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Towards resolving the anonymity of pyramidal slip in magnesium

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ABSTRACT

Plasticity in magnesium crystals oriented for *c*-axis compression has been usually attributed to $\langle c+a\rangle$ dislocation slip on second-order pyramidal $\{11\bar{2}2\}$ planes. Through molecular dynamics simulations, we investigated the formation and slip characteristics of $\langle c+a\rangle$ dislocations on second-order pyramidal planes. It is shown that the critical *c*-axis compressive stress for these dislocations is almost seven times that for $\langle c+a\rangle$ dislocations on first-order pyramidal $\{10\bar{1}1\}$ planes. In particular, it is concluded that first-order pyramidal near-screw $\langle c+a\rangle$ dislocations play a predominant role during the *c*-axis compression of magnesium crystals. Careful reexaminations of published experimental observations show good agreements with the current predictions.

1. Introduction

Hexagonal closed packed (HCP) crystals are anisotropic in their mechanical properties, and mostly exhibit limited ductility [1]. Pyramidal slip has been shown to be very important for improving the ductility of polycrystalline HCP materials. Both titanium [2] and zirconium [3] demonstrate good ductility through commonly observed first-order pyramidal slip. Furthermore, the addition of yttrium in magnesium (Mg) was shown to remarkably improve ductility compared to pure Mg through a high activity of both first-order and second-order pyramidal slips [4].

While Mg and its alloys have been extensively studied over the past few decades, there is still an ongoing debate on the nature of pyramidal slip in these crystals. Many conflicting experimental results have contributed to the confusions on whether $\langle c+a\rangle$ dislocation slip is predominant on first-order pyramidal $\{10\bar{1}1\}$ (Pyramidal-I) or second-order pyramidal $\{11\bar{2}2\}$ (Pyramidal-II) planes. These confusions either originated from incorrect analysis, or claims without sufficient supporting evidences.

One of the most widely cited experiments suggesting Pyramidal-II $\langle c+a\rangle$ slip during *c*-axis loading of Mg is based on surface slip trace analysis by Obara et al. [5]. Fig. 1(a) shows a reproduction of those slip traces nearly on the $\{1\bar{1}00\}$ surface after 2.9% strain at room temperature [5]. The authors have identified the horizontal slip traces coincide with basal slip, and the inclined slip traces make an angle of 55° on average with respect to the basal plane. Based on this, the authors have suggested that these inclined lines coincide with Pyramidal-II slip traces within 5° error. Similar slip trace angles were reported for ZK60 [6] and pure Mg [7] and were also suggested to coincide with Pyramidal-II slip. As shown in Figs. 1(b), (c), and Appendix A, by simple geometric analysis of the HCP lattice, the ideal angles for slip traces of Pyramidal-I and Pyramidal-II planes on the $\{1\bar{1}00\}$ surfaces are in fact 58.4° and 39.1°, respectively. This indicates the reported slip traces in [5–7] probably coincide with Pyramidal-I slip, and not Pyramidal-II slip as commonly cited.

It should be noted that Pyramidal-II slip traces were recently reported during *c*-axis compression of bulk Mg crystals [8]. However, their slip trace observations were performed on samples before yielding, which could suggest they are a result of sample preparation.

Pyramidal-II slip was also passingly suggested to occur in both bulk [9] and micro [10] Mg crystals during *c*-axis compression, while based on TEM observations of *c*-axis compressed micro-pillars, it was suggested that $\langle c+a\rangle$ dislocations may be on Pyramidal-I planes [11]. However, these conclusions are mostly speculative without any conclusive evidences. In addition, in the drop hammer tests of single crystal Mg, only twinning deformation was reported to be effective for *c*-axis compression [12].

Molecular dynamics (MD) simulations have showed that during *c*-axis compression and tension, $\langle c+a\rangle$ dislocations predominantly nucleate on Pyramidal-I planes from free surfaces and cavities [13–15], while discrete dislocation dynamics (DDD)

