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CALCULATIONS OF THE PRESSURE DEPENDENCE OF THE SUPERCONDUCTING TRANSITION TEMPERATURE OF VANADIUM

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An evaluation of the pressure derivative of the superconducting transition temperature of vanadium is presented. These calculations were performed by using detailed band structure results and the rigid-muffin-tin approximation. Good agreement with experiment is obtained.

During the last few years considerable progress has been made in determining superconducting transition temperatures, T_c, from first-principles calculations. Specifically, electronic band structure results have been used together with the rigid-muffin-tin-approximation-theory of Gaspari and Gyorffy[1] to evaluate the electronic part, η, of the electron-phonon coupling constant λ. Using these results together with experimental information on the phonon spectra, λ and T_c have been calculated, the latter from a McMillan-like equation.[2] This approach was used with considerable success to evaluate λ and T_c for most of the elements in the periodic table with Z<50,[3,4] and for compounds such as carbides,[5] A15s,[6] and palladium-hydrogen systems.[7] However, the determination of the pressure dependence of T_c has received much less attention. Early attempts by Hopfield,[8] Garland and Bennemann,[9] and by Evans et al, [10] were primarily qualitative in nature, due to the fact that they did not utilize the detailed band structure information needed in such calculations. More recently, Pickett et al[11] have presented a calculation of T_c for La for three different lattice spacings ignoring any phonon variation.

Here we present calculations of $\partial T_c/\partial p$ where the only experimental information used are phononic properties, i.e. phonon moments and their volume dependences, the bulk modulus, and the normal lattice constant values of λ and T_c. These calculations were based on two sets (I and II) of non-relativistic, self-consistent augmented-plane-wave (APW) calculations at normal and reduced lattice spacings. The first set (I) utilized the Hedin-Lundqvist potentials of Moruzzi et al[12,3] while the second set (II) used self-consistent potentials [13] generated with the Xα exchange-correlation approximation.

In both sets of calculations, APW eigenvalues and wave functions were determined on a mesh of 285 k-points in the 1/48th of the bcc Brillouin zone, and tetrahedral integration was used to obtain the total density of states (DOS), N, as well as the angular momentum decomposed DOS, N_ℓ, within the muffin tin spheres, as needed in the Gaspari-Gyorffy theory.[1] Other quantities needed to evaluate η such as the scattering phase shifts, free-scatterer DOS, etc., were determined from the self-consistent potentials. The results, including the values of $\partial \ell n \eta / \partial \ell n V$ are given in Table I. We note that the values of η and its volume derivatives differ by as much as 10% for the two sets of calculations, pointing out the sensitivity of the results to the exchange-correlation potential and to the fact that sets I and II involve 3% and 1% compressions, respectively. It can also be seen from Table I that $N(E_F)$ decreases under pressure while η increases. This increase in η is obviously due to an increase of the electron-phonon matrix element $\langle I^2 \rangle$.

To calculate $\partial T_c/\partial p$ we differentiate the McMillan equation[2,8] to obtain,

$$\frac{\partial T_c}{\partial p} = \frac{T_c}{B}\left\{\gamma_G - \frac{1.04\lambda(1+0.38\mu^*)}{\chi^2}\left[2\gamma_G + \frac{\partial \ell n \eta}{\partial \ell n V}\right] + \frac{\partial \mu^*}{\partial \ell n V}\,\frac{1.04(1+0.62\lambda)(1+\lambda)}{\chi^2}\right\} \qquad (1)$$

with, $\chi = \lambda - \mu^*(1+0.62\lambda)$.

In Eq. (1) we have used the value 142.9 GPa for the bulk modulus, B, and the value of the Gruneisen parameter, γ_G, has been estimated from thermodynamic data.[14] There is, unfortunately, a good deal of uncertainty in the value of γ_G to be used in Eq. (1), so that we report results in Table I using three different values: $\gamma_G = 1.5 \pm 0.1$ which should bracket the spectrum of "reasonable" choices. For T_c we have used the measured value of 5.3°K and set $\lambda = 0.67$ found by inverting the Allen-Dynes equation[2] using $\mu^* = 0.13$. We have not used the calculated value of λ since it is well known that η is seriously overestimated by the rigid-muffin-tin approximation. We are confident, however, that our calculated values of the pressure derivative $\frac{\partial \ell n \eta}{\partial \ell n V}$ given in Table I are reliable. We have not included the

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volume dependence of any anomalous spin fluctuation[15] terms explicitly, but it could be argued that we have approximately accounted for this effect by using the empirical value of λ together with the inclusion of the term $\frac{\partial \mu^*}{\partial \ell n V}$ discussed below.

Some special mention of our inclusion of a $\partial\mu^*/\partial \ell n V$ term in Eq. (1) should be made. In previous studies of $\partial T_c/\partial p$ it has usually been assumed that this term is negligible, but we have not found this to be the case. The volume variation of μ^* makes a significant contribution and must be handled carefully. To evaluate $\partial \mu^*/\partial \ell n V$ we have used a modified Bennemann-Garland formula,[9]

$$\mu^* = \frac{A\, N(E_F)}{1+ N(E_F)}, \qquad (2)$$

with A determined by using $\mu^* = 0.13$ in both calculations I and II at normal lattice constant (with the appropriate $N(E_F)$ values). The smaller values of μ^* under pressure result from the decrease of $N(E_F)$ upon contraction (see Table I). The dependence of μ^* on $N(E_F)$, given in Eq. (2) although not exact, is reasonable and physically appealing.

The results for $\partial T_c/\partial p$ are also given in Table I where we note the fairly good agreement with the measured[14] value of 0.062°K/GPa especially for calculation I. The sign of $\partial T_c/\partial p$ is predicted correctly in all of the six results shown.

We believe that the present results are very encouraging. It appears that reliable theoretical estimates of $\partial T_c/\partial p$ can be made if reasonable values of γ_G can be obtained from experiment. Further results on different materials will be presented in future publications.

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Table I

Quantities used in the calculation as defined in the text. Note that $\partial T_c/\partial p$ is given for three different choices of the Gruneisen parameter γ_G.

	Calc. I		Calc. II	
a(a.u.)	5.720	5.550	5.713	5.656
$N(E_F)$ (states per Ry-atom-spin)	12.815	11.532	13.035	12.618
η (eV/Å^2)	7.165	8.890	7.177	7.722
$\frac{\partial \ell n \eta}{\partial \ell n V}$	-2.782		-2.558	
μ^*	0.130	0.125	0.130	0.128
$\frac{\partial \mu^*}{\partial \ell n V}$	0.055		0.051	
$\frac{\partial T_c}{\partial p}(\gamma_G=1.4)$°K/GPa	0.071		0.044	
$\frac{\partial T_c}{\partial p}(\gamma_G=1.5)$°K/GPa	0.052		0.024	
$\frac{\partial T_c}{\partial p}(\gamma_G=1.6)$°K/GPa	0.033		0.005	