Experimental and theoretical study of the electronic structures of Ni_3Al , Ni_3Ga , Ni_3In , and NiGa

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The electronic structures of Ni_3Al , Ni_3Ga , Ni_3In , and NiGa are studied by x-ray absorption near-edge spectra (XANES) at the Ni and Ga K edges. The XANES spectra are compared with those calculated with theory. The experimental XANES features for these compounds reflect the Ni- and Ga- p unoccupied density of states. The calculated magnetic moments for Ni_3Al , Ni_3Ga , and Ni_3In are between $0.7\text{--}0.8 \mu_B/\text{cell}$. The number of $3d$ holes per Ni atom is calculated for Ni_3Al , Ni_3Ga , and Ni_3In . These numbers show correlation with heats of formation of the bulk compounds.

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I. INTRODUCTION

Binary intermetallic compounds that contain a transition metal and a group-III metal display interesting electronic and magnetic properties. For instance, the stoichiometric compound Ni_3Al shows weak itinerant ferromagnetism with $T_c = 41.5$ K and a very small magnetic moment ($0.23 \mu_B$ per cell),¹ the stoichiometric compound Ni_3Ga is an exchange-enhanced paramagnetic metal,^{1–3} and NiGa is nonmagnetic. In this article, x-ray absorption near-edge spectra (XANES) at the Ni and Ga K edges of four intermetallic compounds (Ni_3Al , Ni_3Ga , Ni_3In , and NiGa) were measured and compared with theoretical XANES spectra. Such analysis is especially important for establishing a relationship between the experimental XANES spectra and the unoccupied part of the local density of states (DOS) and obtaining quantitative information about hole numbers and charge transfer in these intermetallic compounds. Experimental Ni $L_{2,3}$ -edge and Al and Ni K -edge XANES spectra of Ni_3Al ,^{4–8} Ni_3Ga ,^{5–7,9} Ni_3In ,⁷ and NiGa ^{7,9} have been reported previously. The Ni $L_{2,3}$ near-edge structures of Ni_3Al were also measured by electron-energy-loss spectroscopy.^{10,11} Theoretical analyses of the Ni $L_{2,3}$ -edge and Al and Ni K -edge XANES spectra have been performed on Ni_3Al ,^{6,7,8} Ni_3Ga ,^{6,7} Ni_3In ,⁷ and NiGa ⁷ using either band-structure or multiple-scattering method. Another purpose of this article is to systematically study the electronic structures and the mechanical and magnetic properties of a series of technologically interesting intermetallic compounds, and to compare with available experimental and theoretical results. We note that very few studies were done on Ni_3In and NiGa .

This article is organized as follows. In Sec. II, the experimental and the theoretical methods are described. In Sec. III, the results and discussion are presented. The conclusions of this work are contained in Sec. IV.

II. METHODS

A. Experimental methods

Preparation and characterization of polycrystalline samples of Ni intermetallic compounds were reported previously.^{4,12} Energy-dispersive x-ray (EDX) analysis showed that the Ni atoms concentration deviates by 2, 0, and 3% from the nominal compositions for Ni_3Al , Ni_3Ga , and Ni_3In , respectively; whereas they are rich by 21% for NiGa . We note that our bulk $\text{Ni}_{0.73}\text{Al}_{0.27}$ and Ni_3Ga samples are in the paramagnetic phase.¹ The residual resistivity (ρ) ratio ($\rho_{300\text{ K}}/\rho_{4.2\text{ K}}$) for Ni_3Al and NiGa is 4.5 and 1.32,¹³ respectively. The XANES experiments were carried out on wiggler beamline 17 C at the Synchrotron Radiation Research Center, Taiwan. A Si(111) double-crystal monochromator was used and the typical energy resolution was about 2 eV. The XANES spectra were collected by recording the total yield of secondary electrons from the sample surfaces at room temperature. Standard 5- μm -thick Ni foil was used as a reference for energy calibration. Ni XANES data were also used as a reference spectrum. Data at the Ga K edge for Ni_3Ga and NiGa were internally calibrated by setting the inflection points to 10 367.0 eV. The photon flux was obtained simultaneously by measuring the current of a Au mesh located near the exit slit of the monochromator and used for normalization of the XANES spectra.

