

Density-Functional-Theory Study of Cohesive, Structural and Electronic Properties of Ni-Sb Intermetallic Phases

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Abstract This work has its roots in a long-term theoretical research line aimed at developing a complete database with structural, thermodynamic, cohesive and elastic properties of the intermetallic compounds (ICs) of the type Me_aX_b , where $Me = Cu, Ni$ and $X = In, Sn$ and Sb . The paper reports the results of an ab initio study of various phases occurring in the Ni-Sb phase diagram, viz., the low-temperature Ni_3Sb (orthorhombic oP8), the high-temperature Ni_3Sb (cubic cF16), Ni_5Sb_2 (monoclinic mC28), $NiSb$ (hexagonal hP4) and the $NiSb_2$ (orthorhombic oP6) compounds. The molar volume, bulk modulus and its pressure derivative, the electronic density of states (DOS) and the energy of formation from the elements of these compounds

are calculated ab initio using the relativistic projected augmented wave (PAW) method implemented in the VASP code. The Local Density Approximation of Ceperley and Alder and the Generalized Gradient Approximation due to Perdew and Wang are adopted to treat the exchange and correlation energies. Detailed comparisons between the current and previously reported theoretical and experimental values are reported.

Keywords ab initio calculations · Ni-Sb alloys · *p-d* bonded compounds · thermodynamic properties

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1 Introduction

The current contribution has practical as well as theoretical motivations. On the practical side, the work has its roots on a research line aimed at searching for candidates to be adopted in low-melting Pb-free soldering technology. To this aim various Me-X systems (with $Me = Cu, Ni$ and $X = In, Sn$) have recently been explored theoretically, in particular, by the present authors.^[1-3] The goal of those works was to develop a complete database with structural, thermodynamic, cohesive and elastic properties of the intermetallic compounds (ICs) occurring at the joints between the common contact materials Cu and Ni with the low-melting elements In or Sn. Specifically, Ramos et al.^[3] performed a systematic comparative study of the electronic and cohesive properties of the Cu-In, Cu-Sn, Ni-In and Ni-Sn systems. On these bases, the thermophysical effects of replacing Cu by Ni were established.^[3]

On the theoretical side, the current authors have also been interested in establishing and interpreting microscopically trends in the structural, thermodynamic and

cohesive properties of a large class of Cu_aX_b and Ni_aX_b so-called “*p-d* bonded compounds”. The aim of this complementary research line was to provide information of interest for interpolations and extrapolations, as well as the assessment of the mentioned thermophysical properties.

In addition to the ICs formed with $\text{X} = \text{In}, \text{Sn}$, the effects of incorporating Sb were also investigated. In particular, the phase stability and thermophysical properties of a new $\text{Cu}_{5+x}\text{In}_{2+x}\text{Sb}_{2-x}$ B8-related structure were determined *ab initio*.^[4] In addition, the physical properties of a specific compound of the Ni-Sb system, viz., the high-temperature Ni_3Sb phase were also studied.^[5] By going one step forward in this research line, the current paper focuses on the properties of various ICs occurring in the Ni-Sb system.

The phase diagram of the binary Ni-Sb system has been reviewed by Okamoto.^[6] The following ICs have been detected at low temperature: Ni_3Sb (orthorhombic oP8),

Ni_7Sb_3 (unknown structure), NiSb (hexagonal hP4) and NiSb_2 (orthorhombic oP8). At high temperatures, a non-stoichiometric stable phase usually represented as Ni_5Sb_2 has been reported.^[7-9] In fact, the structure of this phase is still under discussion. This phase was classified by Okamoto^[6] as monoclinic (mC28), whereas in the thermodynamic assessment of the phase diagram by Cao et al.^[10] it was treated as a cubic, cF16 phase, and named as “high temperature (HT) Ni_3Sb ”. Luo et al.^[11] performed low temperature resistivity and magnetization measurements on polycrystalline samples of four of these compounds: Ni_3Sb , Ni_5Sb_2 , NiSb , and NiSb_2 . In addition, *ab initio* band-structure calculations for the same ICs were performed with results which are consistent with those deduced from electrical and magnetic measurements.^[11]