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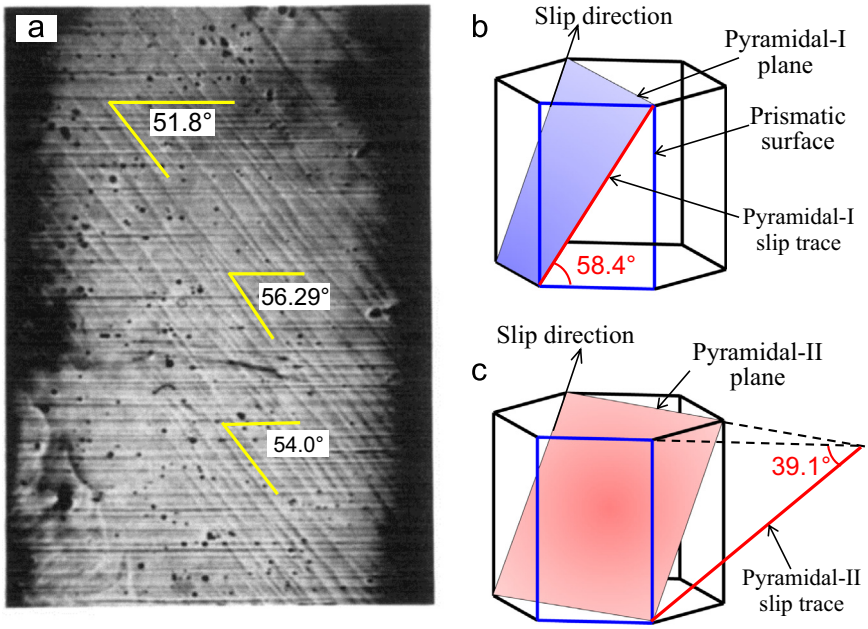

Fig. 1. (a) Slip bands nearly on $\{1\bar{1}00\}$ surface of a Mg single crystal after 2.9% compressive strain along the *c*-axis and at room temperature from Obara et al. [5]. Reprinted with permission from Elsevier Limited. (b, c) Schematics of slip trace angles of Pyramidal-I and Pyramidal-II planes on the $\{1\bar{1}00\}$ surface, respectively. See Appendix A for full schematics of all possible slip trace angles.

simulations support Pyramidal-II slip [16–18]. On the other hand, the transition of slip from Pyramidal-I to Pyramidal-II planes was shown to be plausible through cross-slip or cooperative slip at high applied stresses [13]. These results also agree with the analytical stochastic model proposed by Zhang et al. [19].

These disagreements in experiments and simulations indicate the necessity to critically reevaluate our understanding of pyramidal slip in Mg. This is particularly important since confusions over which slip plane is predominant can lead to inaccuracies in predicting the mechanical response of Mg and its alloys. As such, the aim of this study is to address the perplexing nature of pyramidal slip in magnesium.

2. Simulation methods

MD simulations are utilized to study dislocation slips on both Pyramidal-I and Pyramidal-II planes. These simulations are performed using the MD simulator LAMMPS [20]. Two modified embedded atom method (MEAM) potentials developed by Kim

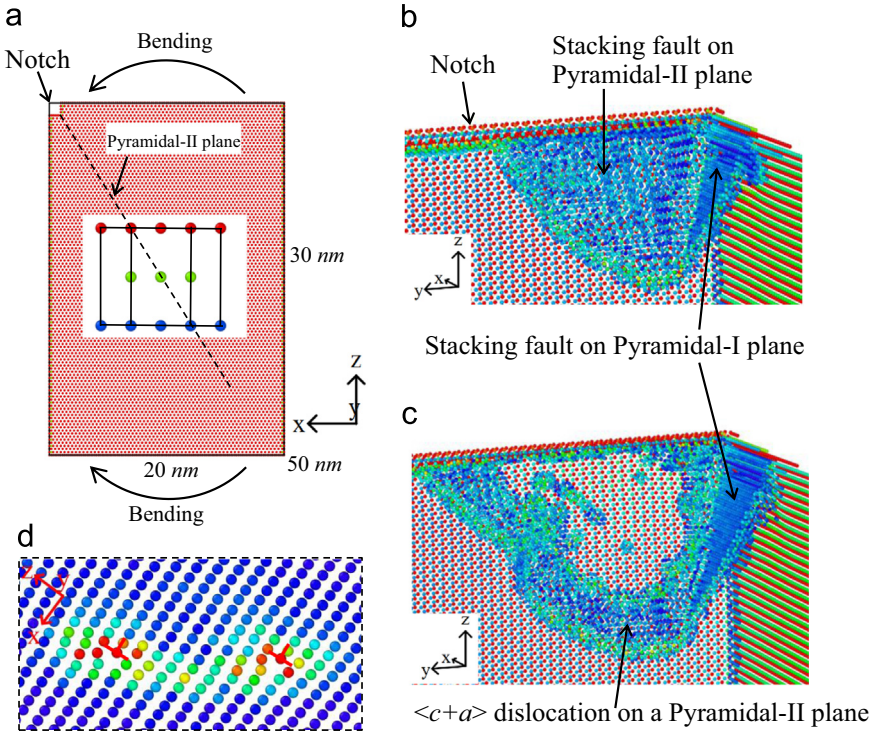

Fig. 2. Nucleation of Pyramidal-II $\langle c+a \rangle$ dislocations from free surfaces during bending simulations: (a) schematic of the simulation cell; (b, c) nucleating Pyramidal-II dislocations; and (d) the core of the nucleating Pyramidal-II $\langle c+a \rangle$ dislocation. The inverted "T" indicates the location of the leading and trailing partial dislocations.