Solid State Communications 149 (2009) 1269–1273

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

Electronic structure and Fermi surfaces of the superconductive A_3B compounds: A = V, Nb; B = Ga, Ge and Sn

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ARTICLE INFO

Article history:
Received 30 March 2009
Received in revised form
5 May 2009
Accepted 9 May 2009 by F. De la Cruz
Available online 18 May 2009

PACS:
71.15.Ap
71.20.Lp
74.25.Jb
74.70.Ad

Keywords:
A. Superconductors
A. Intermetallic compounds
D. Band structure
D. Fermi surface

ABSTRACT

The full-potential linearized augmented-plane wave (FP-LAPW) method is employed in calculations of the band structure and Fermi surfaces of the superconductive A15 (Cr_3O-type) compounds V_3B and Nb_3B, B = Ga, Ge and Sn. A plot of the total density of states shows a minimum above E_F in all studied compounds separating bonding bands from antibonding bands. The V compounds possess higher densities of states at E_F, whereas narrower bandwidths are observed for the Nb compounds. From the results it is inferred that the higher transition temperature T_c experimentally observed for the Nb compounds arises from larger volumes of the Fermi surfaces for electron sheets besides the multi-Fermi-surface structure.

1. Introduction

In the last decades considerable theoretical and experimental work has been devoted to studying the structural and electronic properties of superconductive compounds with the A15 structure (Cr_3Si phase) [1–4]. The crystal structure is cubic with two A_3B formula units per unit cell. The six A atoms lie in pairs on the cube faces and the two B atoms occupy a body-centered lattice. The A atoms, which are transition metals, in this structure form a system of three essentially non-interacting orthogonal linear chains. These are believed to play an important role in the superconductive properties of this class of materials. The composition at which this phase is most likely to occur is influenced by the electron to atom ratio. Band structure calculations for the A15 compounds have shown significant variations even amongst the isoelectronic compounds. An extremely sharp structure is observed in the density of states within which the Fermi level falls, which arises from very flat energy bands or band minima along the symmetry lines Σ and Λ. In the source of this feature is the chainlike structure of the A atoms which could produce a very narrow one-dimensional-like d-band structure [5].

Among the metallic superconductors, the Nb-based A15 compounds, such as Nb_3T, T = Al, Ga, Ge and Sn have a relatively high T_c and high critical field; Nb_3Ge has the highest T_c (23 K). The corresponding V-based compounds have a much lower T_c. Furthermore, Nb_3Sn, V_3Ga, V_3Ge and V_3Sn exhibit a low temperature martensitic transition from the cubic to a tetragonal phase with a smaller cell volume [6]. In Nb_3Sn this has been interpreted as a Jahn–Teller band transition mechanism, in the sense invoked by the Labbé–Friedel model [7], whereupon one assumes that the band structure of the cubic A15 compounds can be represented by three sub-bands of d-type inserted into each other and superposed on a wide band of s-character. For the vanadium compounds the d-subband is less than half-full, so that the Fermi level is near the bottom of the highest d-subband, thus ensuring a high density of states at the Fermi level [8–12]. In this contribution the electronic structure of the A_3B (A15-type) compounds is studied: A = Nb,V; B = Ga,Ge and Sn. A comparative analysis of the band structure and calculated Fermi surfaces (FS) is performed for both vanadium (V_3B) and niobium (Nb_3B) compounds, in order to highlight the peculiarities of the distribution of valence electrons near the Fermi level and to provide a qualitative description of why the Nb compounds have higher T_c than the corresponding V compounds.

2. Method

The calculations were performed with the FPLAPW method [13]. The exchange and correlation effects are treated with the generalized gradient approximation (GGA) using the Perdew–Burke–Ernzerhof (1996) parametrization [14]. No shape approximation

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doi:10.1016/j.ssc.2009.05.011

Table 1
Experimental lattice constant [2,3], Fermi energy (E_F), calculated DOS at the Fermi level ($N(E_F)$), electronic specific heat coefficient (calculated γ^{band} and estimated $\gamma^{\text{expt.}} = \gamma^{\text{band}}(1+\lambda)$), measured electron–phonon coupling constant λ and T_c for A_3B compounds [2–4,11,12,19].

	Lattice constant (Å)	E_F (Ry)	$N(E_F)\left(\frac{\text{states}}{\text{Ry.cell}}\right)$	$\gamma^{\text{band}}\left(\frac{\text{mJ}}{\text{g-at K}^2}\right)$	$\gamma^{\text{expt.}}$	λ	T_c (K)
V_3Ga	4.830	0.62091	270.15	5.86	12.72	1.17	16.5
V_3Ge	4.769	0.71023	254.54	5.52	9.38	0.70	6.1
V_3Sn	4.940	0.66984	279.89	6.07	9.66	0.61	3.8
Nb_3Ga	5.171	0.73251	209.05	4.53	12.41	1.74	20.3
Nb_3Ge	5.166	0.76953	195.80	4.24	11.87	1.80	23.2
Nb_3Sn	5.289	0.77207	230.50	5.00	12.20	1.44	18.0

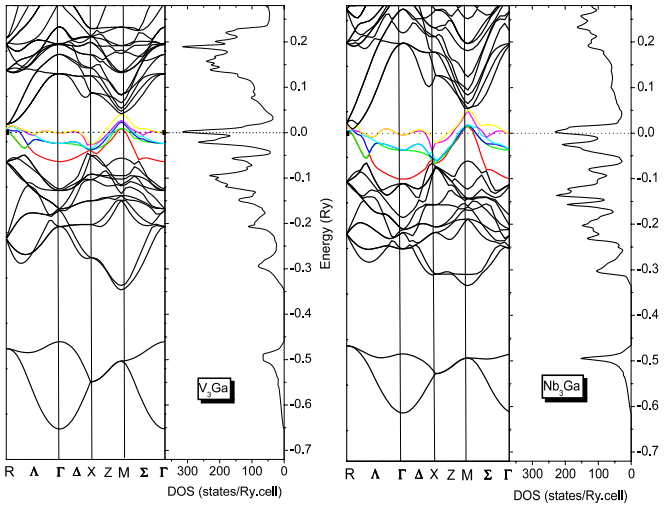

Fig. 1. Band structure around the Fermi level and total density of states (DOS) for V_3Ga (left) and Nb_3Ga (right), where the energy is taken with respect to E_F.