In the present work, the 0 K values of thermophysical and equation-of-state (EOS) parameters such as molar volume, bulk modulus and its pressure derivative, the electronic density of states (DOS), and the energy of formation from the elements of the stable Ni-Sb ICs: Ni_3Sb , Ni_5Sb_2 , NiSb , and NiSb_2 , are established theoretically. The calculations are performed in the framework of the density functional theory (DFT), using the VASP (Vienna Ab Initio Simulation Package) and the Projected Augmented Waves (PAW) method, with the generalized gradient approximation (GGA) and the Local Density Approximation (LDA) to evaluate the exchange and correlation energies. The results of the work are discussed in light of microscopic picture of the bonding trends previously

Table 1 Crystallographic data and typical composition of the stable Ni-Sb phases treated in the present work

System	Phase (typical composition)	Pearson symbol
Ni-Sb	Ni_3Sb (25 at.% Sb)	cF16
	Ni_3Sb (25 at.% Sb)	oP8
	Ni_5Sb_2 (28.57 at.% Sb)	mC28
	NiSb (50 at.% Sb)	hP4
	NiSb_2 (66.66 at.% Sb)	oP6

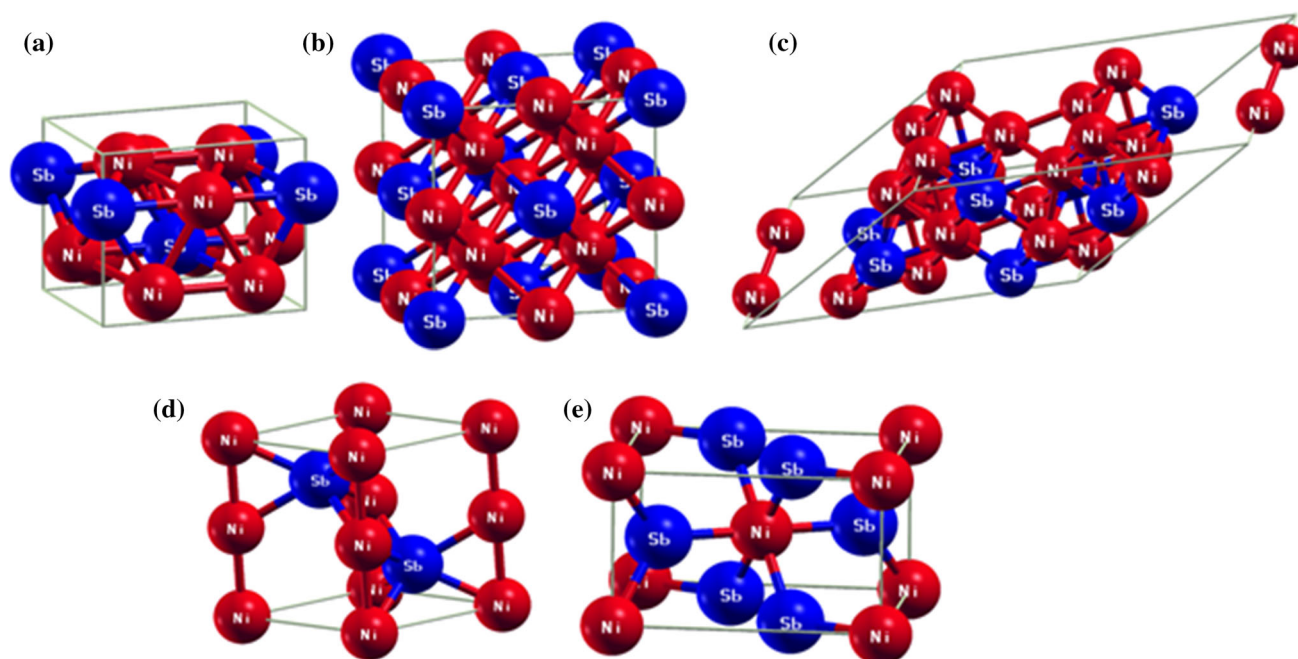


Fig. 1 Structures of the Ni-Sb compounds studied in the present work: (a) Ni_3Sb (oP8), (b) Ni_3Sb (cF16), (c) Ni_5Sb_2 (mC28), (d) NiSb (hP4) and (e) NiSb_2 (oP6). Ni atoms and Sb atoms are indicated

Table 2 Calculated structural and equation of state parameters for the elements Ni and Sb at 0 K, according to the GGA and LDA exchange-correlation (XC) contributions to energy

