

Magnetic Tunnel Junctions II: Half Metallic Ferromagnets

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Half-metallic ferromagnetism in hypothetical semi-Heusler alloys NiVM ($M=P, As, Sb, S, Se, \text{ and } Te$)

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A theoretical study based on first-principle band-structure calculations is carried out for the hypothetical semi-Heusler alloys NiVM ($M=P, As, Sb, S, Se, \text{ and } Te$). For all compounds it is found that the ferromagnetic state is more favorable than the paramagnetic state. NiVAs is predicted to be a half-metallic ferromagnet with a small half-metallic gap of 0.07 eV and an integer magnetic moment of $2 \mu_B$, and NiVP and NiVSb are so-called nearly half-metallic ferromagnets. Furthermore, we find a clear indication that the substitution on the sp atoms influences the hybridization between Ni and V atoms, and can even destroy the half metallicity. © 2004 American Institute of Physics. [DOI: 10.1063/1.1687232]

I. INTRODUCTION

Half-metallic ferromagnets (HMFs), i.e., where one spin band semiconducts with a gap at the Fermi level E_F , while the other spin band behaving like a metal, have attracted increasing interest, since they are expected to be utilized as the ideal materials in spintronic applications. HMFs have been theoretically and experimentally predicted for some Heusler alloys,¹ transition oxides,^{2,3} perovskite manganites, zinc-blende transition-metal pnictides, and transition-metal chalcogenides,^{4,5} and others. Unfortunately, there are some disadvantages in the aforementioned materials, i.e., the Curie temperature of diluted magnetic semiconductors is so low that they have failed in the practical sense,⁶ the spin-polarization decreases sharply with increasing temperature,² and the half-metallic (HM) phases are difficult to obtain due to the high energy barrier with their ground states,⁷ which result in the fact that these materials are not successfully used in spintronics applications until now.

This motivates us to search for new candidates of HMFs in semi-Heusler alloys of the type NiVM ($M=P, As, Sb, S, Se, \text{ and } Te$) by using the first-principle band-structure calculations, since the close structural similarity between the zinc-blende semiconductors and the semi-Heusler alloys makes

the semi-Heusler alloys compatible with the existing conventional semiconductor technology.

II. COMPUTATIONAL DETAIL

First-principles electronic band-structure calculation in the present article is based on the density-functional theory (DFT) within the local spin density approximation (LSDA) for the exchange-correlation potential.⁸ We use the full-potential linearized augmented-plane-wave (LAPW) plus local orbitals method,⁸ where the potential and/or the charge density in the crystal are treated with no shape approximation. The relativistic effect is taken into account in the scalar style except for the spin-orbital coupling. Inside the atomic spheres the charge density and the potential are expanded in cubic harmonics up to $l=6$. The radial basis functions of each LAPW are calculated up to $l=8$ and the nonspherical potential contribution to the Hamilton matrix has an upper limit of $l=4$. The Brillouin-zone integration is done with a modified tetrahedron method⁹ and we use 3000 k points in the Brillouin zone. The density plane-wave cutoff is $RK_{\max}=8.0$.

III. RESULTS

We calculate the total energy as a function of the lattice parameter for the paramagnetic and ferromagnetic configura-

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TABLE I. Calculated properties of NiVM ($M=P, As, Sb, S, Se,$ and Te): equilibrium lattice parameter a_0 of ferromagnetic phases, energy difference ΔE between the paramagnetic states and the ferromagnetic states, spin magnetic moments in μ_B , band gaps and HM gaps.

	a_0 (nm)	ΔE (eV)	$m^{spin} (\mu_B)$			Total (μ_B)	Band gap (eV)	HM gap (eV)
			Ni	V	M			
NiVP	0.566	0.17	0.16	1.64	-0.04	1.76	0.74	
NiVAs	0.585	0.30	0.10	1.94	-0.04	2.00	0.35	0.07
NiVSb	0.589	0.28	0.11	1.85	-0.06	1.90	0.33	
NiVS	0.559	0.07	0.23	2.18	0.04	2.46	0.79	
NiVSe	0.580	0.30	0.14	2.58	0.02	2.73	0.46	
NiVTe	0.584	0.32	0.19	2.43	-0.01	2.62	0.41	

rations. The predicted equilibrium lattice constants and the energy differences between the paramagnetic and ferromagnetic phases are tabulated in Table I. We find for all cases the ferromagnetic phase to be more favorable in energy than the corresponding paramagnetic phase. It is worth noting that all the energy differences are small, therefore, it may be difficult to obtain the single-phase ferromagnetic state in practice, especially for NiVS.

