ELECTRONIC STRUCTURE OF THE Ni_3Al AND Ni_3Ga ALLOYS*

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(Received November 21, 1990; in revised form March 28, 1991)

The results of ab-initio calculations of the electronic density of states and band electronic structure of the Ni_3Al and Ni_3Ga alloys are presented. The calculations are performed with the use of the linear-muffin-tin-orbital (LMTO) method in the atomic sphere approximation. The Barth–Hedin parametrization of the local density exchange correlation energy is used.

PACS numbers: 71.25.Pi

The purpose of this work is to present the results of ab-initio calculations of the electronic density of states and band electronic structure of the Ni_3Al and Ni_3Ga alloys. Ni_3Ga is a strongly exchange-enhanced paramagnet while Ni_3Al is a typical itinerant electron ferromagnet. These materials are very interesting both from theoretical and experimental point of view [1] and the accurate knowledge of the electronic band structure, especially in the immediate vicinity of the Fermi level, seems to be very desirable. The preliminary results of a part of these calculation (i.e. density of states of the paramagnetic Ni_3Al alloy) have recently been reported [2]. However, in those calculations the spin–orbit coupling effects were neglected.

The calculations were performed using the linear-muffin-tin-orbital (LMTO) method [3, 4] with the atomic-sphere-approximation (ASA) for Cu_3Au type structure (simple-cubic unit cell) with Ni atoms located on the face centres and Al on the cube corners. The spin–orbit coupling terms in the scheme of LMTO calculations were included. In ASA the Wigner–Seitz cell is replaced by the sphere with radius s. The radius of the sphere is determined by the condition $4\pi s^2 n/3 = V$, where V is the volume of W–S cell and n is the number of atoms in a primitive cell. In the band calculations we used the Barth–Hedin parametrization of the local density of

*This work was supported by the Institute for Low Temperature and Structure Research Wrocław, from the funds of the Project CPBP 01.12 of the Polish Academy of Sciences.

the exchange correlation energy. The initial potential parameters used to perform the LMTO–ASA band calculation were evaluated from the atomic potentials and the electron charge density was obtained from the energy bands computed on the uniform mesh of 84 K-points in the irreducible wedge of the Brillouin zone.

In the calculations we included s and p states of Al and Ga and s and d states of Ni and we assumed the following initial configuration: for Al — core + $3s^2$, $3p^1$, for Ga — core + $4s^2$, $4p^1$, for Ni — core + $3d^8$, $4s^2$. In the ASA the average sphere radius for Ni_3Al is obtained by minimizing the total energy in the paramagnetic states. From this procedure we obtained $s = 2.63$ a.u. (a = 3.560 Å) for Ni_3Al and $s = 2.64$ a.u. (a = 3.573 Å) for Ni_3Ga while the experimental values are a = 3.568 Å and a = 3.582 Å for Ni_3Al and Ni_3Ga, respectively.

The results of the calculations are given in Figs. 1–6, where total density of states (DOS), total number of states (NOS), l-decomposed partial DOS and NOS and the electronic band structure for Ni_3Al and NI_3Ga are presented. In the Tables I and II the total and l -decomposed partial DOS and NOS at the Fermi level for Ni_3Al and Ni_3Ga, respectively, are given.