Phase	P.S.	V_0	a, b, c	B_0	B'	XC
Stable						
Ni	cP4	10.931(a)	3.523(a)	186.2(a)	5.9(a)	GGA
		10.940(b)	3.524(b)	201.4(b)	3.6(b)	
		10.044(a)	3.425(a)	257.9(a)	5.6(a)	LDA
		10.141(b)	3.436(b)	251.4(b)	4.5(b)	
		10.016(c)	3.422(c)	255.8(c)	5.0(c)	
		10.811(d)	3.510(d)	187.6(e)	5.3(f)	
Sb	hR2	10.857(g)	3.515(g)		4.8(f)	
		31.775	4.377, 11.489	31.6	9.0	GGA
		31.782(h)	(4.377, 11.491)h	31.5(h)	8.8(h)	
		29.168	4.300, 10.927	46.4	8.1	LDA
		30.200(i)	4.308, 11,274i	38.3(j)		

The lattice parameters (a, b, c) are given in Å, the equilibrium volume in (V_0) en Å³/atom, the bulk modulus (B_0) in GPa. The symmetry Pearson space group indicated as P.S.

- (a) Ab initio PAW, Ref 2
- (b) Ab initio US-PP, Ref 21
- (c) Ab initio FP-LAPW, Ref 20
- (d) Experimental data extrapolated at 0 K^[22]
- (e) Experimental data based on C_{ij} at 0 K^[23]
- (f) Reported data at 298 K^[24]
- (g) Experimental data at 0 K^[25]
- (h) Ab initio PAW-PW91 non-spin polarized calculation, Ref 4
- (i) Exp. data, Ref 26
- (j) Exp. data, Ref 27

developed by us for the closely related p - d bonded compounds of the Ni-In and Ni-Sn systems.^[2,3]

2 Theoretical Method, Phases and Structures

Systematic ab initio DFT spin polarized calculations using the projected augmented wave (PAW) method^[12,13] as implemented in the VASP^[14] were performed. Both the LDA of Ceperley and Alder^[15] and the GGA of Perdew and Wang^[16] were adopted to evaluate the exchange-correlation contributions to the energy. We consider ten valence electrons for Ni ($3d^8 4s^2$) and 5 for Sb ($5s^2 5p^3$). The kinetic energy cut-off for the plane wave expansion of the electronic wave function was 330 eV. We use k-points grids defined according to the Monkhorst-Pack method^[17]; the convergency of the k-point grids were checked until getting a precision in the energy higher than 1 meV/atom. We adopt the Methfessel-Paxton technique^[18] with a smearing factor of 0.1 eV to occupy the electronic levels.

The following equilibrium ICs of the Ni-Sb phase diagram were treated: LT Ni₃Sb (orthorhombic oP8), HT

Ni₃Sb (cubic cF16), Ni₅Sb₂ (monoclinic mC28), NiSb (hexagonal hP4) and NiSb₂ (orthorhombic oP6). These compounds are listed in Table 1 and shown in Fig. 1.

For these phases, the following k-point grids were considered: $7 \times 9 \times 9$ for Ni₃Sb (oP8), $11 \times 11 \times 11$ for Ni₃Sb (cF16), $5 \times 11 \times 5$ for Ni₅Sb₂ (mC28), $11 \times 11 \times 9$ for NiSb (hP4) and $7 \times 5 \times 11$ for NiSb₂ (oP6). These k-point meshes mean up to 140 k points in the irreducible Brillouin zone (IBZ), depending on the structure. The convergence criterion for the self-consistent total-energy calculations was 0.1 meV. The lattice parameters as well as the internal coordinates of the unit cell were fully optimized keeping the symmetry space group of the crystalline structure, until the forces were lower than 30 meV/Å, and the energy changes due to the ionic relaxation lower than 1 meV/atom.

