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Atomistic analysis of short range interaction and local chemical order in LPSO structures of Magnesium alloys MARCO FRONZI, HAJIME KIMIZUKA, KAZUKI MATSUBARA, SHIGENOBU OGATA, Osaka University — Magnesium alloys have been object of interest as lightweight material with high strength weight ratio. In particular Long Period Stacking Ordered (LPSO) structure phases show to have a strong influence in enhancing mechanical properties of such kind alloys. However the chemical order of the interacting atomic species in the Mg lattice has not been fully understood. We perform first principles Density Functional Theory (DFT) calculation to compute formation energies as well as interaction energies of the doping atoms in both Faced Centered Cubic (FCC) and Hexagonal Close Packed (HCP) Mg lattices. In particular we consider the Mg-Al-Gd and Mg-Zn-Y ternary systems. We also calculate activation energies for vacancy assisted doping atoms diffusion in order to perform a further analysis of the kinetics of the process. In order to describe short range interaction and cluster formation in the Mg matrix, we build an on lattice potential based on first principles DFT interaction energies. By means of these inter-atomic potentials, we perform Monte Carlo simulations to analyze the chemical order occurring in LPSO Mg-Al-Gd structures.

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