Electron-phonon spectral function and mass enhancement of niobium

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The electron-phonon spectral distribution function $\alpha^2(\omega)F(\omega)$ has been calculated for niobium. The electron energy bands and wave functions were obtained from a self-consistent augmented-plane-wave muffin-tin potential, and the electron-phonon matrix elements were evaluated using the so-called rigid-ion approximation. With this approximation, it is found that $\alpha^2(\omega)$ is constant over the whole energy spectrum. The electron-phonon mass enhancement has also been calculated for local regions of the Fermi surface and found to be anisotropic. The calculated local values of the enhancement do not agree with experimental values available for different orbits from de Haas–van Alphen measurements. The discrepancy seems to arise because the bare-rigid-ion matrix elements are relatively small between states with nearly pure $l = 2$ character.

For d- and f-band materials, the relationship between normal-state and superconducting-state properties is still a major problem. In their phenomenological work, McMillan[1] and, more recently, Allen and Dynes[2] have shown the importance of and the need for a better understanding of such normal-state parameters as the electron-phonon interaction, the density of electron states at the Fermi level, and the phonon spectral distribution. These properties are related in a complicated manner, but the task of sorting out the coupling mechanisms is essential for determining the details governing superconductivity in high-T_c materials. In principle, band-structure calculations yielding accurate energy eigenvalues and wave functions for states on the Fermi surface are capable of dealing with these problems. In this paper, we present first-principles numerical calculations which help to clarify the present difficulties and capabilities of band-structure calculations in determining the relevant normal-state properties. In Sec. I, we discuss the calculational aspects of evaluating the electron-phonon spectral function α^2F, and in Sec. II, we give the results and comment on several recent experimental measurements of this function. The preliminary results of this calculation which were reported at the Second Rochester Conference on d- and f-band Superconductivity[3] contain an error which is corrected in this paper. Section III contains the calculations for the local mass enhancement and the comparison with experiment.

I. CALCULATIONAL DETAILS

The electron-phonon (e-p) spectral distribution function is given by

$$\alpha^2(\omega)F(\omega)=\frac{1}{N(E_F)}\frac{\Omega^2}{(2\pi)^6}\oint_{E_F}\frac{dS'}{|\nabla_k E|}\oint_{E_F}\frac{dS'}{|\nabla_{k'}E|}\sum_j\frac{|\langle\vec{k}|\vec{\nabla}V\cdot\hat{\epsilon}_j(\vec{k}-\vec{k}')|\vec{k}'\rangle|^2}{2M\omega_{\vec{k}-\vec{k}',j}}\delta(\omega-\omega_{\vec{k}-\vec{k}',j}), \tag{1}$$

where the integrals are over the Fermi surface, $\hat{\epsilon}_j$ and ω_j denote the phonon eigenvector and frequency of the jth branch for wave vector $(\vec{k}-\vec{k}')$, and $\vec{\nabla}V\cdot\hat{\epsilon}$ stands for the screened e-p interaction. The e-p mass enhancement is perhaps the single most relevant parameter for superconductivity since it gives an average strength of the electron-phonon coupling. It is given by

$$\lambda=2\int\alpha^2(\omega)F(\omega)\omega^{-1}\,d\omega, \tag{2}$$

where $F(\omega)$ is the phonon density of states. It has been customary to approximate this expression by[1]

$$\lambda=\eta/M\langle\omega^2\rangle, \tag{3}$$

where

$$\eta=\frac{1}{N(E_F)}\frac{\Omega^2}{(2\pi)^6}\oint_{E_F}\frac{dS}{|\nabla_k E|}\oint_{E_F}\frac{dS'}{|\nabla_{k'}E|}\times\langle\vec{k}|\vec{\nabla}V|\vec{k}'\rangle\cdot\langle\vec{k}'|\vec{\nabla}V|\vec{k}\rangle, \tag{4}$$

and the approximation is made by taking

$$\langle\omega^2\rangle = \int F(\omega)\omega\, d\omega \Big/ \int F(\omega)\omega^{-1}\, d\omega\,. \quad (5)$$

The accurate determination of α^2F, η, or λ depends primarily on the quality of the electron-phonon matrix elements. A simple and elegant method of evaluating η has been devised by Gaspari and Gyorffy[4] (hereafter referred to as GG). They used the so-called rigid-ion approximation for the matrix elements in which ∇V is the gradient of the potential used in the calculation of the band structure. This procedure ignores the tails of the "atomic" potentials in the interstitial regions as well as the electronic charge deformation and redistribution associated with the ionic displacements. We have argued that such charge redistributions can be important in metals containing transition elements[5]; however, as a first approximation it seems reasonable to use this much simpler model in which the valence charge within a muffin-tin sphere moves rigidly with the ion. In their procedure, GG averaged wave-function coefficients over the Fermi surface, a procedure which John[6] has shown to be valid for cubic monatomic crystals. A drawback of the GG method is that it precludes the consideration of individual phonons; hence the evaluation of Eq. (1) is not feasible within the GG framework. Application of the GG method for calculating η has been made by Klein and co-workers[7] for a large number of superconductors.

