Comment on "Atomic Shuffling Dominated Mechanism For Deformation Twinning In Magnesium"

Li and Ma [1] concluded on the basis of atomic-scale computer simulation that the mechanism of $\{10\bar{1}2\}$ twinning in hcp metals is not the motion of twinning dislocations (TDs) along the twin boundary (TB), but "atomic shuffling," since it "is unlikely that there could exist such a small partial dislocation" as that required to restore the lattice by shear. These conclusions are incorrect. Li and Ma have not understood the principles of interfacial dislocation theory, failed to report relevant experimental observations and computer simulations that confirm the TD mechanism, and misinterpreted their own simulations.

The topological character of TDs, i.e., their Burgers vector, $\boldsymbol{b}$, and step height, h, has long been appreciated [2]. Motion of a TD along a TB advances the interface by h. Atoms are relocated from matrix to twin sites by a combination of shear (magnitude b/h) and shuffling in the TD core. Use of the term "partial" dislocation in [1] is inadvisable. TDs are "perfect" in the sense that the interfacial structure is identical on either side of the discontinuity. $\boldsymbol{b}$ is the difference between two translation vectors, one each from the matrix and twin [3]. Use of the term "zonal" dislocation is also problematic. The current convention is to use h, as determined by the normal component of the two matrix/twin translation vectors.

It is incorrect to say that b for the $\{10\bar{1}2\}$ twin is too small to have physical significance. Indeed, Burgers vector would not be conserved in dislocation-twin interactions if $\boldsymbol{b}$ of TDs were neglected. Small b simply implies small shear. $\{10\bar{1}2\}$ TDs have been observed by high-resolution TEM [4,5]. Figure 1(a) shows such a defect in Zn: h is twice the spacing of the $\{10\bar{1}2\}$ lattice planes and $\boldsymbol{b}$ given by circuit mapping is $(c^2 - 3a^2)/(c^2 + 3a^2)[10\bar{1}\,\bar{1}]$, i.e., $b = 0.15a$ in Mg. These parameters are consistent with the known twinning elements [2]. This TD has also been studied by computer simulation, e.g., [5–7], and *ab intio* calculation [8]. It has a wide core ($\gg b$) and high mobility, despite the fact that only one in four atoms are moved to their correct sites by the twinning shear [2].

The $\{10\bar{1}2\}$ TD is actually present in the simulations in [1]. Figure 1(b) is taken from Fig. 2(a) of [1] and a circuit around the "step ... formed at the TB" has been superimposed. The labeling emphasizes the close resemblance to the experimental image. Thus, the "step" formed in [1] is not a pure step, for it also has dislocation character. Furthermore, inspection of the simulation movie provided at Ref. [22] in [1] reveals that the $\{10\bar{1}2\}$ TB is translated by h as a TD moves. We have annotated the movie frames by superimposing lines to indicate the location of the TB: the revised movie is at [9]. It is not known how this TD was formed in [1]. The model boundaries were free surfaces, but these can be avoided in a twinned model with periodicity [7], which allows TDs to glide over large distance and the TB to be displaced by h many times over.

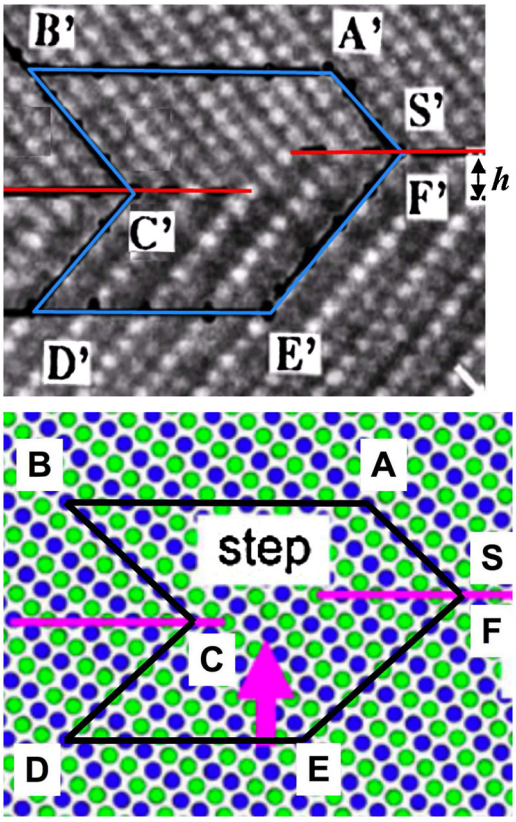

FIG. 1 (color online). Burgers circuit around (a) a $\{10\bar{1}2\}$ TD in Zn from [4] and (b) a "step" found in [1].

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Received 12 September 2009; published 15 January 2010
DOI: 10.1103/PhysRevLett.104.029603
PACS numbers: 61.72.Mm, 62.20.F−

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