theoretical studies, dating back to the early 1950s, [4–6] has been dedicated to the subject. Of particular interest is the question of the activation and the effect of twinning on the plastic response of materials such as magnesium and its alloys. [7–10]

Amongst the three twinning modes experimentally reported in pure and alloyed magnesium, two are of particular interest: $\{\bar{1}102\}$ and $\{\bar{1}101\}$ twins. [8,11–15] The former induces an extension of the *c*-axis while the latter leads to a compression of the *c*-axis. Provided loads are suitably oriented with respect to the texture, these two twin types are readily activated, yet present distinct characteristics. $\{\bar{1}102\}$ Tension twins, an example of which is shown from an atomistic simulation in Figure 1, are commonly observed in several hcp metals (i.e. Ti, Be, Zr, Hf), including pure Mg and Mg alloys AZ31 and ZK60A. [16–18] In the case of Mg, tensile twins are reported to be activated under low critical resolved shear stresses (CRSS) between 2 and 8 MPa. [19,20] These twins can consume

close to the entire parent grains. [8,11,21] The twin morphology depends on the total accumulated shear strain in the twinning shear direction and results from multiple nucleation events followed by growth and coalescence of the twin domains.

On the contrary, $\{\bar{1}101\}$ compression twins, which have been observed in pure Mg as well as in Mg AZ31, [16,17] are activated under relatively high CRSS, between 30 and 100 MPa, [19,23–25] comparable to that required to activate pyramidal slip (30–80 MPa [23,26–29]). Compressive twinning is thus in competition with pyramidal slip. Moreover, even if no quantification of the thickness of $\{\bar{1}101\}$ twins is available in the literature, they typically appear to be narrow. For example, in extruded AZ31, following compressive loading up to 10% strain in the extrusion direction, $\{\bar{1}101\}$ twins were observed to be 2.5 μm thick. [14]

Interestingly, the rationale for these marked differences remains unclear to this date. In the absence of spinoidal mechanisms, understanding the mechanism of twinning requires the study of three phenomena: nucleation, transverse propagation (i.e. propagation of the twin nucleus across the parent phase) and thickening. Twin nucleation has been described, theoretically, in

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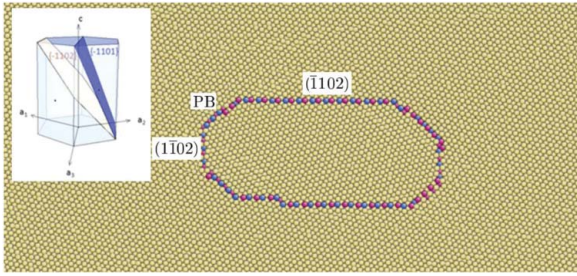


Figure 1. Nucleus of a $\{\bar{1}102\}$ twin from an atomistic simulation. The inset illustrates the mirror planes of the $\{\bar{1}101\}$ and $\{\bar{1}102\}$ twins in hcp crystals. The atoms are coloured according to their coordination number using the Atomeye software.[22]

terms of both homogeneous and heterogeneous processes; the latter being more probable from experimental observations.[17,30,31] The first heterogeneous nucleation model proposed is the pole mechanism of Thompson and Millard,[32] which considers the dissociation of $\langle c \rangle$ dislocations into twinning dislocations. Mendelson [33,34] then developed a similar but more detailed model in which twinning dislocations result from the dissociation of $\langle a \rangle$, $\langle c + a \rangle$ or $\langle c \rangle$ dislocations. Recently, Ghazisaeidi and Curtin [35] studied the dissociation of $\langle c \rangle$ and $\langle c + a \rangle$ dislocations to nucleate $\{\bar{1}102\}$ twins after Capolungo and Beyerlein [36] had studied the conditions to nucleate stable twin loops by dissociating a single $\langle a \rangle$ dislocation. Other potential structures and conditions for generating twin nuclei have also been identified in recent atomistic studies, which are based either on a shuffling mechanism from an existing grain boundary [37] or on the decomposition of particular dislocations, such as the $\{\bar{1}102\}$ twin nucleus resulting from the relaxation of a dipole of partial dislocations suggested by Wang et al.[38] An evaluation of the stresses necessary to nucleate twins was provided by Luque et al. [39] who used molecular dynamics simulations on Mg single-crystal nanopillars.