To determine the EOS parameters, the total energy (E) and external pressure (P) were calculated for different volumes (V) varying around the equilibrium volume (V_0) by up to $\pm 5\%$, letting the relaxation of the internal coordinates. The bulk modulus (B_0) and its pressure derivative (B'_0) were obtained by fitting the P vs V curves to the EOS by Vinet et al.^[19]

Table 3 Structural and elastic properties for Ni-Sb intermetallic compounds at 0 K, according to the GGA and LDA exchange-correlation (XC) contributions to energy

Phase	P.S.	V_0	a, b, c α, β, γ	B_0	B_0'	XC
Stable						
Ni ₃ Sb	oP8	13.023	5.337, 4.288, 4.550	165.5	5.3	GGA
		12.063	5.206, 4.182, 4.432	210.9	6.7	LDA
		12.856(a)	5.321, 4.281, 4.515(a)			Exp.
Ni ₃ Sb	cF16	13.082	5.937	168.0	5.9	GGA
		13.181(b)	5.952(b)	173.4(b)		
		12.133	5.790	209.1	6.2	LDA
		12.124(b)	5.789(b)			
		13.232	5.960(a)			Exp.
Ni ₅ Sb ₂	mC28	13.752	12.985°, 5.463°, 11.484°, 152.10°	148.0	6.6	GGA
		12.755	12.678°, 5.311°, 11.205°, 152.6°	188.3	6.2	LDA
		13.625(a)	12.946°, 5.427°, 11.457°, 151.71°(a)			Exp.
NiSb	hP4	17.655	3.969, 5.177	110.8	3.4	GGA
		16.413	3.881, 5.033	139.9	6.7	LDA
		17.218	3.935, 5.136(a)			Exp.
NiSb ₂	oP6	21.618	5.182, 6.317, 3.840	87.9	6.5	GGA
		20.165	5.126, 6.218, 3.796	107.9	5.7	LDA
		20.952	5.182, 6.317, 3.840(a)			Exp.

The lattice parameters (a, b, c) are given in Å, the equilibrium volume (V_0) in Å³/atom, the bulk modulus (B_0) in GPa

(a) Experimental data^[26]

(b) Ab initio FP-LAPW data^[5]

The energy of formation of the ICs was calculated by computing the difference between the total energy of the compound and the weighted average of the energies of the elements Ni and Sb in their equilibrium structures, viz., the fcc and hR2 phases, respectively.

3 Results and Discussion

We first present and discuss the calculated structural and EOS parameters of fcc Ni and hR2 Sb. In Table 2, we report the currently calculated lattice parameters (LPs), equilibrium volume (V_0), bulk modulus (B_0) and its pressure derivative (B_0'). Experimental data and previously reported theoretical results are also included for comparison.

In accord with our previously reported results,^[1-4] the present PAW results show that the LPs are underestimated by less than 3% with LDA, and overestimated by less than 0.3% with GGA, with respect to the experimental results. On the other hand, these LPs agree well with those predicted by the FP-LAPW method^[20] and other ab initio results based on ultra-soft pseudo potentials (US-PP).^[21] As stated in previous works,^[1,2,21] the calculated B_0 show larger discrepancies with experiments, and better agreement is found when the GGA is adopted.

The calculated LPs and cohesive properties for the Ni-Sb ICs studied in the present work are presented in Table 3, together with the experimental data and other theoretical results reported in the literature.

The calculated LPs deviates positively respect to the experimental results by less than 1.2% in the GGA approximation, whereas those given by the LDA are lower than the experimental ones by less than 3%. The calculated internal coordinates (Table 4) agree well with the experimental ones.

In Fig. 2 the GGA and LDA values of V_0 and B_0 of the Ni-Sb ICs of various Sb contents are compared with the experimental data available. The GGA approximation systematically overestimates V_0 while LDA underestimates it, as already found in other related systems.^[1,2]

The ab initio calculated V_0 and B_0 of the Ni-Sb ICs (Fig. 2) indicate, in general, a smooth variation with composition. The V_0 values tend to deviate negatively from the linear interpolation between the values corresponding to the elements. The B_0 values present positive as well as negative deviations with respect to the corresponding linear interpolation.

