

CALCULATIONS OF THE SUPERCONDUCTING PROPERTIES OF $\text{NbC}_{1-x}\text{N}_x$

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The electron-phonon interaction, η , and superconducting transition temperature, T_c , for the system $\text{NbC}_{1-x}\text{N}_x$ have been calculated as a function of x using the rigid-muffin-tin (RMT) method of Gaspari and Gyorffy (GG) (1972). These calculations are based on the densities of states (DOS) and scattering phase shifts resulting from self-consistent, augmented-plane-wave (APW) band structure calculations of NbN and NbC. Our band structure results of NbC have been reported previously (Klein, Papaconstantopoulos, and Boyer, 1980). The NbN APW calculation was performed in a similar manner i.e. by the spin-independent relativistic APW method with the exchange potentials determined using the $X\alpha$ parameters of Schwarz (1972). The lattice constant was taken equal to 8.273 a.u. (Skelton 1980) and the muffin-tin sphere radii ($R_{\text{Nb}} = 2.308$ a.u., $R_{\text{N}} = 1.828$ a.u.) were chosen so that the starting potentials were matched at the point of contact of the spheres. The states originating from the Nb(4s, 4p, 4d, 5s) and N(2s, 2p) atomic orbitals were treated as bands while the inner core states were calculated atomic-like. Self-consistency to within 1mRyd was achieved after six iterations. In each iteration 20 k-points in the irreducible Brillouin zone (BZ) were included. The inclusion of 20 and not 6 k-points in each iteration and the fact that the present calculation incorporates relativistic effects should account for small differences from a similar calculation performed by Schwarz (1977).

The final iteration was done for 89 k-points in the irreducible BZ and the tetrahedron method of Lehmann and Taut (1972) was used to obtain the DOS. Figure 1 shows the total DOS and its angular momentum components per site inside the muffin-tin spheres. The first peak at $\sim -0.3\text{Ryd}$ is due to s-like N states; the second peak at $\sim 0.4\text{Ryd}$ is a mixture of p-like N and d-like Nb states with the N states dominating by approximately a factor of two; the third peak at $\sim 1.0\text{Ryd}$ consists mainly of Nb d states. At the Fermi level, E_F , the states have predominantly Nb d-like character.

In the present work the DOS were used, in the rigid band approximation, to obtain at E_F the values of the DOS and of the scattering phase shifts δ_l needed to evaluate the electron-phonon interaction by the GG theory. In this scheme in the range $0 < x < 0.5$ the DOS and δ_l 's of NbC were used while in the range $0.5 < x < 1.0$ the corresponding quantities from NbN were used. These values of x correspond to a total energy range of only 0.08Ryd above the E_F of NbC and below the E_F of NbN. The resulting values of the electron-phonon interactions η_{Nb} and $\eta_{\text{N(C)}}$ are plotted in Fig. 2. One should note the almost constant value of $\eta_{\text{N(C)}}$ and the increase of η_{Nb} until it reaches a maximum value at $x \sim 0.85$, and the drop as x approaches 1.0. The results of this calculation at the NbN end are in semi-quantitative agreement with a recent self-consistent cluster approach reported by Rietschel, Winter, and Reichardt (1980). For example $N(E_F)$, the total DOS at E_F , was found from the APW results to be $N(E_F) = 0.96$ states/eV/unit cell and from the cluster results $N(E_F) = 0.88$ states/eV/unit cell.