To date, transverse twin propagation has attracted much less attention. To the authors' knowledge, Wang et al. [38] and Xu et al. [40] provided the only studies of this phenomenon. In both works, only $\{\bar{1}102\}$ twins were considered. In [40], a specific low-energy interface, which was systematically found at the front of the growing twin, is observed to drive transverse propagation. This interface places face-to-face a basal plane of the matrix and a prismatic plane of the twin (or vice versa) and is consequently referred to as prismatic-basal (PB) interface. This interface was also identified in [37] and observed experimentally in cobalt in [41]. One open question is whether a similar interface is involved in either the transverse propagation or the thickening of $\{\bar{1}101\}$ twins.

Twin thickening has been extensively studied and occurs through the propagation of disconnections along the twinning plane.[42–45] Disconnections are line defects characterized by a Burgers vector in the twin

interface and a step normal to the twinning plane. In the case of $\{\bar{1}101\}$ twins, Christian and Mahajan,[1] Serra et al.,[45] Serra and Bacon [46] and Wang et al. [47,48] reported the disconnections to be two or four crystallographic planes high. Similarly in the case of tensile twins, disconnections were fully characterized in work of Serra et al.,[45] Serra and Bacon [46] and Pond et al.[49]

The purpose of the present article is to rationalize the experimentally observed structural differences between $\{\bar{1}101\}$ and $\{\bar{1}102\}$ twins. To this end, molecular statics simulations were performed, using the embedded atom method interatomic potential developed by Liu et al.[50] First, twin transverse propagation is studied by extending the results of Xu et al. [40] to $\{\bar{1}101\}$ twins. In particular, we investigate whether a specific interface, analogous to the PB interface, exists for $\{\bar{1}101\}$ twins. The second part of this article focuses on thickening. Energies necessary to propagate two-layer and four-layer twinning disconnections are investigated on the two types of twin interfaces (i.e. $\{\bar{1}102\}$ and $\{\bar{1}101\}$). Our work points to an extrinsic growth mechanism for $\{\bar{1}101\}$ twins mediated by plasticity, while the growth mechanism of $\{\bar{1}102\}$ twins is compatible with an intrinsic mechanism (i.e. not mediated by the interaction with other defects).

2. Transverse propagation As stated above, our investigations start from the results obtained by Xu et al.[40] Since the real nature of twin nuclei is still unknown, twin transverse propagation was studied from two hypothetical initial nuclei. In this part, we first recall the results found in [40] for $\{\bar{1}102\}$ and apply a similar methodology to $\{\bar{1}101\}$ twins.

The first method to generate a nucleus consists in introducing a dipole of partial dislocations in a perfect crystal and letting the system relax under an applied shear strain via energy minimization. The Burgers vector of the partials, $\pm b_n$, matches the minimum of the γ -line calculated on the twinning plane along the $[1\bar{1}01]$ direction, as suggested by Wang et al.[38] Upon imposing a sufficiently large shear strain parallel to the twin interface, growth of the nucleus can be activated. The resulting twinned structure is bounded by $\{\bar{1}102\}$ and $(1\bar{1}02)$ planes and PB interfaces, as shown in Figure 1. The second type of nucleus created in [40] was inspired by Eshelby's inclusion problem.[51] The nucleus is obtained by cutting a sub-domain, applying mirror symmetry to the atoms inside the sub-domain and placing the atoms back in the original space with an additional strain applied to recover the initial shape of the sub-domain. Such nucleus was also found to grow under sufficiently large shear strains parallel to the twin plane. These two methods revealed the importance of PB interfaces to transverse propagation of $\{\bar{1}102\}$ twins in [40]. One particularly important feature is that PB interfaces readily form regardless of the method used to build the initial nucleus.

