A First-principles Study of Twin Boundary and Surface Energies of Magnesium Alloys

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Magnesium (Mg) and its alloys have attracted much attention as a potential candidate for light-weight mobility and energy-related applications. For wide industrial application of Mg, the poor formability at room temperature should be improved. It has been reported that the addition of rare earth elements in solid solution improves the mechanical properties. In this study, we investigate effects of solute atoms on twin boundaries and surfaces of Mg alloys by using first-principles calculations. Solute atoms are stable or unstable at the twin boundary sites, depending on the atomic radius. The interaction of solute atoms and twin boundaries could suppress migration of the twin boundaries. On the other hand, the surface energy is lower for the basal, prism, and {10-11} planes than for the {10-12} and {11-22} planes. The surface energies are varied by solute atoms and the qualitative trend is related to the difference in the valence electron density between Mg and the solute element solid.

Keywords: First-principles calculations, Magnesium, Twin boundary, Surface energy