Electronic Structure of Nb_3Sn

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The electronic band structure of Nb_3Sn has been calculated by means of the augmented-plane-wave method. Comparison with a variety of experimental data suggest that the band model is highly accurate.

Primarily because of its high superconducting critical temperature,[1] the A-15 material Nb_3Sn has continued to interest experimentalists and theorists. Recent interest has focused on a number of anomalous properties in the normal state. Theoretical models have been used to correlate or make these anomalous properties understandable. Many models have focused on point-group symmetry of selected points in the Brillouin zone (BZ); others have invoked the use of tight-binding schemes with a variety of couplings within or between the dominant Nb chains.[2] Clogston and Jaccarino[3] suggested that the temperature dependence of the susceptibility and the Knight shift in V-based A-15's could be understood by a narrow peak in the density of states, $N(E)$, close to the Fermi energy E_F.

In this Letter we report an *ab initio* calculation of the electronic structure, density of states, and Fermi surface of Nb_3Sn. Our technique and methodology is similar to the well-known work of Mattheiss.[4] Without adjustment, we find good agreement with a number of experiments including the temperature dependence of the susceptibility and a recent measurement of the de Haas–van Alphen (dHvA) effect.[5]

The crystal potential was constructed from overlapping neutral atomic charge densities and exchange was treated in Slater's ($\alpha = 1$) local approximation; this technique, the "Mattheiss prescription," has produced good agreement with self-consistent local density exchange calculations in Nb.[6] Since the linear chains distort severely the spherical symmetry about the Nb sites, we have incorporated nonspherical corrections inside the MT's (muffin-tin potential). The interstitial potential deviations from a constant MT floor were incorporated as Fourier terms.[7] We have found that the contours of potential were similar to a potential constructed from the experimental charge density,[8] if appropriate cores were added.

A length ordered basis of more than 300 augmented plane waves (APW) was used to form the secular matrix. Using our potential, tests showed that all bands were converged to better than 3 mRy. Globally, the resultant band structure of Nb_3Sn was the same as that of Ref. 4 and compared equally well with XPS (x-ray photoelectron spectroscopy) data.[9] Microscopically it differed in that the Γ_{12} level (intersecting E_F) has dropped by approximately 30 mRy relative to a host of levels at M. In Fig. 1 is given the band structure in the immediate vicinity of the Fermi level, showing multiple hole structure at the point M and an intersection of the flat bands associated with Γ_{12} symmetry.

The band structure for the lowest 24 bands was found at 56 equally spaced independent points in the irreducible $\frac{1}{48}$th of the BZ. The structure was fitted to 28 symmetrized Fourier terms ("stars") and the density of states was calculated by a linear gradient method using 1728 tetrahedrons in the irreducible BZ. In Table I are listed (bare) values of the experimentally derived $N(E_F)$'s. Our results are fortuitously close to Junod's specific-heat value.[10] NMR-derived[11] results give similar agreement.

We have used $N(E)$ near E_F to calculate the temperature dependence of the Pauli contribution to the susceptibility, which depends on the derivatives of $N(E)$. Linear interpolation was applied between a $N(E)$ grid spaced by 1.25 mRy. The Fermi level was calculated at every temperature by a self-consistent procedure; it varied by more than 4 mRy nonmonotonically as T varied between 0 and 300°K. In Fig. 2 is given the temperature dependence of the susceptibility χ of Rehwald *et al.*[12] The relationship between χ and the martensitic phase transformation has recently been considered,[13] using parametrized Hamiltonians and the group symmetries of special points in the zone. Most previous discussions of $\chi(T)$ have relied on the model of Ref. 3 which utilized a large orbital contribution to explain the anomalous temperature dependence of the Knight shift. Recently,[8] it was found that in forming the related compound V_3Si, approximately two electrons transfer from each Si site to the V chains. This removes the necessity of a large