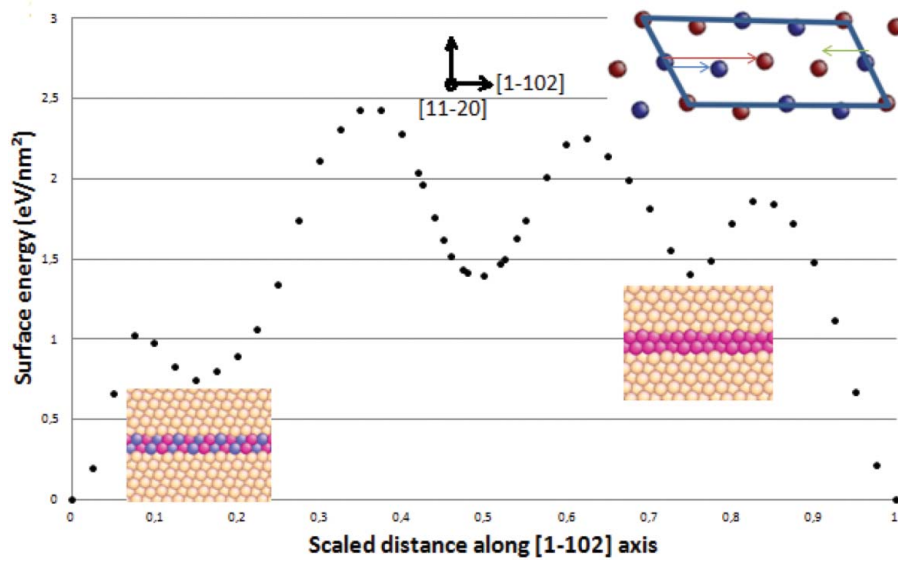


Figure 2. γ -line calculated in the $\{\bar{1}101\}$ twin interface along the $[1\bar{1}02]$ direction. Distances are given as a fraction of the length of the $[1\bar{1}02]$ vector. The atomic configurations correspond to the two stable stacking faults. The unit cell is given as an inset, arrows corresponding to the fault vector of the minima.

In the present letter, the two above methods were applied to $\{\bar{1}101\}$ twins. We first calculated the γ -line on the twinning plane along the $[1\bar{1}02]$ direction in order to apply the dipole method. The result is shown in Figure 2. The γ -line has three local minima, generically noted b_m , located at $0.17*[1\bar{1}02]$, $0.5*[1\bar{1}02]$ and $0.75*[1\bar{1}02]$, resulting in five potential Burgers vectors: $0.17*[1\bar{1}02]$ ($0.17-1$)* $[1\bar{1}02]$, $0.5*[1\bar{1}02]$, $0.75*[1\bar{1}02]$ and $(0.75-1)*[1\bar{1}02]$. For each minimum, we chose the lowest absolute value between b_m and (b_m-1) since the smaller b_m has a lower energy.

Referring to the unit cell in Figure 2, one can notice that all three minima correspond to displacements essentially positioning atoms at previously occupied sites, accordingly to the topological approach of Pond et al.[49] We then introduced the corresponding dipoles of partial dislocations into periodic cells of dimensions $58.8 \times 24.4 \times 0.32 \text{ nm}^3$, containing approximately 20,000 atoms. Unlike $\{\bar{1}102\}$ twins where there is a minimal length for the dipole that results in the growth of a twin, all dipole lengths provide the same result for the $\{\bar{1}101\}$ twin. The $0.17*[1\bar{1}02]$ Burgers vector results in a stable stacking fault of low energy, given by the absolute minimum of the γ -line. This Burgers vector is represented by the blue arrow in the unit cell given in Figure 2. The $0.5*[1\bar{1}02]$ Burgers vector, represented by the red arrow, yields an unstable structure, relaxing into the previously identified stable stacking fault outside of the initial dipole. The $(0.75-1)*[1\bar{1}02]$ Burgers vector, represented by the green arrow, results in another stable configuration but with a higher stacking fault energy. No dipole of partial dislocations thus leads to the formation of an incipient twin, even under applied shear strains up

to 10%. It is consequently not possible to use the dipole method to make a $\{\bar{1}101\}$ twin grow.