The calculations presented in this paper used the augmented-plane-wave (APW) energy bands and wave functions of a self-consistent muffin-tin potential for which the Slater exchange parameter α was equal to $\frac{2}{3}$.[8] An expression for the e-p matrix elements is given by Sinha.[9] As in the GG method, we neglected the interstitial potential and screening effects. For states on the Fermi surface, it can be shown that our matrix elements should be equivalent to those assumed by GG before averaging; however, in evaluating radial integrals of the type

$$\int_0^{R_{MT}} R_\ell(r)\frac{dV(r)}{dr}R_{\ell\pm1}(r)r^2\,dr\,, \quad (6)$$

GG chose to integrate to just beyond the muffin-tin sphere radius, thus including the unphysical step discontinuity in the potential caused by the muffin-tin approximation. We have chosen to integrate just up to the muffin-tin radius for our calculations. This is a technical detail and does not make a very significant difference in the matrix elements, as can be seen in Table I, in which the various angular momentum contributions to η have been listed. The row labeled GG(1) gives the results using the GG method as published,[4] while GG(2) labels the results for which the step discontinuity of the potential is not included. The small differences between our results using Eq. (2) and GG(2) are probably due to the lack of total convergence in our summations, which were terminated because of computational expense. Our calculation includes cross terms[6] [arising from p-d transitions in one matrix element in Eq. (4) but d-f transitions in the other] and yields a total value for η of 10.33 eV/Å^2.

TABLE I. Comparison of the results of Eq. (4) using 816 651 matrix elements with the results using the method of Ref. 4. Units are eV/Å^2.

η	s-p	p-d	d-f
Eq. (2)	0.80	4.91	4.18
GG(1)	0.61	3.78	4.53
GG(2)	0.82	4.83	4.11

In addition to the matrix elements, there may be some concern as to the appropriateness of a muffin-tin potential for these calculations. The question naturally arises: How good are the wave functions and eigenvalues (Fermi surface) obtained from a muffin-tin potential? The question has been thoroughly investigated very recently by Elyashar and Koelling, who performed a relativistic, self-consistent, $\alpha = \frac{2}{3}$ APW calculation using a completely general potential.[10–12] They found that the energy eigenvalues were surprisingly accurate within the muffin-tin approximation (e.g., the Fermi energy changed by only 3 mRy in going from a muffin-tin self-consistent potential to a completely general self-consistent potential.[12] The wave functions (and therefore the charge density) did show some sensitivity to the nonspherical terms in the potential. There was an increased contribution to the $L = 4$ angular component of the density and nonuniform shifts of the order of (2–3)% in the angular momentum character of the wave functions—generally in the direction of increased anisotropy.[10,11] Although these changes are significant for accurate x-ray analysis or for understanding the anisotropy in accurate induced magnetic form factor measurements by neutron diffraction, the changes are not as important for our calculations. Thus, the greatest significance of the Elyashar-Koelling results is to give confidence in the wave functions from the muffin-tin potential. Of particular concern (as emphasized in the GG technique) is the l character of the wave functions at the Fermi surface. A comparison between the $\alpha = \frac{2}{3}$ muffin-tin and general self-consistent potential results indicated that there were less than 2% differences in the different l components of the density of

states at the Fermi level.[12,13]

The integrations over the Fermi surface were accomplished by adopting the tetrahedron methods which have been developed for evaluating the density of states.[14,15] The irreducible $\frac{1}{48}$ of the Brillouin zone is divided into many small tetrahedrons. Inside each tetrahedron the energy bands are linearly interpolated between the four corner energies. As the number of small tetrahedrons increases, the linear approximation converges to the correct analytic results. Within a tetrahedron, a constant energy surface is a plane whose area can easily be obtained, as can the gradient, $\nabla_k E$. In our calculations the Fermi surface cut through 231 tetrahedrons in the $\frac{1}{48}$ of the Brillouin zone. Wave functions were evaluated at the center of mass of each of the 231 planes comprising the $\frac{1}{48}$ section of the Fermi surface. The summation over $\vec{k}'$ in Eq. (1) requires $\vec{k}'$ to vary over the entire Fermi surface so that group theory is required to rotate those wave functions obtained in the $\frac{1}{48}$ into the other sections of the complete zone. Our procedure then was to pick a $\vec{k}$ in the $\frac{1}{48}$ for which the incremental area ΔS and the gradient were known and let $\vec{k}'$ vary over the other 231×48 independent wave functions. In this manner, $\alpha^2(\omega) \times F(\omega)$ or $\lambda_{\vec{k}}$ can be obtained for each $\vec{k}$. In principle, we should have summed over all 231 $\vec{k}$ in the $\frac{1}{48}$, but because of computational expense the summation was truncated. The 73 $\vec{k}$ which had the largest weight ($\Delta S/|\nabla_k E|$) were included. These account for 67% of the total density of states at the Fermi energy, and result in 816 651 total matrix elements. Because each $\lambda_{\vec{k}}$ was calculated, the convergence of the average λ could be watched and was found to be stable after about 50 $\vec{k}$ points had been included. We believe our final results are accurate to within 3%. This is supported by the comparison with the calculation of η by the GG method as described above. The phonon frequencies and eigenvectors were obtained for each of the 816 651 matrix elements using an eighth-nearest-neighbor force constant fit.[16] It was in fact the use of the transpose of the phonon-eigenvector matrix rather than any mistake in the electron-phonon matrix elements which caused the error in Ref. 3.