B. Theoretical methods

The theoretical XANES spectra, the electronic structures, and the mechanical and magnetic properties of these intermetallic compounds are calculated using the highly accurate all-electron full-potential linear augmented-plane-wave (FLAPW) method.¹⁴ The calculations are based on first-principles density-functional theory with the generalized

FIG. 1. The experimental (open circles) and theoretical paramagnetic (solid lines) Ni *K*-edge XANES spectra for (a) Ni₃Al, (b) Ni₃Ga, (c) Ni₃In, and (d) NiGa. Also shown is the Ni *p* partial DOS (dashed lines).

gradient approximation (GGA) to the exchange-correlation potential.¹⁵ We find that using the GGA is essential to bring the calculated lattice constants and bulk moduli of these compounds into good agreement with the experimental values. We begin the calculations by determining total energies at several values of the lattice constants near the experimental one for each compound. These energies are then fitted to the Murnaghan equation of state¹⁶ to obtain the theoretical equilibrium lattice constants and bulk moduli. The calculations are done for both paramagnetic and ferromagnetic states of these materials. The muffin-tin radius of 1.22 Å is used for all the atoms. The wave functions, the charge densities, and the potentials are expanded in terms of the spherical harmonics inside the muffin-tin spheres. The cutoff angular momentum (l_{max}) is ten for the wave functions and six for the charge densities and the potentials. The Brillouin zone (BZ) integration is carried out by using the improved tetrahedron method.¹⁷ The number of the augmented plane waves included is about 80 per atom, i.e., $R_{\text{mt}}K_{\text{max}}=9$.¹⁴ The number of the *k* points in the irreducible BZ wedge (IBZW) used in the self-consistent calculations is 56. To calculate the DOS curves and the theoretical XANES spectra, the experimental lattice constants for these intermetallics and 165 *k* points in the IBZW were used. We have checked the conver-

gence of the calculated eigenvalues with respect to the number of augmented plane waves used and the number of *k* points used.

III. RESULTS AND DISCUSSIONS

The experimental (open circles) and theoretical paramagnetic (solid lines) XANES spectra of Ni *K* edge for Ni₃Al, Ni₃Ga, Ni₃In, and NiGa are displayed in Figs. 1(a)–1(d), respectively, those of Ga *K* edge for Ni₃Ga and NiGa are shown in Figs. 2(a) and 2(b), respectively. The Ni *K*-edge XANES spectra for Ni₃Al and Ni₃Ga are similar to those reported previously.^{5,6,8} Also shown in Figs. 1 and 2 are Ni and Ga *p* partial DOSs (dashed lines), respectively, calculated for these intermetallic compounds. The maxima of the XANES spectra in Figs. 1 and 2 coincide, respectively, with the peaks in the Ni and Ga *p* partial-DOS curves, which correspond to Ni and Ga 1*s* to ϵp transitions. The zero energies correspond to the inflection points of the respective Ni and Ga *K*-edge absorption edges. The experimental data were normalized to theoretical spectra in the region 10–20 eV above the absorption edges. The absolute energies of the Ni and Ga *K*-edge white lines and the energy separations of the subsequent XANES structures for these four compounds

FIG. 2. Same as Fig. 1 except for Ga *K*-edge XANES spectra for (a) Ni₃Ga and (b) NiGa. Also shown is the Ga *p* partial DOS (dashed lines).

are listed in Table I. Overall, we have a reasonable good agreement between theory and experiment. The decrease in peak height after the maxima is due to the finite-sized, linearized energy-dependent basis sets in the muffin-tin spheres used in the present calculations. With the exception of NiGa, all major features of the absorption peaks, as well as white-line positions and intensities, are well reproduced. The disagreement between experimental and theoretical Ni and Ga *K*-edge XANES spectra found for NiGa is caused by high concentration of antistructure defects (0.75 at. %) present in

TABLE I. The absolute energies (in eV) of the Ni and Ga *K*-edge white lines for Ni₃Al, Ni₃Ga, Ni₃In, and NiGa, and the energy separations of the subsequent XANES structures.

Edge	Ni ₃ Al	Ni ₃ Ga	Ni ₃ In	NiGa
Ni <i>K</i>	8331.6	8331.6	8334.0	8334.0
	1.4	2.5		
	16.0	15.5	15.8	17.3
	26.8	23.4	22.8	
Ga <i>K</i>		48.4	46.0	
		10 372.1		10 371.7
		4.9		3.5
		12.9		13.0
		23.9		
		45.9		47.7