One may also wonder if a mechanism similar to the propagation of PB interfaces in $\{\bar{1}102\}$ twins could result in $\{\bar{1}101\}$ twin propagation. In order to search for potential low-energy interfaces that would be comparable to PB interfaces, we computed the energy of the twin interface as a function of its orientation with respect to the $\{\bar{1}101\}$ mirror plane, as done in [40] for $\{\bar{1}102\}$ twins. To do so, the first step is to be able to produce a twinned domain of arbitrary shape. For that, we noticed that a twinned domain can be obtained starting from a perfect crystal by propagating a screw dislocation of Burgers vector $[11\bar{2}0]/6$ every other dense pyramidal plane and letting the system relax. This is equivalent to propagating two-layer disconnections on the twinning plane, since the latter have the same $[11\bar{2}0]/6$ screw component and the edge component (approximately $0.16a$ in Mg [46]) that is necessary to recover the entire twinning dislocation forms during the energy minimization. We then created a cylindrical volume in which the interface between the matrix and the twin corresponds to a diameter of the cylinder (Figure 3). The energy of each interface was calculated by summing the energies of all atoms in the volume and subtracting their cohesive energy. Boundary effects were minimized by including the cylinder of interest (blue) in a larger one (red). The angle between the interface and the twinning plane is referred to as θ and we chose to set $\theta = 0$ when the interface coincides with the twinning plane. One obtains the energies of the interfaces as a function of their orientation with respect to the $\{\bar{1}101\}$ mirror plane by making θ vary between 0° and 180° (Figure 3(a)).

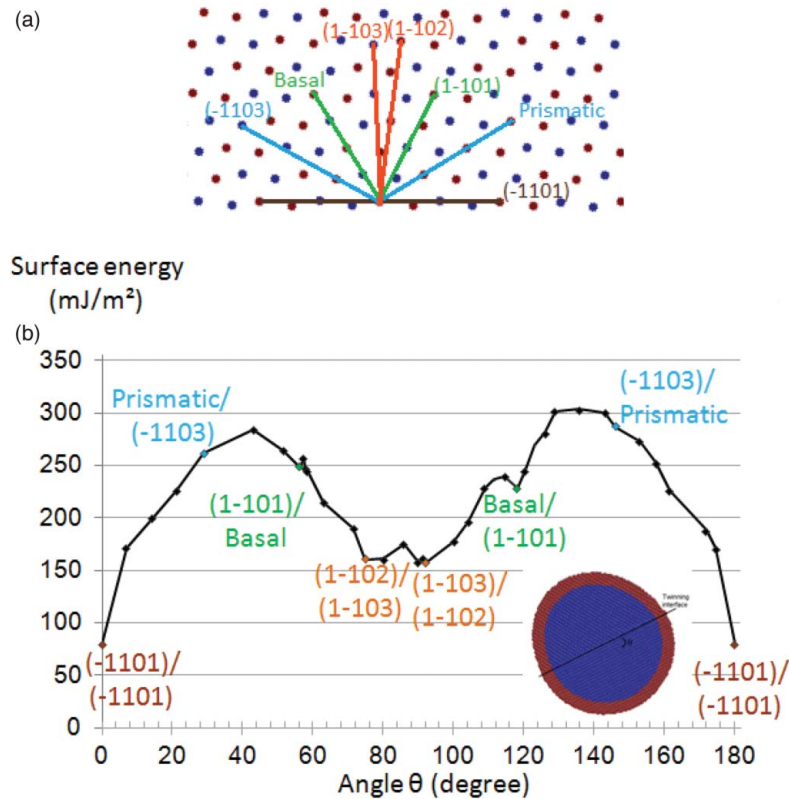


Figure 3. Planes with symmetry properties with respect to the normal to the $\{1\bar{1}01\}$ twinning plane (a) and energies of twinned interfaces as a function of their angle θ with respect to the horizontal $[1\bar{1}02]$ direction (b).

Several low-index planes are identified in Figure 3(a) that are close to symmetrical with respect to the normal to the twinning plane and result in particular interfaces. Such relationship between symmetrical planes is purely geometrical since symmetry operations with respect to the twinning plane or with respect to its normal result in the same crystal reorientation. The $\{1\bar{1}01\}$ mirror plane is the orientation of minimum energy. Three other pairs of particular conjugated planes were identified from Figure 3(a) and used as boundaries to build hexagonal twin nuclei with the method inspired from Eshelby's inclusion problem. $(1\bar{1}02)/(1\bar{1}03)$ interfaces were studied first since they are the second lowest energy interfaces. They are reminiscent of the PB interfaces for $\{1\bar{1}02\}$ twins since they correspond to marked minima in the energy curve. Prismatic/ $\{1\bar{1}03\}$ interfaces were investigated because of their high energy that suggests that they may be unstable. Finally, $(1\bar{1}01)/\text{basal}$ interfaces were considered since they are local minima and may present properties similar to PB interfaces.