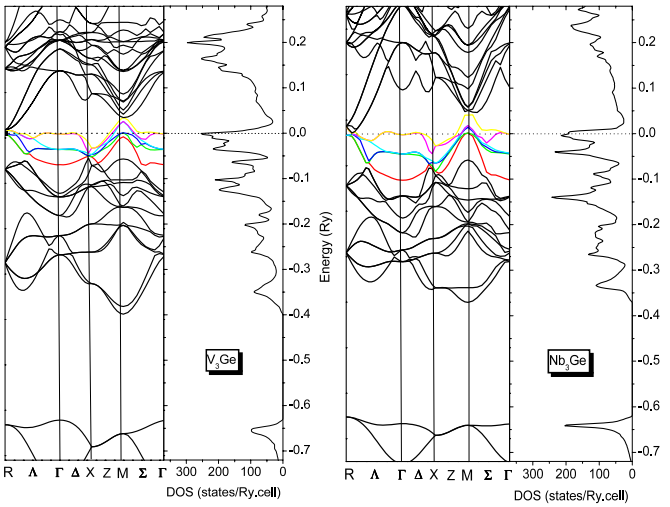

Fig. 2. Band structure and total DOS for V_3Ge and Nb_3Ge.

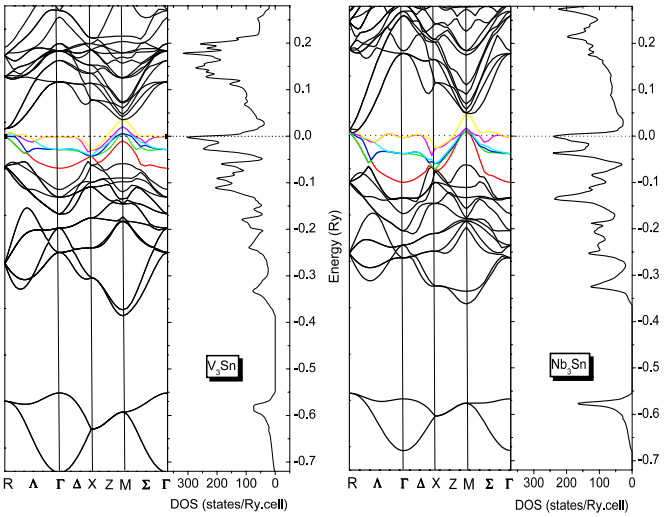

Fig. 3. Band structure and total DOS for V_3Sn and Nb_3Sn.

is used for either the potential or the electronic charge density in this method. Atomic-sphere muffin-tin radii $R_A = 2.22$ a.u. and $R_B = 2.33$ a.u have been chosen. For the A atoms this is the maximum possible radii for non-overlapping spheres. 6000 k-points were used in the calculations, which yields 226 k-points in the $\frac{1}{48}$ irreducible part of the Brillouin zone (IBZ). The experimental lattice constants for these compounds are listed in Table 1. The atomic wave function expansion was set up to $l = 10$, and the charge density Fourier expansion cutoff is taken as $G_{\max} = 12$. In order to achieve a satisfactory degree of convergence, the cutoff parameter was taken as $R_{mt}K_{\max} = 8.0$, where $K_{\max}$ is the maximal value of the reciprocal lattice vector used in the plane wave expansion, and R_{mt} is the smallest atomic sphere radius in the unit cell. The energy was used as the convergence criterion, taken to 10^{-2} mRy.

3. Results

In Figs. 1–3 are shown plots of the band structure along symmetry directions and the total densities of states (DOS) for the studied compounds. For the sake of comparison, the V_3B and Nb_3B compounds are shown together for the same B atom. A sharply peaked structure near the Fermi level E_F in the bonding region can be seen in all the DOS diagrams, as is typical for these compounds. Moreover, another common feature which can be seen in these diagrams is a somewhat flat band structure at E_F, as well as an accumulation of bands around M points in the IBZ. The flattened characteristic of the bands along Γ and Δ lines near E_F is responsible for the sharp peak observed in the DOS plots. The structure which appears at lower energies in these diagrams is due to the contribution of s-electrons from the B atom. The V d-states are found within a energy range of ≈0.2 Ry below E_F. The resonances in the DOS diagrams observed between about 0.3–0.2 Ry below E_F consist primarily of an admixture of p-states from both (A, B) atoms. A minimum is observed above E_F, which separates bonding bands from antibonding bands. Narrower bandwidths are observed for the 3d states around E_F. The observed trends are in good agreement with results of earlier calculations [8,9,12,15–19].

For the V-based compounds it can be seen in Figs. 1–3 that the center of gravity of the antibonding region is closer to the Fermi level, as compared with the corresponding Nb compounds. There is a propensity to form degenerate bands around M points. The admixture of Ga p-states and V d-states occurs within a energy