the sample,¹³ which were not considered in the present theory. The same disagreement was also found in NiGa of the Ni *L*-edge XANES spectrum and that obtained from multiple-scattering theory.⁷ Small discrepancies in peak positions and intensities might be due to the use of muffin-tin approximation in calculation of the potentials and to the neglect of the dipole transition-matrix elements. For example, the theoretical Ni *K*-edge XANES spectra for Ni₃Al and Ni₃Ga well produce the three experimental peaks at approximately 16, 25, and 49 eV above the white lines. The same features are present in the calculated Ni *K*-edge XANES spectra for Ni₃In, though less pronounced and in less agreement with the experimental data of the peak positions. Another source of error is that the GGA eigenvalues are not the true excitations of the XANES spectra, and the errors in peak positions are comparable to the self-energy correction between GGA and more sophisticated methods such as GW.¹⁸ As for the source of the discrepancy in peak width, the hot-electron lifetime is strongly energy dependent so that it mostly damps peaks about 20 eV above the absorption edge. Since the dipole transition-matrix element is not a very sharp function of energy above 40 eV of the Ni-*K* white line for Ni₃Al,⁸ the difference in intensity of the XANES features at roughly 49 eV above the Ni-*K* white lines for Ni₃Al and Ni₃Ga can be explained solely by the larger Ni *p* DOS for the latter compound. For Ni₃Ga and NiGa, the unoccupied Ga *p* DOSs also affect the intensity variations of the features at roughly 4 and 13 eV above the Ga-*K* white lines.

In Table II, we list the calculated and experimental values of the equilibrium lattice constants of these materials, along with their crystal structures. Ni₃Al, Ni₃Ga, and Ni₃In have the cubic *L*1₂ structure, while NiGa has the B2 structure. It was reported¹⁹ that Ni₃In has the ordered *D*0₁₉ structure isotypic with Ni₃Sn. However, the Ni *L*_{2,3} XANES spectrum of Ni₃In calculated using this latter structure resulted in a much worse agreement with the experimental spectrum than using the cubic *L*1₂ structure for Ni₃In.⁷ Our FLAPW results for the equilibrium lattice constants in Table II are within 1% of the experimental values, and weak ferromagnetism affects the structural properties of Ni₃Al, Ni₃Ga, and Ni₃In only slightly. The theoretical and experimental values of the bulk modulus (*B*) for these intermetallic compounds are listed in the last column in Table II. Our calculated *B* values for Ni₃Al and Ni₃Ga are about 8% and 25% larger than the experimental *B* values for Ni₃Al [1.707,²⁰ 1.71,²¹ and 1.73 (Ref. 22) Mbar] and Ni₃Ga (1.46 Mbar),²¹ respectively. Here, only experimental *B* values obtained from the stoichiometric single crystals at room temperature are used to compare with our calculated values, since it is reported²³ that the elastic constants of nonstoichiometric polycrystals Ni₃Al are rather different from each other and from those of Ni₃Al single crystals. Our calculated *B* value for Ni₃Al (1.847 Mbar) agrees better with the experimental values than other theoretical calculated values [1.75,^{24,25} 1.743,²³ 2.10,²⁶ and 2.34 (Ref. 27) Mbar] do. Our calculation for Ni₃Ga overestimates the *B* value by 25%, which is much less than previous local spin-density approximation (LSDA) calculation (over 70%)²⁷ did. This means that it is important to include GGA in LSDA calculations.

TABLE II. Crystal structure, lattice constant a , total magnetic moment M_s , density of states at the Fermi energy $n(E_F)$, and bulk modulus B for Ni_3Al , Ni_3Ga , Ni_3In , and NiGa . The first, second, and third line for each material is the theoretical (paramagnetic), theoretical (ferromagnetic), and experimental values, respectively.

Material	Crystal structure	a (Å)	M_s (μ_B /cell)	$n(E_F)$ (states/eV cell)	B (Mbar)
Ni_3Al	$L1_2$	3.571	0.0	5.82	1.863
		3.573	0.75	3.29	1.847
		3.568	0.23	11.02	1.707
Ni_3Ga	$L1_2$	3.589	0.0	6.66	1.836
		3.591	0.81	3.19	1.835
		3.576		10.22	1.46
Ni_3In	$L1_2$	3.745	0.0	7.02	1.570
		3.747	0.73	4.66	1.564
		3.750			
NiGa	$B2$	2.9231	0.0	0.87	1.530
		2.9230	0.0	0.87	1.522
		2.8952		1.48	