Interestingly, regardless of the specific interfaces chosen to construct the twinned subdomain (i.e. high energy or low energy), the direction of the strain (i.e. shear strain or strain normal to the twinning plane or in the direction of the plane), the amount of strain (up to 10%) and the geometry of the nucleus (i.e. from 2-layers to more than 15-layers thick and from a ratio length/thickness

from about 2 to about 10), none of these nuclei grew. The fact that we did not succeed in making a $\{1\bar{1}01\}$ twin nucleus grow suggests that $\{1\bar{1}01\}$ twin transverse propagation might not be driven by a particular interface, in contrast with $\{1\bar{1}02\}$ twins.

3. Thickening As stated above, twin thickening is mediated by the propagation of disconnections on the twin interfaces. The rate of twin growth is then a direct consequence of (1) the geometrical characteristic of the disconnections (e.g. their Burgers vector and step height), (2) the process of disconnection generation and (3) the mobility of the disconnections. To appreciate the potential difference in growth rate of tensile and compressive twins, these three points are addressed in what follows.

The following potential thickening defects were considered: two-layer steps, four-layer steps and finite size interfaces. For the latter case, the PB interface was chosen for the $\{1\bar{1}02\}$ twin while the basal/ $(1\bar{1}01)$ interface—naturally forming as a result of energy minimization—was selected for the $\{1\bar{1}01\}$ twin, with either 6- or 8-layer thickness.

To study the steps, we consider a bi-crystal geometry illustrated in Figure 4 with one half of the crystal twinned with respect to the other half. Figure 4 is given as an illustration, however the real simulation cells were

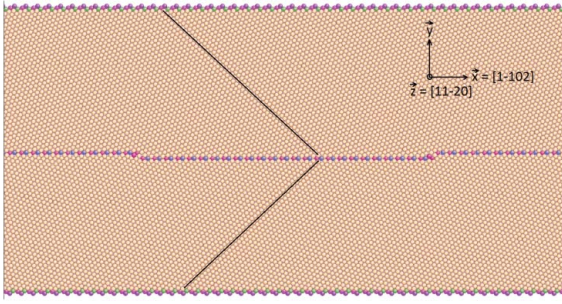


Figure 4. Simulation cell used to study the propagation of $\{\bar{1}102\}$ twins. The black lines indicate the orientations of the basal planes in the two parts of the crystal.

chosen large enough to avoid border effects and interaction between the steps. Due to the symmetry with respect to the twinning plane, periodic boundary conditions along the y -axis were removed. We introduced a pair of steps on the interface in order to maintain periodicity along the x -axis. The steps on the $\{\bar{1}101\}$ interfaces were created using the method described earlier in this letter. For $\{\bar{1}102\}$ twins, we repositioned the atoms as tracked by Wang et al. [37] during a nucleation event.

Following energy minimization, steps higher than two layers on $\{\bar{1}102\}$ twin interfaces systematically decompose into two-layer steps, even under an applied shear strain. This is particularly interesting as it shows that the stability of PB interfaces depends on the geometry of their extremities. Indeed, our calculations show that PB interfaces are not stable when they connect two parallel $(\bar{1}102)$ twin interfaces. However, they were found to be stable when they are connected with other PB interfaces or with $(\bar{1}102)$ conjugate planes, as seen in the nuclei of Figure 1. As a result, the PB interface cannot be regarded solely as a stack of two-layer disconnections. For the sake of the study on twin thickening though, in which case PB interfaces are unstable, the only defect pertaining to tensile twins considered in what follows is the two-layer step.

On $\{\bar{1}101\}$ twin interfaces, all steps reached stable configurations after relaxation. The four- and eight-layer steps were always stable, regardless of the amount and direction of the applied strain, while six-layer steps, depending on the initial configuration used before energy minimization—and in particular the initial position of the screw components of the disconnections—, may decompose into either a two-layer step and a four-layer step or into a two-layer step and an eight-layer step. Note that the later was found to be a stack of two four-layer steps.