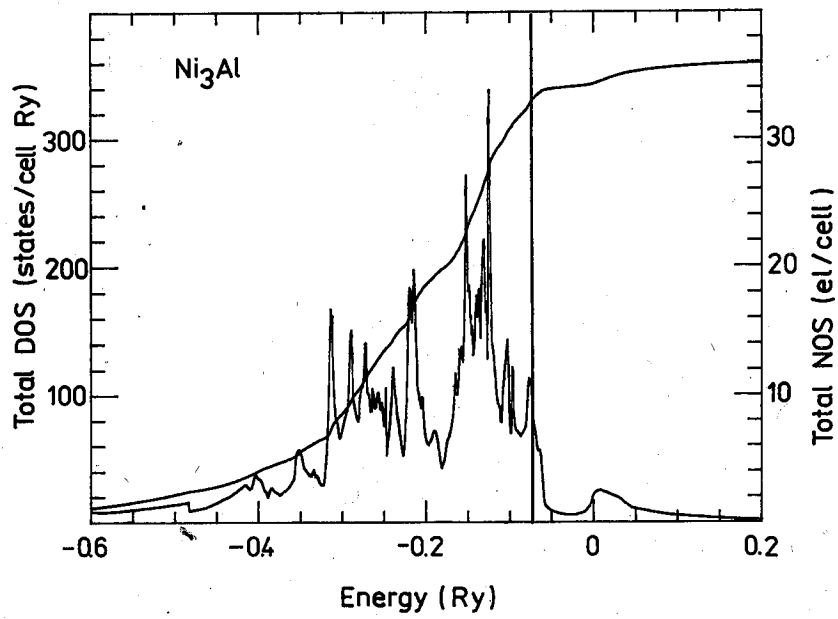

Fig. 1. Total DOS and NOS of paramagnetic Ni_3Al.

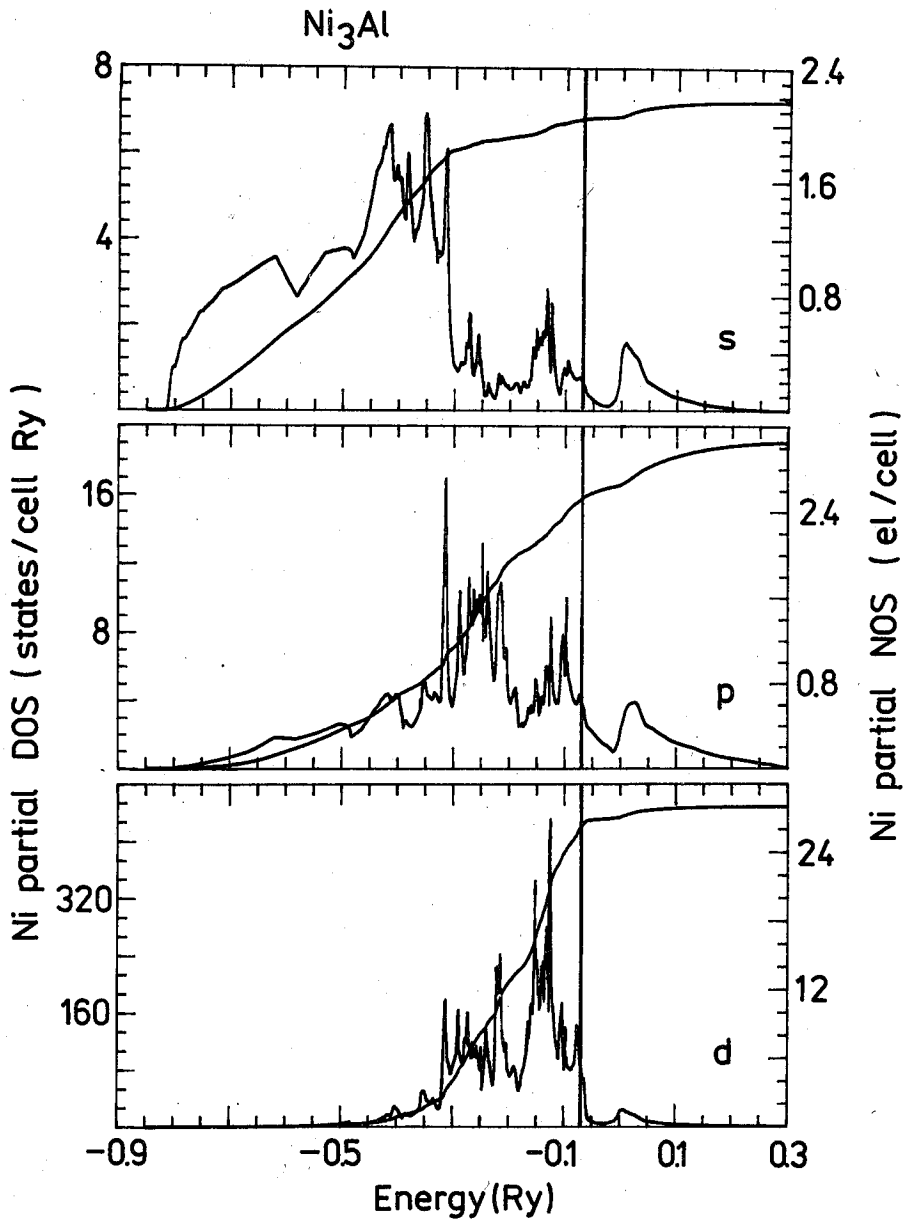

Fig. 2(a). Partial DOS and NOS per cell of Ni_3Al at the Ni atoms.

