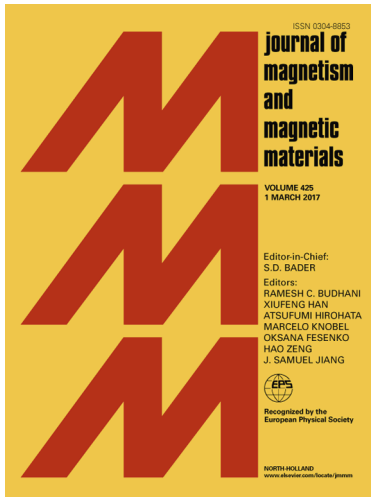

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Electronic structure and magnetic properties of manganese-based $MnAs_{1-x}P_x$ ternary alloys

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Abstract

Full potential band structure calculations have been performed on the NiAs (hexagonal), MnP (orthorhombic) and Zinc-blende structures of $MnAs_{1-x}P_x$ ($0\leq x\leq 1$) alloys. The stability of the ferromagnetic state is investigated by comparing the total energies for paramagnetic (P), ferromagnetic (F) and antiferromagnetic (AF) state, where different types of AF state are assumed. The stability of the different phases of $MnAs_{1-x}P_x$ ($0\leq x\leq 1$) is found to depend mainly on the volume and on the amount of magnetic order. It is found that for large lattice constants the ferromagnetic state is favored, whereas for small lattice constants different antiferromagnetic states can be stabilized. In the ferromagnetic state, the structure with minimal energy is always hexagonal, whereas it becomes orthorhombically distorted under pressure. The calculated total magnetic moment can be explained from the large charge transfer of electrons from the Mn cations to their neighbor As and P anions, and the strong p (As or P)-d(Mn) hybridization. We found that a particular Mn-Mn separation plays also the significant role in determining the change from antiferromagnetic to ferromagnetic order in such systems. It is also found a true half-metallic phase for zinc-blende MnAs and $MnAs_{0.75}P_{0.25}$ when the lattice constant expanded beyond 5 Å, otherwise, $MnAs_{1-x}P_x$ ($0\leq x\leq 1$) alloys were found to be metals.

Keywords: First-principle study; LAPW; Phase transition; alloying; magnetic stability

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