The energies involved in disconnection generation were investigated using the nudged elastic band (NEB) method.[52] This method consists in minimizing the energy on intermediate configurations between an initial and a final state in order to identify the energy barrier to overcome when going from one state to the other. To study the nucleation of disconnections on both types

of interfaces, we started from a perfectly flat twin interface and ended with two steps—to be consistent with the periodic conditions (Figure 4). The energies necessary to create these two steps are given in Figure 5(a). We found that the energy barrier is about three times higher for $\{\bar{1}101\}$ twins so that it is easier for steps to nucleate on $\{\bar{1}102\}$ twin interfaces. The energies necessary to create these two steps are given in Figure 5(a). We found that the energy barrier is about three times higher for $\{\bar{1}101\}$ twins so that it is easier for steps to nucleate on $\{\bar{1}102\}$ twin interfaces. As a consequence, we infer that two-layer steps on $\{\bar{1}102\}$ twin interfaces may nucleate by an intrinsic process not requiring, for example, interaction of the interface with glide dislocations. The functional dependence of the step nucleation energy on stress will require further study to decipher the relative roles of stress and temperature on twin thickening. Note that such thermal effect may not exist for the generation of the twin nucleus. On the contrary, steps on $\{\bar{1}101\}$ twin interfaces are probably mediated by extrinsic defects, possibly the interaction and absorption of screw dislocations.[46,53,54]

Finally, we focused on the mobility of these disconnections by calculating the energies necessary for their propagation using the NEB method. These calculations, shown in Figure 5(b) and 5(c), revealed that the energy necessary to propagate four-layer steps on $\{\bar{1}101\}$ twin interfaces is about ten times higher than the energy necessary to propagate two-layer steps (Figure 5(b)), confirming the stability of four-layer steps. The different nature of the two kinds of steps is also underlined by a metastable configuration for four-layer steps that does not exist for two-layer steps. This type of curve is consistent with the results of Wang et al. [47] for two-layer steps. For four-layer steps, the order of magnitude differs and the metastable configuration is more pronounced in our case. We checked the accuracy of our calculations by running the simulations again using the potential developed by Sun et al. [55] and found a similar behaviour. The structure of the eight-layer step was identified to be equivalent to two superimposed four-layer steps of either the stable or the metastable configuration. The intermediate configurations computed by the NEB method reveal that the propagation of an eight-layer step is equivalent to the simultaneous propagation of two four-layer steps. The differences in energies involved in step propagation suggest that $\{\bar{1}101\}$ twin growth, which is already difficult to activate as discussed previously, is hindered by the stability of high steps. As a consequence, these twins appear to be thin.

The critical resolved shear stress associated with the propagation of two-layer steps on $\{\bar{1}101\}$ twin interfaces, directly measured by applying a shear stress to the simulation cell, was found to be 310 MPa with a positive stress and −400 MPa with a negative stress. The difference between these two values can be explained by the non-symmetric character of the step with respect to