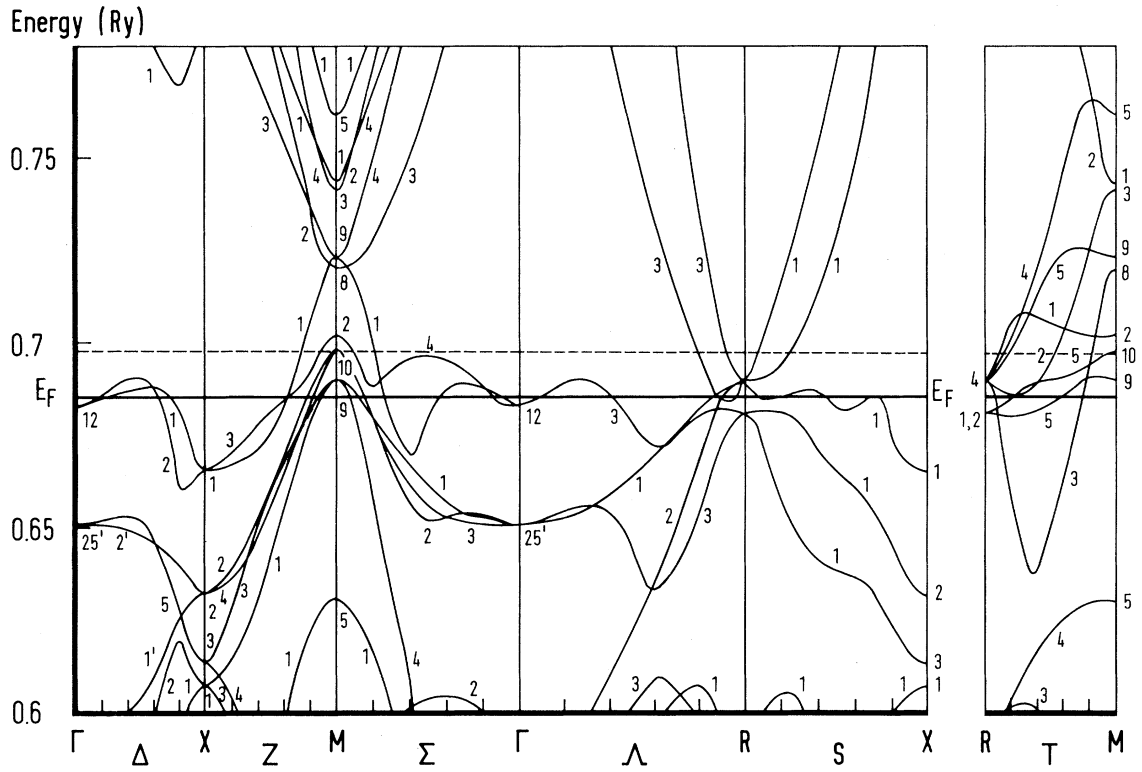

FIG. 1. The band structure of Nb_3Sn near E_F. The dashed line is E_F appropriate to Nb_3Sb.

orbital term. We plan to return to this important point. We find that by applying a constant enhancement[14] of $3.69S = \chi/\chi_0 \equiv 1/(1-\mu)$, the temperature dependence of the susceptibility is consistent with a Pauli term, where $\chi_0 = \mu_B{}^2 N(E_F)$, shown in Fig. 2 as the dashed curve.

For purposes of comparison, we consider an enlarged cell of six atoms of pure bcc Nb. Taking data from McMillan[15] ($\chi = 514$ and $\gamma = 269$ in states/Ry "cell"), and using $\lambda = 0.82$ we find a pure Nb Stoner factor of $(1+\lambda)\chi/\gamma$ or 3.38. Deriving an effective exchange interaction[14] per Nb site from $I = 12(1 - 1/S)N(E_F)$, we find 0.79 eV for bcc Nb compared with a value of 0.49 eV for Nb in Nb_3Sn. This difference reflects two competing effects: (1) The Nb-Nb nearest-neighbor distance is 7.3% smaller in Nb_3Sn (2.65 Å) than in bcc Nb (2.86 Å); (2) the number of nearest neighbors is far less in Nb_3Sn (2) than in bcc Nb (8). The second effect dominates the first.