Figures 1 and 2 show the spin-dependent density of states (DOS) and energy band for NiVAs. As seen in Fig. 1, the As atoms provide s - p states to hybridize with d electrons and determine the degree of occupation of the p - d orbitals. In the majority-spin component, V $3d$ states are mostly occupied and hybridized with Ni $3d$ electrons; in the minority-spin part, local and mostly nonhybridized V $3d$ states are found at about 1 eV above E_F . In Fig. 2, at about -3.5 eV the threefold bands are mainly due to As p electrons that transform following the Γ_{15} representation and have a strong admixture of Ni d states. The next twofold Γ_{12} bands at

about -2.7 eV mainly originate from the Ni $3d$ electrons. Finally, in the minority bands the threefold Γ_{15} bands just below E_F are created by the bonding t_{2g} states of Ni and V with a small part of As p states. Above the band gap antibonding twofold $V e_g \Gamma_{12}$ states and threefold $t_{2g} \Gamma_{15}$ states can be found. It is clear that the majority-spin band is strongly metallic, while the minority-spin band shows a semiconducting gap, 0.35 eV, around E_F . Unfortunately, the HM gap is only 0.07 eV, which results in an unstable half metallicity, which will be lost for any contraction of the lattice or atomic disorder, but obviously a lattice expansion will make the half metallicity more robust.⁷ The origin of the gap is mainly attributed to the covalent hybridization between the d states of the Ni and V atoms, leading to the formation of bonding and antibonding bands with a gap in between. The bonding hybrids are localized mainly at the Ni atoms whereas the antibonding states are mainly at the V sites.

Figure 3 shows the spin-dependent DOS of NiVM ($M=P, Sb, S, Se,$ and Te). The band gaps, HM gaps, and spin magnetic moments are tabulated in Table I. Since the Fermi levels of NiVP and NiVSb are both located in the conduction

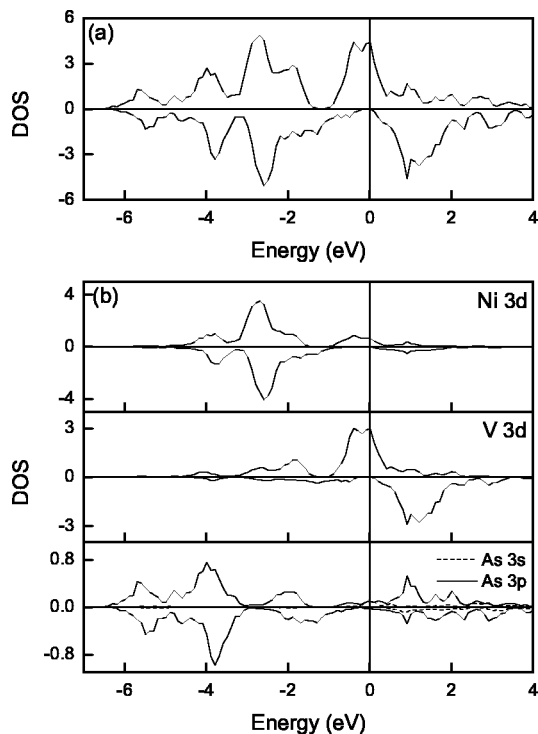


FIG. 1. The spin-dependent total (upper panel) and partial (lower panel) DOS of NiVAs at its predicted equilibrium lattice constant. There is a gap of around 0.35 eV around the Fermi level for the minority-spin bands.

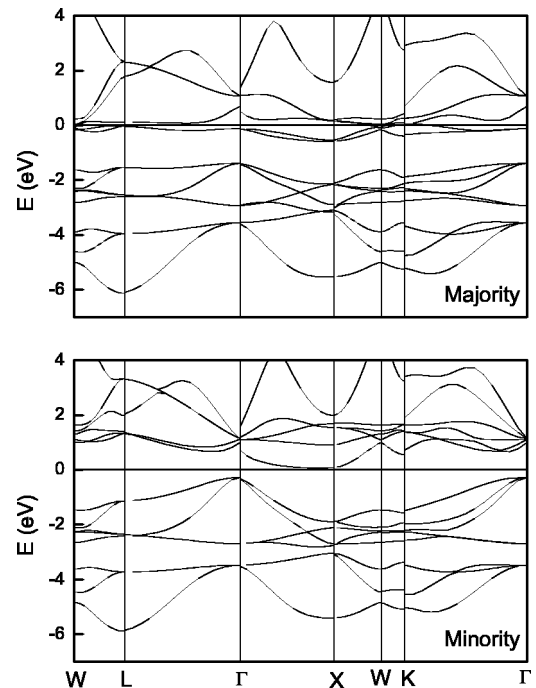


FIG. 2. Band structure of NiVAs as calculated for the predicted equilibrium lattice constant.