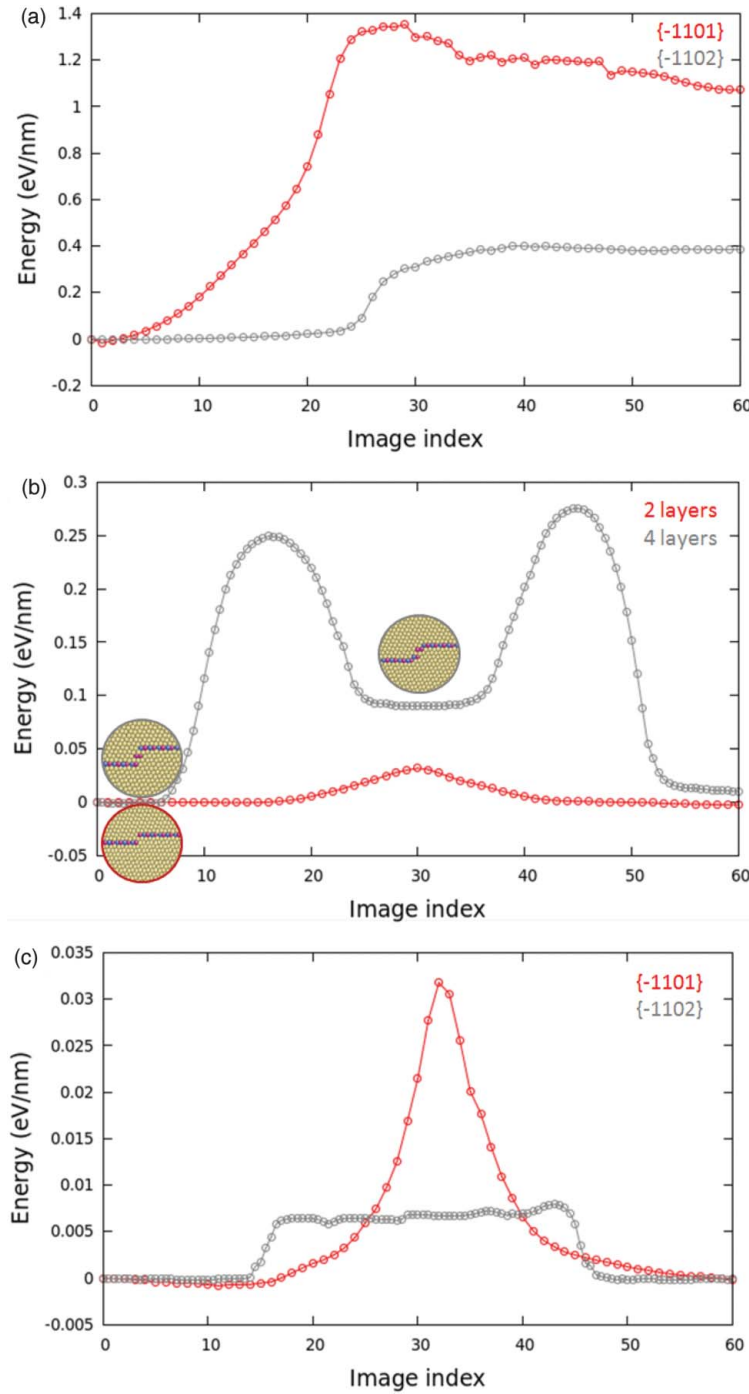


Figure 5. Energy necessary to nucleate two-layer steps on $\{\bar{1}101\}$ and $\{\bar{1}102\}$ twin interfaces obtained using the NEB method (a), propagation of two-layer and four-layer steps on $\{\bar{1}101\}$ twin interfaces with atomic configurations (b) and energy necessary to propagate two-layer steps on $\{\bar{1}101\}$ and $\{\bar{1}102\}$ twin interfaces (c).

the y-axis. Incidentally, this asymmetry may be related to detwinning. However, it has to be kept in mind that our simulations are conducted at 0 K, such that we have no temperature effect and in particular no effect of thermal activation on step mobility. Also, our calculations were performed in two dimensions, forcing the steps to move as straight lines, while in three dimensions, a

step may glide by a nucleation/propagation mechanism similar to the kink-pair mechanism of high Peierls stress dislocations.[56]

Regarding tensile twins, it was found that the energy barrier to be overcome to propagate two-layer steps on $\{\bar{1}102\}$ twin interfaces is about 0.007 eV/nm (Figure 5(c)), which is about four times lower than for

$\{\bar{1}101\}$ twins, hence its easy propagation. The associated critical resolved shear stress was found to be 190 MPa when we apply a positive stress and -230 MPa when the stress is negative. These values stay below the CRSS of $\{\bar{1}101\}$ twins, which is consistent with the lower energy involved in the propagation of this type of twins.

These energy considerations provide two more arguments in favour of the more frequent appearance of $\{\bar{1}102\}$ twins since it is easier both to nucleate and to propagate two-layer steps on their interfaces. Moreover, while four-layer steps on $\{\bar{1}101\}$ twin interfaces significantly hinders the growth process, four-layer steps on $\{\bar{1}102\}$ twin interfaces decompose into mobile two-layer steps, which profits to twin growth.

4. Conclusion The different natures of $\{\bar{1}101\}$ and $\{\bar{1}102\}$ twins have been underlined, providing an explanation to their experimentally observed differences. The transverse propagation of $\{\bar{1}102\}$ twins was found in [40] to be driven by the propagation of PB interfaces. By way of contrast, the new results presented earlier in the present article show that $\{\bar{1}101\}$ twin transverse propagation may not be driven by such a process, which increases the singularity of $\{\bar{1}102\}$ twins. Focusing on twin thickening, we found that the glide of two-layer steps is the main mechanism controlling growth in both cases. Energy considerations on step propagation revealed that it is much easier to nucleate and propagate steps on $\{\bar{1}102\}$ twin interfaces, pointing towards an intrinsic mechanism involving thermal activation. On the contrary, the nucleation of $\{\bar{1}101\}$ twins has to be mediated, possibly by the interaction with lattice dislocations or other twins.

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