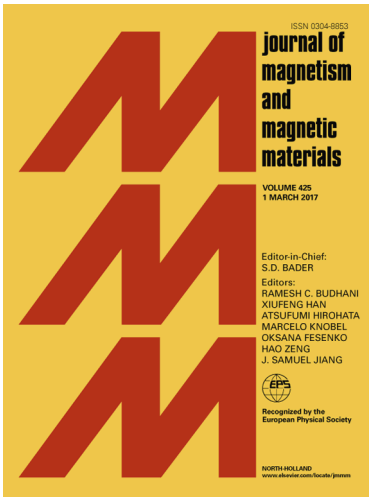

Prediction of possible martensitic transformations in all-*d*-metal Zinc-based Heusler alloys from first-principles

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Prediction of possible martensitic transformations in all-*d*-metal Zinc-based Heusler alloys from first-principles

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Several newly designed Zinc-based all-*d*-metal Heusler alloys have been predicted, and their XA- and $L2_1$-type atomic-site preferences, electronic structures, magnetic properties, as well as their possible martensitic phase transformations, have been studied theoretically from first principles. For cubic-type Zn_2MMn (M = Ru, Rh, Pd, Os, Ir) alloys, their $L2_1$-type phase is more stable than the XA phase, that is, the two Zn atoms prefer to locate at the A (0,0,0) and C (0.5, 0.5, 0.5) positions in the lattice. Their magnetic state is ferromagnetic (FM), with a large total magnetic moment (>3 μ_B/***f.u***), and the total magnetic moment arises mainly from the Mn atom due to its strong exchange splitting. Remarkably, Zn_2MMn alloys with a tetragonal martensitic structure can lower their total energies and show more stable behaviour than cubic systems. The energy difference ΔE_M is defined as the difference in total energy between the martensitic and cubic states. ΔE_M can be tuned under uniform strain, namely, as the lattice constant increases, ΔE_M also increases. Moreover, in the case of martensitic-type Zn_2RuMn and Zn_2OsMn alloys, quite large c/a ratios (1.41, 1.43, respectively) can be found, which is preferable for the transformation strain effect. It is hoped that this work can motivate researchers to look for new spintronic and magnetic-intelligent materials among all-*d*-metal Heusler alloys.