Using these results we find estimates of μ^*, the Coulomb pseudopotential[15,16] of Morel and

TABLE I. Comparisons of $N(E_F)$ and results.

$N(E_F)$	Density of states	This work	243 states/Ry cell	
N_0	NMR	Fradin *et al.*[a]	264 states/Ry cell	
γ_0	Specific heat	Junod[b] $\gamma/(1+\lambda)$	240 states/Ry cell	
χ	Susceptibility (extrapolated)	Rehwald *et al.*[c]	896 states/Ry cell	
			Nb_3Sn	Nb
S	Stoner factor	χ/χ_0	3.69	3.48
I	Exchange interaction per Nb atom-spin	$12\mu/N(E_F)$	0.49 eV	0.79 eV
μ^*	Coulomb pseudopotential		0.25	0.18

[a]Ref. 11. [b]Ref. 10. [c]Ref. 12.

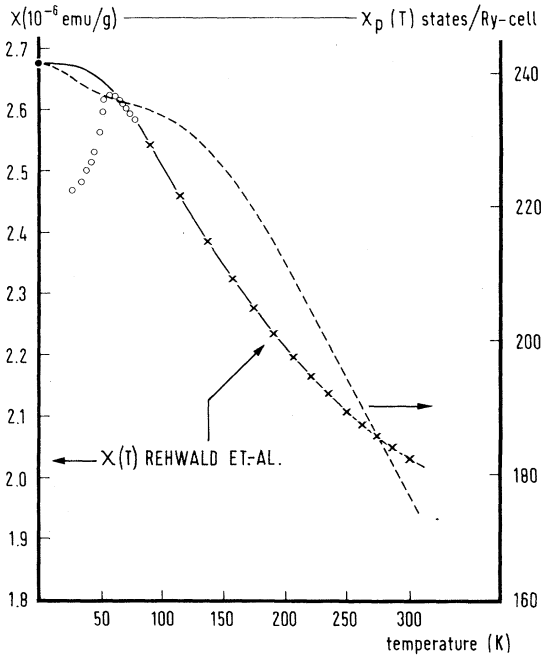

FIG. 2. The temperature dependence of the susceptibility of Nb_3Sn. The circles are the data of Rehwald *et al.* (Ref. 12) taken in the tetragonal phase, the crosses in the cubic phase, and the solid line their extrapolation function (left-hand scale). Note that both left- and right-hand scales share a common zero.

Anderson,

$$\mu^* = \frac{\mu}{1 + \mu \ln(E_B/\omega_0)}, \tag{1}$$

of 0.18 and 0.25 for Nb and Nb_3Sn, respectively. We have assumed that $\omega_0 = \omega_D/1.2$ and have used the values of 0.11 Ry[6] and 0.02 Ry (Fig. 1) for the band width E_B (near E_F), and the values[10,15] of 277° and 227° for ω_D, for Nb and Nb_3Sn, respectively.

In Fig. 3 we present the Fermi surface of Nb_3Sn (intersecting bands 15–21) in the principal symmetry planes. Because of the sensitivity of small energy shifts (especially bands 19 and 20) we have used the APW secular itself as an "interpolation scheme." Two features are noteworthy compared to the previous V_3Si isoelectronic Fermi surface[4]: (1) the greater confluence of osculated structure at *M*, and (2) the flat "boxlike" structures centered at Γ. A microscopic test of band structure near E_F is provided by the dHvA effect. Recently Arko *et al.*[5] found dHvA oscillations in Nb_3Sn single crystals using 400-kG pulsed fields. Within their accuracy and insensitivity to small pieces we find that the rich structure exhibited in Fig. 3 is consistent and can be used to interpret their data (the *M*-centered pieces).