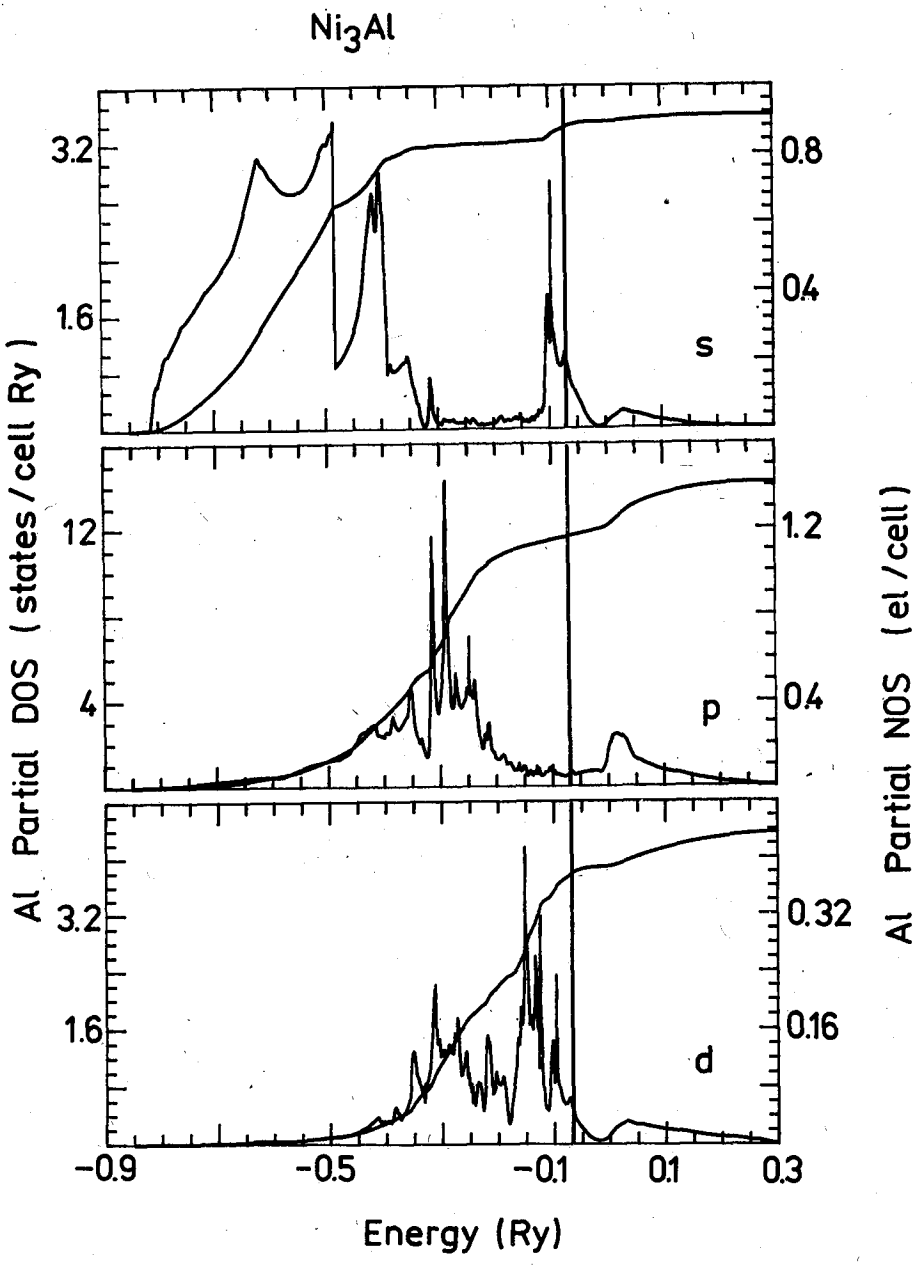

Fig. 2(b). Partial DOS and NOS per cell of Ni_3Al at the Al atom.