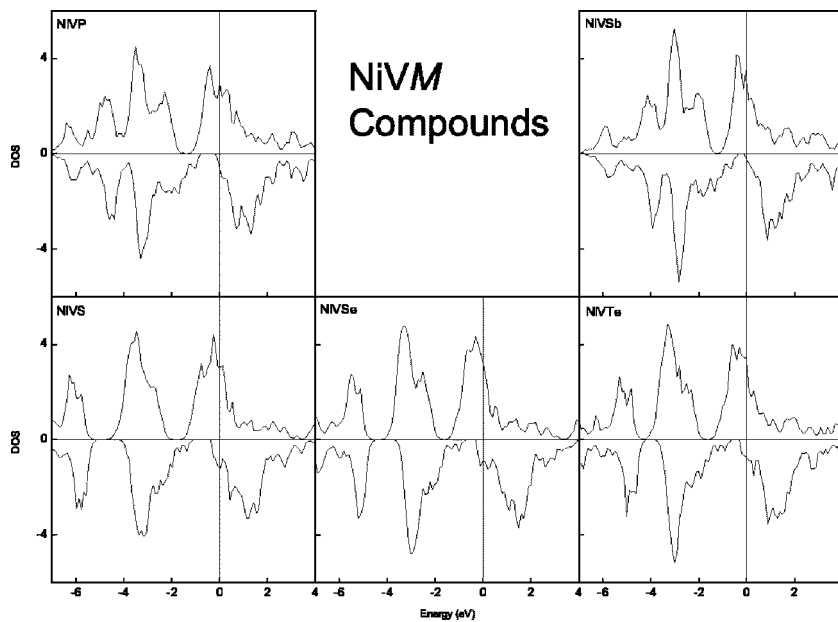


FIG. 3. The spin-dependent total DOS of NiVM ($M = \text{P, Sb, S, Se, and Te}$) as calculated for their predicted equilibrium lattice constants.

bands, but are very close to the right edge of gaps, NiVP and NiVSb are so-called nearly HMFs. In contrast, the minority-spin DOS at the Fermi level of NiVS, NiVSe, and NiVTe are all relatively high, which implies that NiVS, NiVSe, and NiVTe do not display half metallicity. In the rigid-band regime, obviously the half metallicity will be reobtained when the lattice is expanded for NiVP, NiVSb, NiVS, NiVSe, and NiVTe.⁷ Hence, they may still be useful for spintronic applications when the appropriate substrates are chosen.

As seen in Figs. 1 and 3, the DOS of these compounds are mainly characterized by the large exchange splitting of the Vd states, which leads to the localized spin moment at the V site. In HMFs, the total magnetic moment should be an integer. As given in Table I, we notice that the total magnetic moment per unit is an integer Bohr magneton, $2\mu_B$, for NiVAs, which is in agreement with the aforementioned HM behavior. Asada *et al.*,¹⁰ Continenza *et al.*,¹¹ and Zhao *et al.*¹² have all reported that the LSDA calculated magnetic moments at fixed volume are always smaller (not more than 5%) than the corresponding experimental values. Hence, we think that NiVSb may still turn out to be a HMF. We suppose that a more accurate result can be expected if a better BZ k -point sampling (more k points are involved) is adopted. It is worth noting that for these compounds the spin moments of Ni and V are inversely proportional. This is due to the fact that the weaker hybridization between Ni and V results in a smaller Ni spin moment and a bigger V spin moment, and eventually makes the V moment more localized. The substitution of sp atoms produces similar DOS and leads to a shift of the Fermi levels, thus the change of sp atoms can destroy the half metallicity, but the substitutions of sp atoms are not responsible for the occurrence of the band gap since all compounds have gaps near the Fermi levels.

IV. CONCLUSION

We have investigated the electronic band structures for the semi-Heusler alloys NiVM ($M = \text{P, As, Sb, S, Se, and}$

Te) to search for new HMFs. The total-energy calculations show that for all compounds the ferromagnetic state is more favorable than the paramagnetic state. We predict that NiVAs is likely to be a true HMF and NiVP and NiVSb are nearly HMFs. The substitution of sp atoms can kill the half metallicity.

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