The magnetic properties of the intermetallic compounds we investigated in this work depend sensitively on the lattice constants, as shown in the fourth column in Table II for the total magnetic moments (M_s). We note that our calculated M_s value for Ni_3Al ($0.75 \mu_B/\text{cell}$) is three times larger than the experimental value ($0.23 \mu_B/\text{cell}$).^{1,28} An attempt was made to include spin-orbit coupling in the self-consistent calculation for Ni_3Al , but no significant change of the M_s value was observed. We should point out that LSDA and GGA calculations tend to overestimate the M_s value for other materials, too.²⁹ We should also mention that controversy has remained about the magnetic moment of Ni_3Al with the M_s values ranging from 0 to $0.7 \mu_B/\text{cell}$.²⁹ The one ($0.71 \mu_B/\text{cell}$)²⁶ closest to our value was calculated by means of the all-electron semirelativistic linear muffin-tin orbitals method. Since the ferromagnetic state is slightly lower in energy than the paramagnetic state by about 20 meV/cell for Ni_3Al , Ni_3Ga , and Ni_3In , all three materials should show weak itinerant ferromagnetism. This assertion agrees with that obtained from structural-stability study for Ni_3Al .²⁶ However, experimentally Ni_3Ga is an enhanced paramagnet.³ All these differences are a direct consequence of the small energy difference associated with magnetic polarization and the difficulty of conventional spin-polarized calculations to discriminate between nonmagnetic and ferromagnetic solutions. Magnetic measurements on Ni_3In may be able to clarify the magnetic behavior of this material. NiGa on the other hand is paramagnetic. Site-decomposed magnetic moment at the Ni, Al (Ga, In), and interstitial sites for Ni_3Al , Ni_3Ga , and Ni_3In are listed in the first row for each material in Table III. One can see that the main contribution for the magnetic moments of these three compounds comes from that of the Ni $3d$ electrons; while uncompensated Al p electrons and electrons in the interstitial region are polarized slightly negatively.

The calculated and experimental DOSs at the Fermi energy [$n(E_F)$] for Ni_3Al , Ni_3Ga , Ni_3In , and NiGa are listed in the fifth column in Table II, while the site-decomposed partial DOS at the Fermi energy are listed in the second and third rows for spin-up and spin-down band, respectively, in Table III. The main contribution for the $n(E_F)$ values for

these compounds comes from the spin-down Ni $3d$ electrons. For Ni_3Al and Ni_3Ga , we chose the $n(E_F)$ values derived from the specific-heat measurement³⁰ neglecting electron-phonon interaction as the experimental ones. The reason we chose these values in Table II is because the authors who reported these $n(E_F)$ values were the only ones that studied both compounds in the same paper. Higher-experimental $n(E_F)$ values [12.86,²⁸ 13.08,³¹ and 13.84 (Ref. 32) states/(eV cell)] derived from specific-heat measurements on Ni_3Al were also reported. It should be pointed out that all the experimental $n(E_F)$ values for Ni_3Al are much larger than our calculated paramagnetic one [5.82 states/(eV cell)], which is close to other theoretical paramagnetic values [5.18,³³ 5.53,³⁴ 6.56,²⁷ 7.40,²⁶ and 7.72 (Ref. 35) states/(eV cell)]. Our ferromagnetic value for Ni_3Al [3.29 states/(eV cell)] is also close to other theoretical ferromagnetic ones [4.35 (Ref. 36) and 4.39 (Ref. 26) states/(eV cell)]. For Ni_3Ga , our calculated paramagnetic $n(E_F)$ value [6.66 states/(eV cell)] is essentially the same as previous theoretical ones [5.45,³⁷ 6.25,³ and 6.47 (Ref. 35) states/(eV cell)]. However, all these theoretical values are much smaller than the experimental $n(E_F)$ values [9.71 (Ref. 38) and 10.22 (Ref. 31) states/(eV cell)]. The discrepancy between the $n(E_F)$ values calculated by band-structure calculations and those determined calorimetrically for Ni_3Al and Ni_3Ga is too

TABLE III. Magnetic moment M_s (the first line in units of μ_B/atom) and density of states at the Fermi energy $n(E_F)$ (the second and third lines for spin-up and spin-down states, respectively, in units of states/eV cell) at different sites for Ni_3Al , Ni_3Ga , and Ni_3In .

Material	Ni-site	Al (Ga, In)-site	Interstitial
Ni_3Al	0.27	-0.03	-0.04
	0.44	0.05	0.06
	2.62	0.05	0.07
Ni_3Ga	0.29	-0.02	-0.04
	0.47	0.05	0.05
	2.48	0.06	0.08
Ni_3In	0.267	-0.02	-0.05
	0.51	0.06	0.07
	3.85	0.06	0.11

large for any reasonable electron-phonon enhancement correction. The strong renormalization of these $n(E_F)$ values may point to the importance of exchange-enhanced spin fluctuations arising essentially from the effect of a molecular field which is local in space and time.³ For NiGa, the experimental $n(E_F)$ value¹³ is also much larger than our calculated value. This latter discrepancy may be attributed to the electron-phonon mass enhancement. Further study is needed to explain these discrepancies found in the intermetallic compounds.