In Fig. 3 the ab initio calculated composition dependence of the energy of formation from the elements (ΔE_f) is compared with experimental data and with the results of CALPHAD (i.e., Calculation of Phase Diagrams)

Table 4 Calculated and experimental internal coordinates of Ni₃Sb (oP8), Ni₅Sb₂ (mC28) and NiSb₂ (oP6) IPs

Phase	Site	Internal coordinates		
		(x, y, z): calculated	(x, y, z): calculated	(x, y, z): Exp.(a)
Ni-Sb		GGA	LDA	
Ni ₃ Sb	Ni:2b	0.000, 0.500, 0.316	0.000, 0.500, 0.315	0.000, 0.500, 0.345
	Ni:4f	0.250, 0.000, 0.172	0.250, 0.000, 0.171	0.250, 0.000, 0.150
	Sb:2a	0.000, 0.000, 0.678	0.000, 0.000, 0.677	0.000, 0.000, 0.655
Ni ₅ Sb ₂	Ni:2a	0.000, 0.247, 0.000	0.000, 0.248, 0.000	0.000, 0.249, 0.000
	Ni:2a	0.000, 0.749, 0.000	0.000, 0.749, 0.000	0.000, 0.750, 0.000
	Ni:4c	0.722, 0.498, 0.848	0.724, 0.498, 0.852	0.710, 0.509, 0.846
	Ni:4c	0.302, 0.998, 0.405	0.300, 0.999, 0.403	0.305, 1.000, 0.407
	Ni:4c	0.028, 0.247, 0.257	0.028, 0.247, 0.258	0.028, 0.240, 0.255
	Ni:4c	0.028, 0.749, 0.257	0.028, 0.749, 0.258	0.025, 0.743, 0.257
	Sb:4c	0.723, 0.000, 0.849	0.721, 0.000, 0.847	0.723, 0.000, 0.850
	Sb:4c	0.298, 0.498, 0.401	0.299, 0.498, 0.402	0.297, 0.497, 0.401
NiSb ₂	Ni:2a	0.000, 0.000, 0.000	0.000, 0.000, 0.000	0.000, 0.000, 0.000
	Sb:4g	0.221, 0.359, 0.000	0.221, 0.358, 0.000	0.219, 0.359, 0.000

(a) Experimental data^[26]

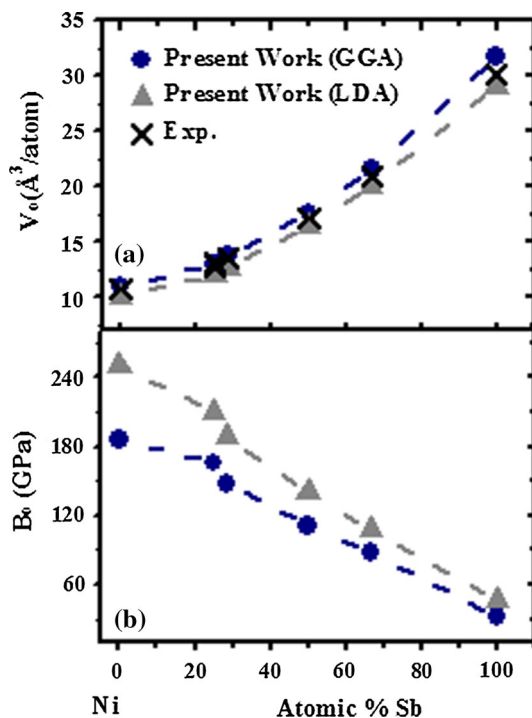


Fig. 2 (a) Equilibrium volume per atom (V_0) and (b) Bulk modulus (B_0) of Ni-Sb compounds as functions of Sb atomic concentration. Filled symbols correspond to values calculated in this work (PAW method) by LDA (triangles) and GGA (circles). The crosses correspond to experimental values indicated in Table 1

assessments. All the phases studied in the present work are found to be thermodynamically stable with respect to the pure elements. Moreover, a very good qualitative agreement is found for the composition dependence of ΔE_f . In particular, the most stable compound is correctly placed by

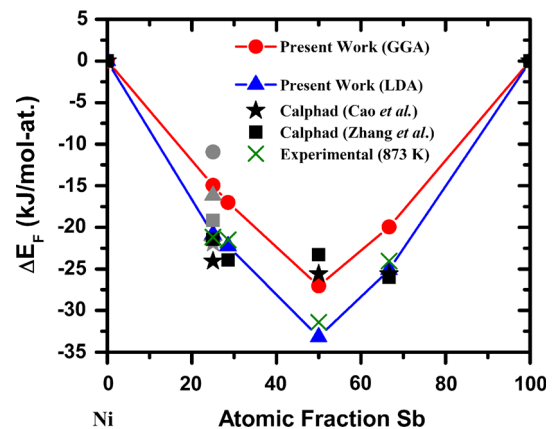


Fig. 3 Energy of formation of the Ni-Sb compounds as a function of Sb concentration. Filled circles and triangles correspond to the GGA and LDA values for the LT ground state phases, respectively, whereas symbols in grey correspond to those for HT phases. Squares and stars represent CALPHAD results extrapolated at 0 K^[9,10] Crosses correspond to experimental results at 873 K^[28]

