# Mg prismatic and basal dislocation/solute interactions from first principles

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New lightweight, ductile, strong Mg alloys which can be formed at room temperature are of considerable interest to the transportation industry for improved fuel economy. In Mg, the prismatic slip system is two orders of magnitude stronger than the basal slip system resulting in low ductility. Accurate first-principles calculations of dislocation cores on the basal and prismatic systems provide useful information for improving ductility. We present first-principles calculations of relaxed $a$-type basal edge and screw dislocations, a relaxed $a$-type prismatic edge and a constricted $a$-type screw dislocation which is constrained such that cross-slip on the prismatic plane is possible. The atomistic basal dislocation geometries provide the basis for a quantitative solute/dislocation interaction prediction from size and stacking fault energy changes. We use this data to construct a solute-strengthening "design map" for Mg in the basal plane based upon Fleischer's weak obstacle strengthening model[1]. The constriction energy is extracted by comparing the two core energies using the energy density method[2], and compared to *in situ* experimental data[3] using the Friedel-Escaig cross-slip model. Direct Al interaction with the prismatic edge core and the constricted screw geometries are also computed for comparison.

[1] R. L. Fleischer, *The Strength of Metals* (Reinhold, 1964), chap. 3, pp. 93–140.

[2] M. Yu, D. R. Trinkle, and R. M. Martin, in preparation (2010).

[3] A. Couret, and D. Caillard, Acta Metall. 33, 1455 (1985).