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Pathways for tailoring the magnetostructural behavior of FeRh-based systems[1]

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The prediction of phase transition temperatures in functional materials provides dual benefits of supplying insight into fundamental drivers underlying the phase transition, as well as enabling new and improved technological applications that employ the material. In this work, studies focused on understanding the magnetostructural phase transition of FeRh as a function of elemental substitution, provides guidance for tailoring phase transitions in this compound, with possible extensions to other intermetallic-based magnetostructural compounds. Clear trends in the magnetostructural temperatures (T_t) of alloys of composition $Fe(Rh_{1-x}M_x)$ or $(Fe_{1-x}M_x)Rh$ (M = 3d, 4d or 5d transition metals), as reported in literature since 1961, were identified and confirmed as a function of the valence band electron concentration (($s+d$) electrons/atom) of the system. It is observed that substitution of 3$d$or 4$d$elements ($x \leq 6.5$ at%) into B2-ordered FeRh compounds causes $T_t$to increase to a maximum around a critical valence band electron concentration (e_v*)of 8.50 electrons/atom and then decrease. Substitution of 5$d$elements echoes this trend but with an overall increase in $T_t$and a shift in $e_v*$to 8.52 electrons/atom. For e_v>8.65 electrons/atom, FeRh-based alloys cease to adopt the B2-ordered crystallographic structure in favor of the chemically disordered A1-type structure or the ordered $L1_0$-type structure. This phenomenological model has been confirmed through synthesis and characterization of FeRh alloys with Cu, Ni and Au additions. The success of this model in confirming existing data trends in chemically-substituted FeRh and predicting new composition-transition temperature correlations emphasizes the strong interplay between the electronic spin configuration, the electronic band structure, and crystal lattice of this system. Further these results provide pathways for tailoring the magnetostructural behavior and the associated functional response of FeRh-based systems for potential technological applications.

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