EVAN-R 73-0015

LETTER TO THE EDITOR

A calculation of the pressure dependence of the superconducting transition temperature T_c in niobium and vanadium

R Evans†, V K Ratti‡ and B L Gyorffy

H H Wills Physics Laboratory, Tyndall Avenue, Bristol BS8 1TL, UK

Abstract. The electronic part, η, of the electron–phonon mass enhancement is calculated at normal and reduced volumes for Nb and V. We find that η increases rapidly with decreasing volume and the coefficients $d\ln\eta/d\ln V$ are in good agreement with empirical analyses of the pressure dependence of T_c in these transition metals.

Unlike superconducting simple metals where the pressure derivative dT_c/dp is, in general, negative, this derivative varies in sign as well as magnitude between different transition metals (for a comprehensive review see Smith 1972a). Recently, Hopfield (1971) has analysed some of the experimental results for transition metals using the McMillan (1968) equation for T_c:

$$T_c = \frac{\theta_D}{1\cdot45} \exp\left(\frac{-1\cdot04\,(1+\lambda)}{\lambda - \mu^*(1 + 0\cdot62\lambda)}\right) \tag{1}$$

where θ_D is the Debye temperature and μ^* is the electron–electron interaction parameter. The electron–phonon enhancement λ can be written as:

$$\lambda = \frac{n(E_F)\langle I^2\rangle}{M\langle\omega^2\rangle} = \frac{\eta}{M\langle\omega^2\rangle} \tag{2}$$

where M is the atomic mass, $\langle\omega^2\rangle^{1/2}$ is an appropriate average phonon frequency, $n(E_F)$ is the electronic density of states at the Fermi energy E_F and $\langle I^2\rangle$ is the square of the electron–phonon matrix element averaged over the Fermi surface. Neglecting the variation of μ^* with volume Hopfield obtained from equation (1):

$$\frac{d\ln T_c}{dp} = \frac{1}{B}\left[\gamma_g + \left(\frac{1\cdot04\lambda}{\lambda - \mu^*(1 + 0\cdot62\lambda)} - \frac{1\cdot04\lambda(1+\lambda)(1 - 0\cdot62\mu^*)}{[\lambda - \mu^*(1 + 0\cdot62\lambda)]^2}\right)\left(2\gamma_g + \frac{d\ln\eta}{d\ln V}\right)\right] \tag{3}$$

where B is the bulk modulus, γ_g is the *effective* Gruneisen $\gamma = -d\ln\langle\omega^2\rangle^{1/2}/d\ln V$ and $\theta_D/1\cdot45$ has been replaced by $\langle\omega^2\rangle^{1/2}$.

Since the first large parentheses in equation (3) is $-2\cdot0$ or less the sign of dT_c/dp is determined *mainly* by the magnitude of γ_g. Roughly speaking for $\gamma_g > 1\cdot7$ this sign is negative and is positive for smaller values of γ_g. Taking experimental values of dT_c/dp and B and estimates of γ_g from Gschneider (1964) Hopfield inverted equation (3) to obtain

† Present address: Institut für Theoretische Physik, Freie Universität Berlin, 1 Berlin 33, West Germany.
‡ Present address: Institute of Theoretical Physics, University of Alberta, Edmonton, Alberta, Canada.

d ln η/d ln V for several transition metal superconductors. He found this quantity was fairly constant; a typical value being -3.5. This is in contrast to simple metals for which d ln η/d ln $V \sim -1.0$ and dT_c/dp can be well understood using pseudopotential theory, eg Trofimenkoff and Carbotte (1970), Carbotte and Vashishta (1971) and Coulthard (1971).

In this letter we present *ab initio* calculations of d ln η/d ln V for Nb and V using the theory of Gaspari and Gyorffy (1972). This model gives a simple expression for the electronic parameter η in terms of quantities which can be obtained from band theory:

$$\eta = \frac{2mE_F}{\hbar^2\pi^2} \left(\frac{2 \sin^2(\delta_1 - \delta_0)}{n(E_F)} + \frac{[4 \sin^2(\delta_2 - \delta_1) + 6 \sin^2\delta_2]n_2(E_F)}{n_2^{(1)}n(E_F)} \right) \qquad (4)$$

where δ_0, δ_1, δ_2 are the angular momentum phase shifts of the appropriate muffin-tin potential evaluated at E_F, n_2 is the d component of the density of states and $n_2^{(1)}$ is the d component of the 'single scatterer' density of states (see Evans *et al* 1973):

$$n_2^{(1)} \simeq \frac{5}{\pi} \frac{\mathrm{d}\delta_2}{\mathrm{d}E} (E_F). \qquad (5)$$

Calculations based on equation (4) have been carried out by Evans *et al* (1973) for several transition metals and the results for η are in qualitative agreement with the empirical estimates obtained by McMillan (1968) from the inversion of equation (1). Evans *et al* have also discussed the approximations and assumptions involved in the Gaspari–Gyorffy scheme.

In order to apply this theory to the calculation of d ln η/d ln V we require muffin-tin potentials, densities of states and Fermi energies for metals at different lattice spacings. A few non self-consistent band structure calculations have been carried out at reduced lattice spacings eg Davis *et al* (1968) on Cu, O'Sullivan *et al* (1971) on the noble metals and Das *et al* (1973) on Pd. These calculations are based on the Mattheiss (1964) prescription for the lattice potential and give successful descriptions of the pressure variation of the Fermi surface and electronic specific heat. Similar self-consistent calculations are reported by Kmetko (1971) and recently by Papaconstantopoulos *et al* (1972) for V and by Anderson *et al* (1973) for Nb.

We have used the self-consistent muffin-tin potentials of these latter authors to calculate the phase shifts δ_l at normal and reduced lattice spacings for Nb and V. This procedure is the same as that used by Stocks *et al* (1972) in their calculation of T_c for Cs under pressure. The phase shifts are given in Table 1 along with the densities of states calculated by Papaconstantopoulos *et al* and Anderson *et al*.

Table 1. Phase shifts δ_l and energy derivative δ_2' evaluated at the Fermi energy E_F. $n(E_F)$ is the density of states and R_s is the Wigner–Seitz radius

	R_s (au)	E_F (Ryd)	δ_0	δ_1	δ_2	δ_2' (Ryd^{-1})	$n(E_F)$ (spin states/atom/eV)
Nb (normal)	3.071	0.75	-1.0437	-0.4403	1.0336	4.551	1.037
Nb (reduced)	2.918	0.935	-1.254	-0.584	1.0483	3.147	0.853
V (normal)	2.813	0.76	-0.7978	-0.232	0.8945	7.062	0.978
V (reduced)	2.672	0.92	-0.961	-0.325	0.9606	5.552	0.794