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First-principles study of energy, structure and atomic solubility of twinning-associated boundaries in hexagonal metals ANIL KUMAR, JIAN WANG, CARLOS TOME, Los Alamos National Laboratory — HCP metals are widely used as structural materials in many industries, ranging from transport and energy to biomedical applications due to their low density, high specific strength. Twining is one of the important plastic deformation modes in HCP metals. Understanding atomic structure and chemistry of twin-associated boundaries is very crucial to improve mechanical properties of these HCP metals. In this work, using first-principles density function theory, we study twinning-associated boundaries (TBs), $\{10\bar{1}n\}$ coherent twin boundaries (CTBs) and coherent basal-prismatic boundary (CBP) in six hexagonal metals (Cd, Zn, Mg, Zr, Ti and Be), with a focus on structure and solute's solubility at twin boundaries. We find that the formation of TBs is associated with creation of an excess volume. All the six metals show positive excess volume associated with $(10\bar{1}1)$ and $(10\bar{1}3)$ CTBs, but the excess volume associated with $(10\bar{1}2)$ CTBs and CBP can be positive or negative depending on metal. To understand solubility at TBs, we calculated solubility of solute atoms in Mg, Ti, and Zr for solute positions in bulk, $(10\bar{1}2)$ CTB and CBP boundaries and show that, in general, solute atoms have better solubility at CTB and CBP than in bulk.

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