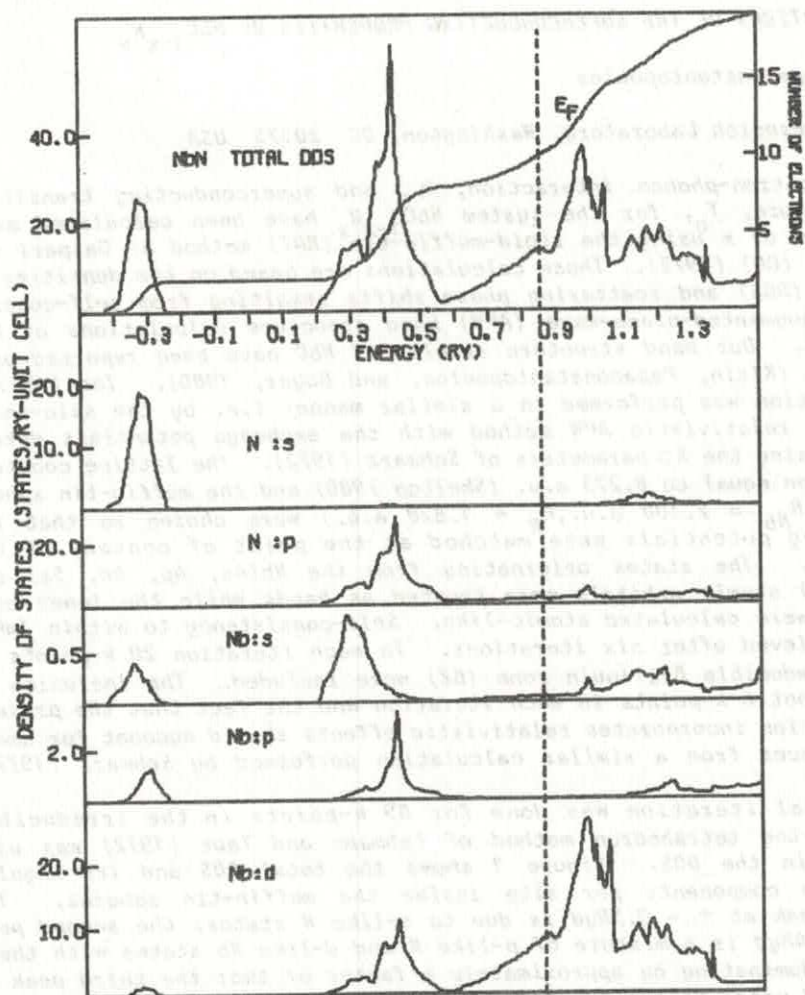


Fig. 1 The NbN total DOS and its λ -components per site inside the muffin-tin spheres.

Having calculated η_{Nb} and $\eta_{N(C)}$ as a function of x , the following expression is then used in order to compute the electron-phonon coupling constant:

$$\lambda(x) = \frac{\eta_{Nb}(x)}{M_{Nb} \omega_{Nb}^{-2}} + \frac{\eta_{N(C)}(x)}{M_{N(C)} \omega_{N(C)}^{-2}} \quad (1)$$

This equation decouples the acoustic-mode from the optic-mode scattering and is a good approximation to λ due to the large mass difference between Nb and N or C (Klein and Papaconstantopoulos, 1976).

The phonon moments ω_{Nb}^{-2} in the first term of Eq. 1 were determined from the measured phonon dispersion curves of NbC (Weber 1973; Feldman and Skelton 1974) by a linear extrapolation to the NbN end, utilizing the measured Debye temperatures of NbC $_{1-x}N_x$ (Roedhammer et al 1977).

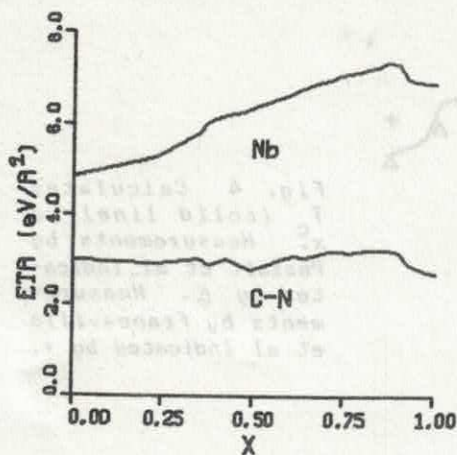


Fig. 2 Electron-phonon interactions vs N content.