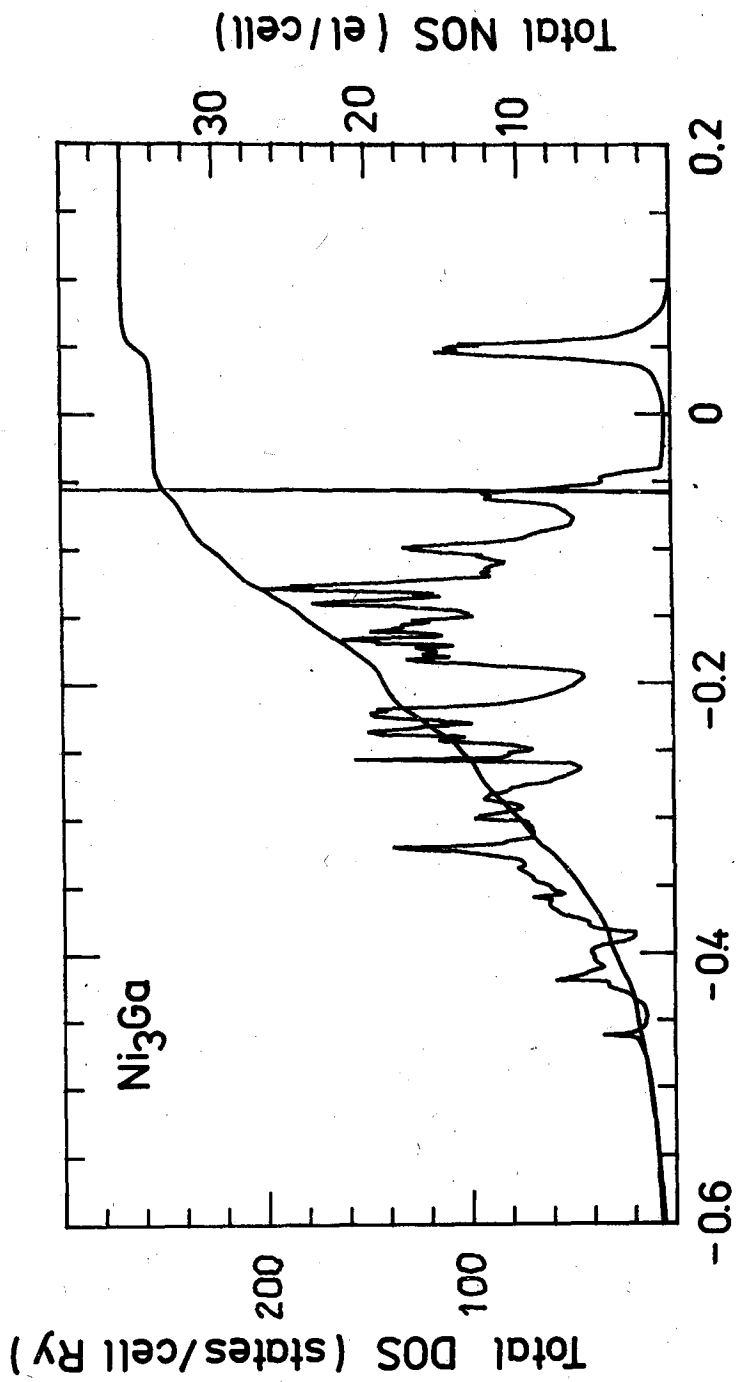

Fig. 3. Total DOS and NOS of Ni_3Ga.