the calculation at 50 at.%Sb. However, systematic quantitative discrepancies amounting at about 6 kJ/mol-atom between the GGA calculated ΔE_f and the experimental data are found for the Ni₃Sb oP8 phase. It is to be remarked that comparable discrepancies have already been reported for related systems (Ni-X, X = In, Sn).^[2] A better agreement is found for the ΔE_f obtained in the LDA approximation. In this case, the discrepancies between calculations and the available data amount at about 2 kJ/mol-atom. The systematically better prediction of the ΔE_f values by LDA calculations for Ni-X (X = In, Sn) has already been reported.^[2] Also, the present results reproduce a well

Table 5 Energy of formation (in kJ/mol-atom) for Ni-Sb ICs at 0 K obtained ab initio in PAW calculations using both the GGA and LDA exchange-correlation (XC) contributions to energy, compared with results of CALPHAD assessments extrapolated at 0 K and with experimental data

Phase	P.S.	Ab initio ΔE_f PAW-LDA (this study)	Ab initio ΔE_f PAW-GGA (this study)	ΔE_f Calphad	ΔE_f Exp.
Ni ₃ Sb	oP8	-20.852	-14.951	-24.062(a) -21.460(b)	-21.163(c)
Ni ₃ Sb	cF16	-16.183	-10.934	-21.881(a) -19.150(b)	
Ni ₅ Sb ₂	mC28	-22.255	-17.007	-23.929(b)	-21.497(c)
NiSb	hP4	-33.203	-27.041	-25.600; -12.493(a) -23.310; -3.182(b)	-31.411(c)
NiSb ₂	oP8	-25.121	-19.942	-25.603(a) -26.020(b)	-24.059(c)

The reference states are fcc Ni and hR2 Sb

(a) CALPHAD results at $T = 0$ K.^[10] Details of this comparison are given in section 3

(b) CALPHAD results at $T = 0$ K.^[9] Details of this comparison are given in section 3

(c) Experimental results at $T = 873$ K^[28]

