Ferromagnetism and half-metallicity of some 3- and 4-*d* transition metal alloys

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We have studied the occurrence of half-metallic (HM) ferromagnetism in some binary and ternary alloys containing 3- and 4-*d* transition metals, with a view to their potential application in spintronics. Among the 3-*d* binary alloys we present results for some Cr-based chalcogenides and pnictides (CrX, X=AS, Sb, S, Se, Te) in zinc blende (ZB) structure, which show the promise of robust half-metallic ferromagnetism with regard to both lattice parameter variation and the Curie temperature Tc. The exceptions occur for the alloys involving S, Se and Te at some low values of lattice parameters, where significant inter-atomic antiferromagnetic exchange interactions indicate ground states to be either antiferromagnetic or of complex magnetic nature. A comparison of total energies for the ferromagnetic (FM), disordered local moment (DLM), and three ZB antiferromagnetic configurations (AFM[001], AFM[110, and AFM[111]) show the lowest energy configuration to be AFM[111] for CrS and CrSe for compressed lattice parameters. The mixed pnictide-chalcogenide alloys $CrAs_{50}X_{50}$ (X=Sb, S, Se and Te) do not show any tendency to antiferromagnetic spin fluctuations for the entire range of the lattice parameter studied. For CrTe, a comparison of ZB, rock salt (RS) and NiAs-type hexagonal structures and total energy comparison for the FM, and AFM configurations shows the lowest energy configuration to be FM in all the three structures. The RS phase is found to be more stable than the ZB phase. Although both ZB and RS structures exhibit HM behavior, ferromagnetism is stronger with a higher Tc in the RS phase.

Among the 4-*d* transition metals we consider Tc-based binary alloys TcC, TcSi and TcGe in hypothetical ZB structure. Among the three, magnetism is found to be most robust in TcGe, in the sense that the magnitude of the moment for a given lattice parameter in TcGe is more or less independent of the magnetic configuration. The FM state is found to be energetically favorable to the NM and the AFM states. Exchange calculations show that the magnetism is dominated by nearest neighbor interaction. Estimated Curie temperatures lie in the range ~100K, 200K and 300K for TcC, TcSi and TcGe, respectively.

Another system studied was the semiconductor GeTe in both ZB and RS structures doped with the 3-d transition metal alloys: V, Cr, and Mn. For both structures, it is the Ge sublattice that is doped with the transition metals. Some of these compounds are found to be half-metallic at their optimized cell volumes. The Cr-doping case is the most promising, as in both RS and ZB structures FM interactions dominate, and these remain FM with changes in the lattice parameter. The next promising case is V-doping in the ZB structure, the RS counterpart showing strong AFM interactions, particularly at and around the equilibrium lattice parameter. These AFM interactions weaken on both sides of the equilibrium lattice parameter value and become FM only at much higher volume. Our calculations for $Ge_{75}Mn_{25}Te$ shows the substance to be AFM (for the ordered as well as disordered compounds, with the gap being narrower in the disordered case). We show that this AFM behavior is linked to the substance being a narrow/zero gap semiconductor/semimetal at this Mn concentration. We further establish that the presence of uncompensated carriers should drive the material toward ferromagnetism. The origin of these carriers could be vacancies, impurity atoms, and/or structural imperfections.