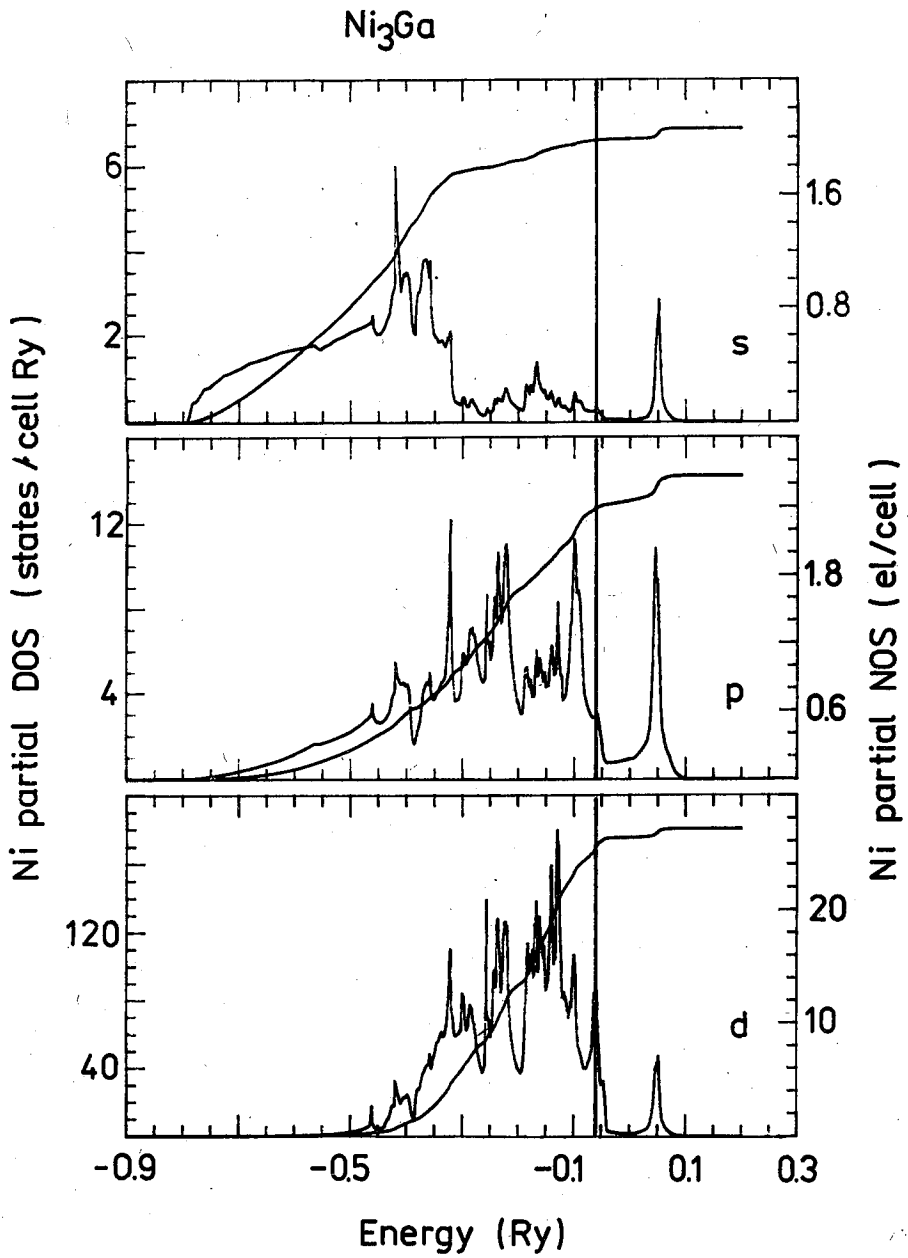

Fig. 4(a). Partial DOS and NOS per cell of Ni_3Ga at the Ni atoms.

