Structure, Energetics, and Transformations of $\langle \mathbf{a} \rangle$ and $\langle \mathbf{c}+\mathbf{a} \rangle$ Dislocations in HCP Metals

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HCP metals such as Ti, Mg, and Zr are of high technological importance, but the mechanisms of deformation are complex due to the HCP crystal structure. Fundamental understanding of the dislocations in HCP metals is thus lacking, particularly for the $\langle \mathbf{c}+\mathbf{a} \rangle$ dislocations. The $\langle \mathbf{c}+\mathbf{a} \rangle$ slip is the only mode capable of providing slip in the crystallographic $\langle \mathbf{c} \rangle$ direction, and is therefore essential to enabling generalized plastic flow in polycrystalline HCP metals. Here, we present a systematic study of slip modes, and the competition and transformation between different possible dissociated dislocation structures having the same Burgers vector. We first present careful DFT results on the stacking fault energies for the basal, prism, and pyramidal I and II systems, which is a first step toward rationalizing operative slip systems in each individual HCP metal. Results show that the $\langle \mathbf{c}+\mathbf{a} \rangle$ stacking fault involves significant multi-plane relaxations, such that standard methods to compute the γ surface are inadequate. We then use anisotropic elasticity to analyze competing dissociation paths for full $\langle \mathbf{a} \rangle$ and $\langle \mathbf{c}+\mathbf{a} \rangle$ dislocations. We show that both Pyr. I mixed and Pyr. II edge dislocations should undergo a transformation from dissociation on the Pyramidal plane to dissociation along the basal plane separated by a basal stacking fault, with the resulting dislocation being immobile. This prediction explains experimental observations in Mg, Ti, Ti-Al, and Zr. Direct MD studies using a validated interatomic potential for Mg show the thermally activated transition directly, with a relatively small energy barrier, thus rationalizing the proliferation of such dislocations in Mg and the consequential rapid strain hardening and low ductility in Mg. The analysis also shows the energy difference between Pyr. I and II screw dislocations, which determines the ability of $\langle \mathbf{c}+\mathbf{a} \rangle$ dislocations to cross-slip. The analysis further shows that the Pyramidal screw dislocations dissociate into pure or nearly-pure screw partials. An NEB analysis in Mg then shows that $\langle \mathbf{c}+\mathbf{a} \rangle$ cross-slip occurs by a mechanism entirely different than that in fcc metals (which also have dissociated partials). In Mg, cross-slip barriers are also found to depend on non-Schmid/non-Escaig stresses, thus affecting the relative prevalence of Pyr. I vs. Pyr. II slip in Mg, and explaining tension/compression asymmetry in the Pyramidal slip deformation of Ti. All of these results point toward directions for alloy design to prevent unfavorable phenomena and encourage favorable phenomena, so as to achieve desired strength and ductility in HCP alloys. Overall, our studies demonstrate how the combination of density functional theory, anisotropic elasticity, and targeted molecular simulations can provide in-depth insight into competing slip modes in complex metals.

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