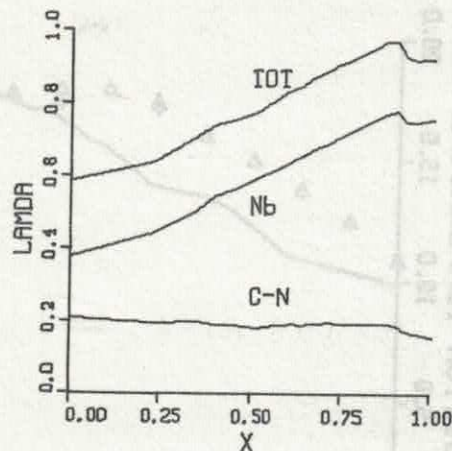


Fig. 3 Electron-phonon coupling constant vs N content.

The phonon moments $\bar{\omega}_{N(C)}^2$ in the second term of Eq. (1) were set equal to the value at the NbC end, while the mass $M_{N(C)}$ was taken as an average of the nitrogen and carbon atomic masses. Figure 3 shows $\lambda(x)$ as well as the components $\lambda_{Nb}(x)$ and $\lambda_{N(C)}(x)$. These graphs show similar behavior as those for $\eta(x)$ with $\lambda(x)$ varying more rapidly due to the inclusion of the x dependence of the phonon moments.

Finally $T_c(x)$ was calculated using the Allen-Dynes (1975) equation with $\omega_{log}(x)$ determined from the phonon moments discussed above and the Coulomb pseudopotential $\mu^*(x)$ calculated from a modified version of the Bennemann-Garland (BG) (1972) formula:

$$\mu^*(x) = \frac{AN(E_F)}{1+N(E_F)} \quad (2)$$

The modification to the above formula consists of reducing the constant A from the value 0.26 given by BG to the value 0.20. This reduction of A makes the results for T_c approximately 1°K higher and in better overall agreement with experiment. It seems that it makes physical sense to have μ^* depend on $N(E_F)$ and not to set it equal to a constant as is often done. The values of μ^* resulting from Eq. (2) and used in the present work range from 0.08 to 0.10.

The calculated T_c versus x is plotted in Fig. 4 where it is compared with the measured values of Pessall, Gold and Johansen (1968) and those of Francavilla, Wolf and Skelton (1980). The calculation reproduces very well the overall variation of T_c shown in the measurements. This calculation predicts that a maximum $T_c(max)$ of 17.8°K is found at $x = 0.87$. This result does not agree with the earlier experiments (Pessall et al 1968) which gave the $T_c(max)$ at $x \sim 0.75$. However, the more recent measurements of Francavilla et al (1980) are in very good agreement with the present theory regarding the location of this maximum. Both sets of experiments seem to show a broader peak than that found in the calculations. This discrepancy may be due to deviations from stoichiometry in the samples. It should be noted that

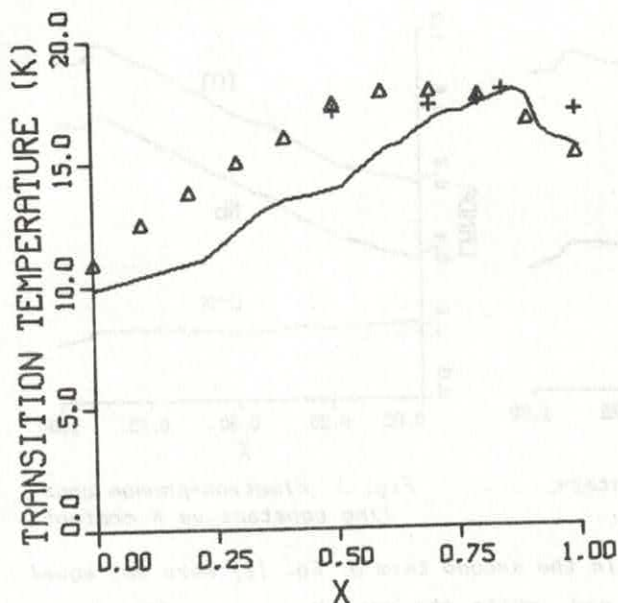


Fig. 4 Calculated T_c (solid line) vs x . Measurements by Pessall et al indicated by Δ . Measurements by Francavilla et al indicated by +.

what is important here is the trend of T_c and not the absolute numerical values which are sensitive to the details of the calculation (RMT approximation, phonon spectra data and μ^*).

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