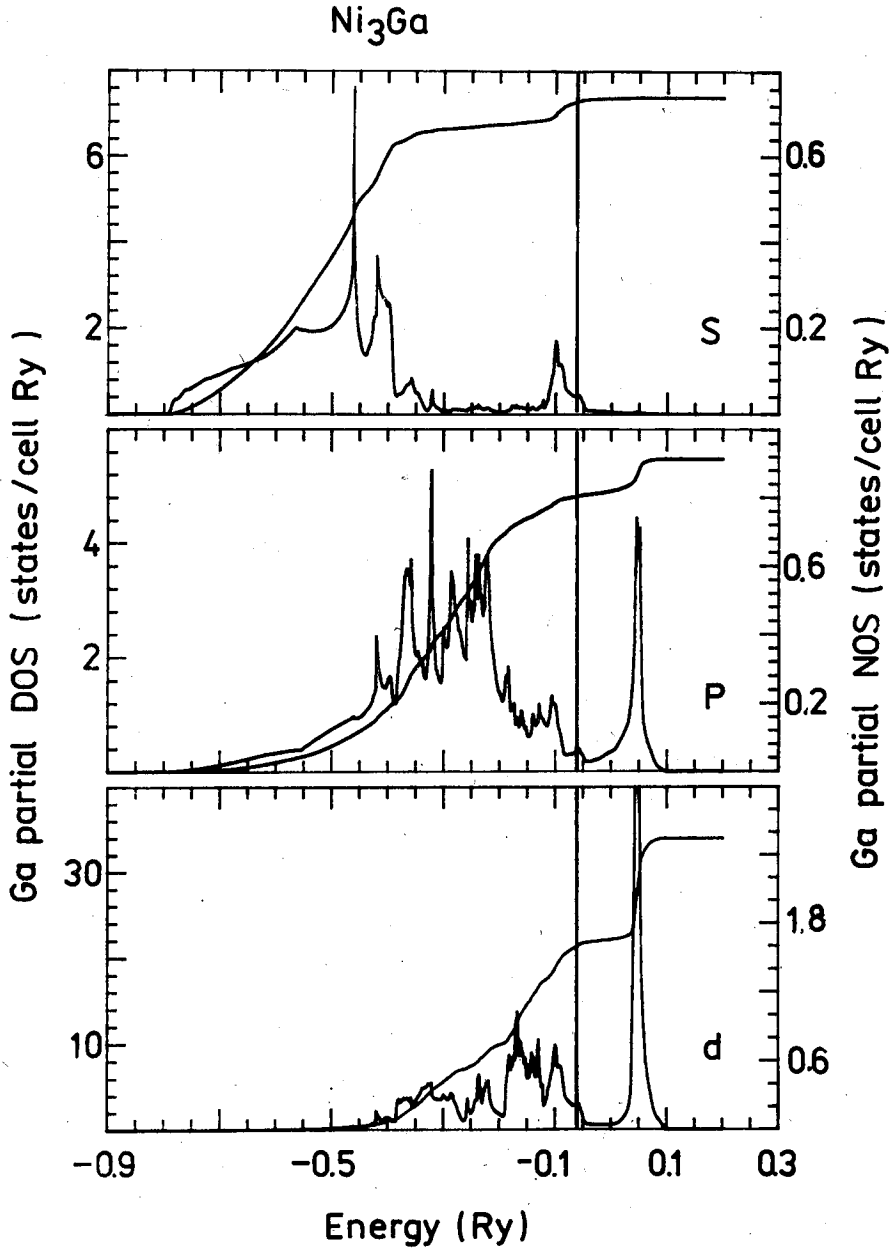

Fig. 4(b). Partial DOS and NOS per cell of Ni_3Ga at the Ga atom.

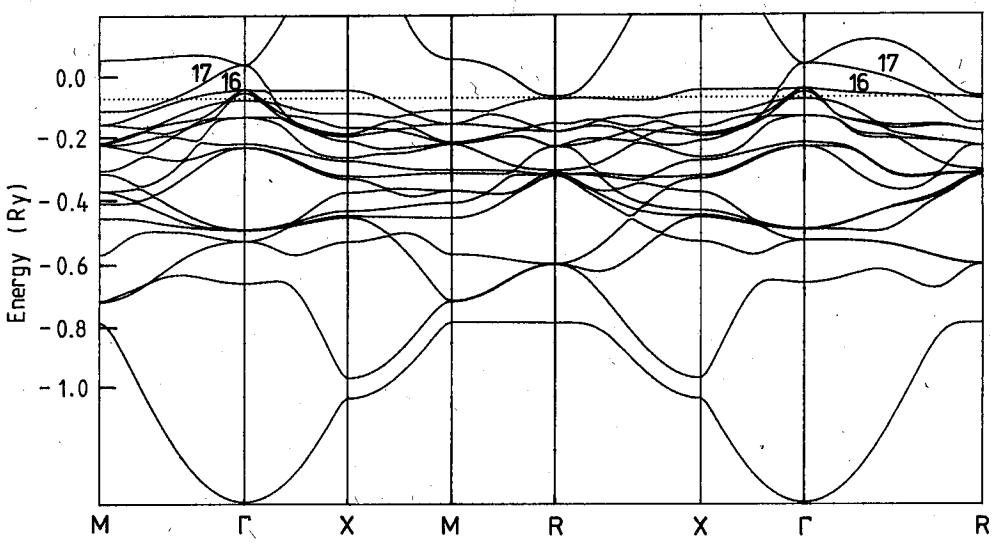

Fig. 5. Energy bands of paramagnetic Ni_3Al. The Fermi level is denoted by the dotted line.