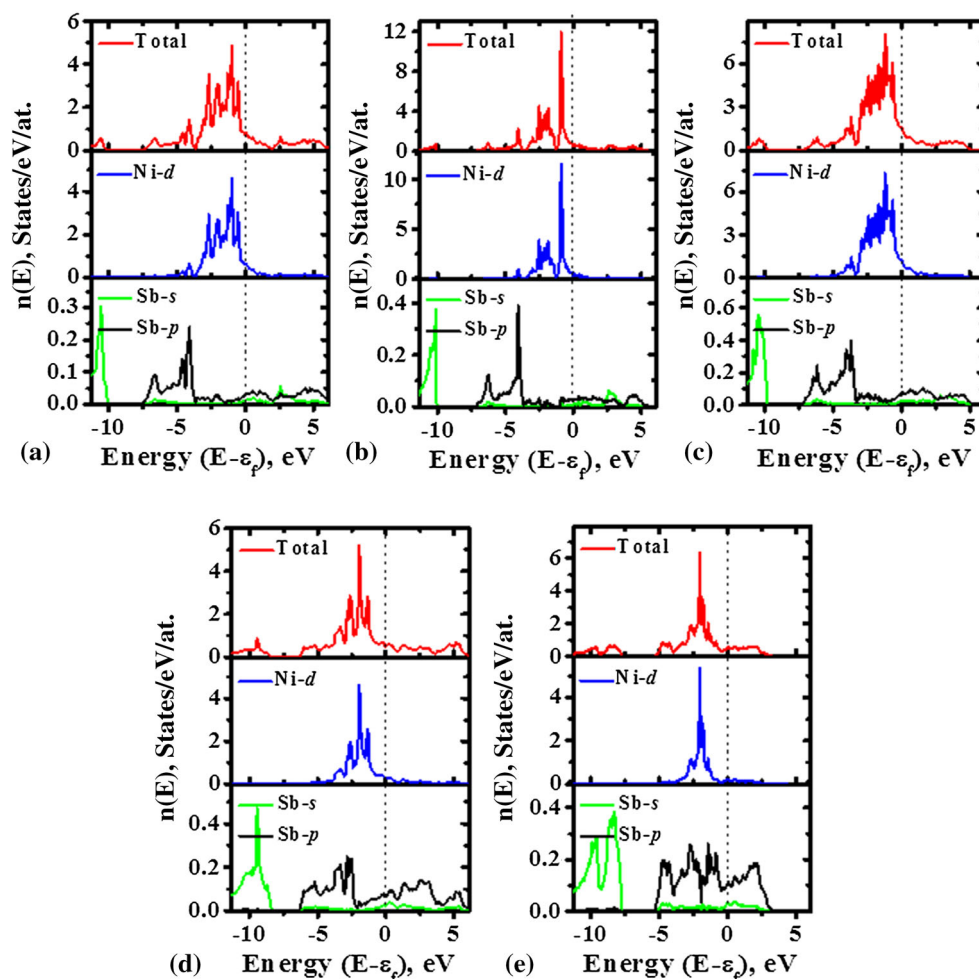


Fig. 4 Electronic DOS for the Ni-Sb compounds: (a) Ni₃Sb-oP8, (b) Ni₃Sb-cF16, (c) Ni₅Sb₂-mC28, (d) NiSb-hP4 and (e) NiSb₂-oP6. The partial site contributions to the DOS of Ni 3d electrons, and Sb

5s and 5p electrons are also included. The origin of the energy scale corresponds to the Fermi level

established trend, with LDA calculated ΔE_f being more negative than the GGA ones.^[21]

We close the comparisons for ΔE_f by focusing on the results for the NiSb compound. The current values are compared in Table 5 with two sets of CALPHAD estimates, which correspond to end-members of the three sublattice model $(\text{Ni}, \text{Va})_{1/3}(\text{Sb})_{1/3}(\text{Va}, \text{Ni})_{1/3}$ yielding the “NiSb” stoichiometry, viz., the $(\text{Ni})_{1/3}(\text{Sb})_{1/3}(\text{Va})_{1/3}$ and $(\text{Va})_{1/3}(\text{Sb})_{1/3}(\text{Ni})_{1/3}$ ICs.^[9,10] The present calculations come closer to the CALPHAD estimates for the first compound.^[9,10]

In Fig. 4 we plot the electronic DOS for the Ni_3Sb -oP8, Ni_3Sb -cF18, Ni_5Sb_2 -mC28, NiSb -hP4 and NiSb_2 -oP6 ICs of the Ni-Sb system. We include the total DOS, and Ni-*d*, Sb-*s* and Sb-*p* partial DOS contributions.

The ICs treated in this work have a finite, relatively low value of the DOS at the Fermi level, indicating metallic character. The DOS for the current Ni-Sb ICs suggest an electronic behavior similar to that found in the related systems Ni-X^[2] and Cu-X, (X = In, Sn).^[1] Specifically, the main band in the DOS of this class of systems is determined by the high contribution of Ni-*d* electrons, whereas the contributions of the *s*- and *p*-electrons of Sb are relatively small. However, as found in related Me-X systems, the hybridization occurring between the Ni-*d* and Sb-*p* electrons is expected to contribute significantly to cohesion in this type of compounds.^[1-3,21]

4 Summary and Concluding Remarks

The present study is part of a long-term research line focusing on the thermophysical properties of the compounds formed by Cu or Ni with In, Sn or Sb. By means of the ab initio methodology used in previous studies, the structural and thermodynamic properties of various Ni-Sb compounds have been determined. The calculated values agree reasonably well with the available experimental data. More specifically, the LPs of the currently studied compounds are better predicted by the GGA PW91 than by the Ceperley-Alder LDA treatment of the exchange-correlation contributions to the energy. However, the reverse is true for the energy of formation from the elements, for which the LDA results are closer to the experimental values. In addition, the study of the electron density of states obtained for the Ni-Sb intermetallics indicate that they may also be classified as “*p-d* bonded compounds”.

Finally, we emphasize that the present results open up the possibility of investigating the effects of varying the X alloying element of the Ni-X compounds in the sequence X = In → Sn → Sb. This problem will be dealt with in a forthcoming paper.

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