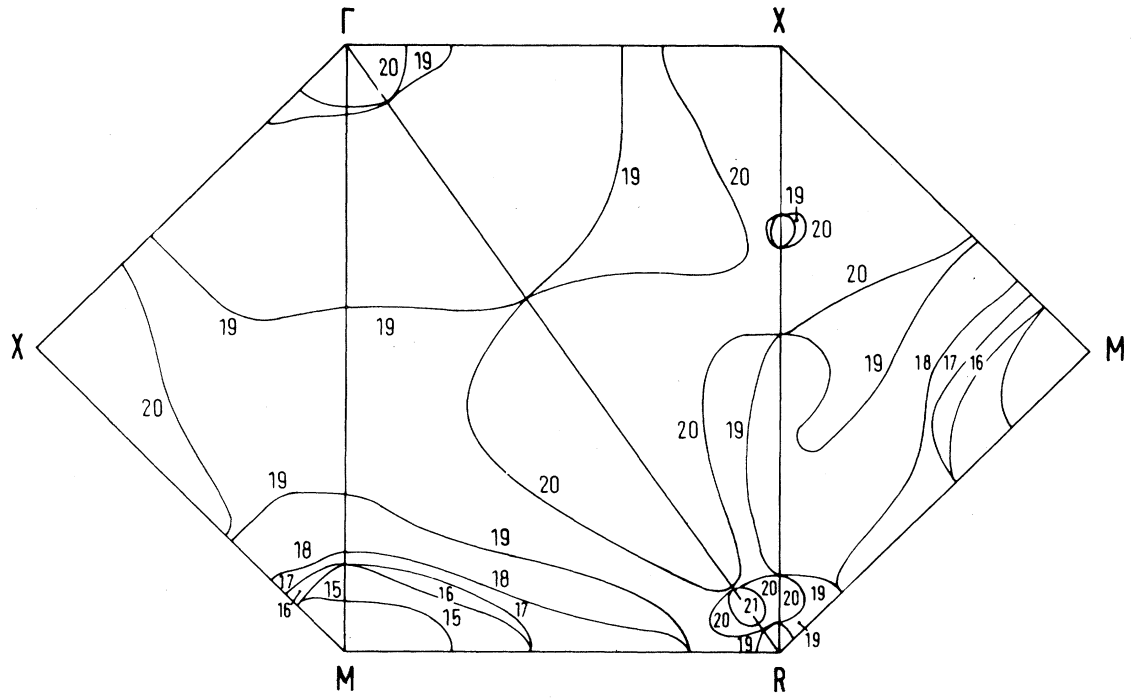

FIG. 3. The Fermi surface of Nb_3Sn. The band indexing follows Ref. 5. The positions of the labels follows the filling of $\vec{k}$ space volumes so that band 20 near Γ is an electron piece and band 15 near *M* is a hole piece.

Other band models[17] show frequencies with neither the correct magnitude nor angular variation. The pieces at M have band masses ranging from 0.23 to $1.03m_e$; those centered at Γ, 2 to 3; and those at R, 0.2. Our R-centered pieces have dHvA frequencies smaller than any seen.[5] The high mass of the Γ-centered pieces inhibits observation in the dHvA effect. Samoilov and Weger[18] have reported structure in V_3Si, using positron annihilation, in the [100] direction at 0.2, 0.6, and 0.8 π/a units. The intersections of the "flat" sheets along Γ–X are 0.15 and 0.64 π/a units in good agreement with the first pieces of structure. The twentieth band near X and surrounding the X–R line is a possible candidate for the third structure.

We conclude that our results compare well with available experimental data. In addition, the intersections of E_F for pseudo Nb_3Sb (shown in Fig. 1) are in quantitative agreement with dHvA data.[19]

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