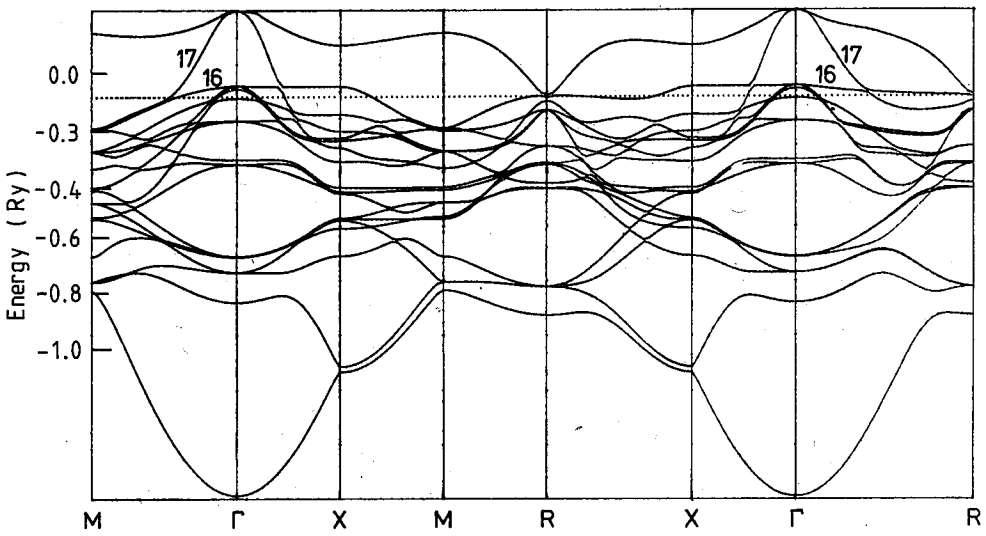

Fig. 6. Energy bands of Ni_3Ga. The Fermi level is denoted by the dotted line.

TABLE I

The l-decomposed DOS at the Fermi level N_l (E_F) and the partial charge occupancies Q_l of paramagnetic Ni_3Al.

		s	p	d	total
$N_l(E_F)$	3Ni	0.76	4.32	85.4	
					92.4
(Ry cell)$^{-1}$	Al	0.8	0.48	0.64	
	3Ni	2.06	2.4	26.2	
Q_l					33.0
	Al	0.8	1.16	0.38	

TABLE II

The l-decomposed DOS at the Fermi level N_l (E_F) and the partial charge occupancies Q_l of Ni_3GA.

		s	p	d	total
N_l (E_F)	3Ni	0.49	2.86	85.0	
					92.0
(Ry cell)$^{-1}$	Ga	0.41	0.37	2.83	
	3Ni	1.96	2.38	25.5	
Q_l					33.0
	Ga	0.74	0.8	1.62	

For Ni_3Al we can compare our results with those obtained recently by Min et al. [5] by the full-potential linearized-augmented-plane wave (FLAPW) method. As we can see the shape of the DOS, the position of the Fermi level on the sharp peak and the picture electronic band structure are very similar. The calculated density of states at the Fermi level for Ni_3Al is 92.3 states/(Ry cell) and is higher than that of Min et al. [5] (75.2) but is still too small in comparison with the experimental value determined from specific-heat measurements (approximately 150 states/(Ry cell) [6].

Ni_3Al and Ni_3Ga alloys have the similar electronic configuration. The Fermi level is located on the left side of peak (Figs. 1 and 3) and the shape of the densities of states in the both systems is similar.

The magnetic properties of transition metal-based alloys depend strongly on the band structure and particularly from the number of bands near the Fermi level. In the band calculations we included the S–O interaction in order to show which bands are located near the Fermi energy.

The S–O interaction does not modify the shape of the density of states but it changes the band structure.

The analysis of the electronic band structure (Figs. 5 and 6) leads to the conclusion that in the case of both the Ni_3Al and Ni_3Ga alloys only two bands (16 and 17) give non-negli-gible contribution to the density of states at the Fermi level. This information is very important if the finite-temperature properties of these materials are considered [7].

We thank Professor N.E. Christensen for the computer programs used to

calculate the band structure.

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