We also calculated the hole numbers in order to analyze charge transfer in these Ni intermetallic compounds. The number of 3d holes per Ni atom calculated for Ni₃Al, Ni₃Ga, Ni₃In, and NiGa is 1.60, 1.59, 1.59, and 1.49, respectively. The hole number for bulk Ni calculated in this work is 1.44. As expected, the filling of the Ni 3d bands in these compounds is incomplete. This conclusion is consistent with previous x-ray photoemission spectroscopy, bremsstrahlung isochromat spectroscopy, and resonant photoemission spectroscopy (RESPES) studies on these compounds.^{4,5,9} The changes in the number of Ni d electrons from bulk Ni to Ni₃Al, Ni₃Ga, and Ni₃In are consistent with that (0.1 ± 0.15 electrons/atom)¹⁵ reported for other Ni compounds. One also finds that the hole number decreases in the series Ni, Ni₃Al, Ni₃Ga (Ni₃In), and NiGa. Previous RESPES⁴ and core-level photoemission⁵ studies on these materials predicted the hole number decrease in the series bulk Ni (1.56), Ni₃Al (1.37), Ni₃In (1.34), and Ni₃Ga (1.30). We note that the order for Ni₃In that obtained from the present theoretical calculation is not consistent with that obtained from previous experimental data. The maximum difference between these two sets of hole numbers for Ni₃Al, Ni₃Ga, and Ni₃In is found for Ni₃In, and is only about 4%. This observation seems to suggest that the uncertainty in determining the hole number for Ni₃In, both theoretically and experimentally, is higher than that for Ni₃Al and Ni₃Ga. The higher uncertainty for Ni₃In may be due to defects present in the sample.

It is well known that the cohesive energy can be predicted from the filling of the d band, and a phenomenological relationship between the number of 3d holes per Ni atom and the heat of formation (ΔH) was established recently for Ni₃Al.¹⁰ Following Muller *et al.*'s method,¹⁰ we estimated that the ΔH values for Ni₃Al, Ni₃Ga, Ni₃In, and NiGa are -0.48 , -0.02 , -0.06 , and -0.14 eV/atom, respectively. Therefore, the order of compound stability is Ni₃Al, NiGa, Ni₃In, and Ni₃Ga. It is also worth noting that the general rule,³⁹ that the strongest bond is for an exactly half-filled DOS, holds for the Ni–Ga compounds. The ΔH values for Ni₃Al and Ni₃In are close to the experimental values of -0.43 and -0.087 ± 0.017 eV/atom, respectively.⁴⁰ There are two other reported ΔH values for Ni₃Al: -0.41 (Ref. 41) and -0.40 (Ref. 42) eV/atom, which are within 7% to the above cited value. Surprisingly, the estimated ΔH value for Ni₃Al is exactly the same as that calculated previously.²⁶ We also note that our calculated hole number per Ni atom for Ni₃Al (1.36 in Table I) differs by only 2% with that (1.33) obtained previously.²⁶ Thus, the simple approach used in this work is capable of predicting the heat of formation for these intermetallic compounds.

IV. CONCLUSIONS

The electronic structures of Ni₃Al, Ni₃Ga, Ni₃In, and NiGa were studied jointly by XANES measurements at the Ni and Ga K edges and by theoretical analysis using FLAPW method. Except for NiGa, a reasonably good agreement between theory and experiment was found. The experimental XANES features for these compounds reflect the Ni- and Ga-p unoccupied states. The disagreement between experimental and theoretical Ni and Ga K-edge XANES spectra found for NiGa is caused by a high concentration of anti-structure defects present in the sample. The magnetic moments, the DOS at the Fermi energy, and the equilibrium lattice constants and bulk moduli for these intermetallics are calculated and compared with previous theoretical and experimental results. Discrepancies between calculated and experimental-derived DOS at the Fermi energy for these compounds come from electron-phonon mass enhancement and localized magnetic fluctuations. The number of 3d holes per Ni atom is 1.36, 1.34, and 1.28 in the unoccupied bands of Ni₃Al, Ni₃Ga, and Ni₃In, respectively. These numbers show correlation with heats of formation of the bulk compounds.

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