II. DISCUSSION OF $\alpha^2 F$ RESULTS

The calculated $\alpha^2 F$ function, Eq. (1), is given as a histogram in Fig. 1 along with the phonon density of states.[16] For comparison, both curves are shown normalized to the same area. It is clear from this figure that α^2 is independent of energy within the precision of the calculation. The value of λ obtained from Eq. (2) was 1.58, which is considerably larger than the range of values (~ 0.9–1.0)

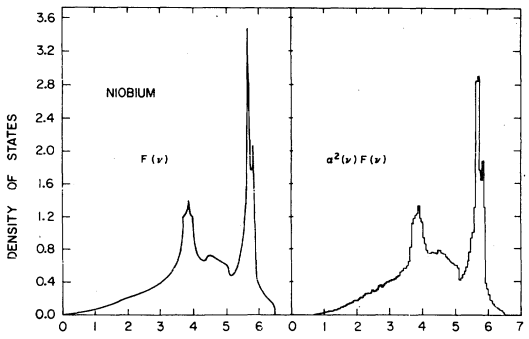

FIG. 1. Phonon density of states F for Nb using the force constant fit of Ref. 16, and the calculated electron-phonon spectral function $\alpha^2 F$, which for comparison has been normalized to the same area.

commonly accepted for Nb.[1,2] It is also slightly larger than recent calculations[8,17] which used different muffin-tin potentials and included the potential step discontinuity in the electron-phonon matrix elements. An earlier and less precise calculation of λ by Yamashita and Asano[18] yielded $\lambda = 1.7$. In considering all the calculations and the various approximations, it seems fair to conclude that first-principles calculations overestimate λ by 20–50%. It is quite likely that screening beyond that implicitly included in the rigid-ion approximation could account for this difference. If λ cannot be so accurately calculated at present, one may hope to learn more from calculations of $\alpha^2 F$ which provide considerably more information than the single number λ. Unfortunately, the experimental situation regarding the $\alpha^2 F$ of Nb is not completely resolved.

There have been to our knowledge three recent independent superconducting tunneling measurements of $\alpha^2 F$ for Nb.[19–22] The three experiments used different techniques to make the tunnel junctions, and the results differ in the measured value of gap energy. The values of λ and μ^* which are obtained from the data using the inversion program of McMillan and Rowell[23] were also different, with λ varying from ~0.4 to 1.0 and μ^* from ~ −0.08 to +0.1. In spite of these differences, the shape of $\alpha^2 F$ obtained from each of these measurements was remarkably similar. The most noticeable feature of the measured $\alpha^2 F$ curves is the attenuation of the high-energy longitudinal peak relative to the transverse peak. This is a common feature in many tunneling spectra, and Shen has argued that the high-energy phonon induced structure is smeared because the high-energy electrons have a shorter mean free path and are thus affected proportionately more by any surface irregularities.[19] There is evidence that better junctions produce more longitudinal peak structure. However, no

measured α^2F has come close to giving the relative peak strengths shown in Fig. 1; thus, it is still an open question as to how much of the longitudinal attenuation is intrinsic. It should be noted that a broadening of the calculated α^2F or $F(\omega)$ cannot account for the experimental results, and that there is an actual decrease in the strength α^2 or loss (by surface scattering?) of tunneling electrons at higher energies.

The high-energy structure in α^2F is not as important in determining the superconducting properties as the very-low-energy regions because of the ω^{-1} weighting [see Eq. (2)]. The experiments which give $\mu^* > 0$ do seem to have some enhancement above $F(\omega)$ in Fig. 1 for the low-energy region below the transverse peak. It is not known whether this enhancement is due to variations of α^2 or the observed softening (~15%) of the low-energy transverse phonon branches as T is lowered from room temperature to below T_c(Ref. 24) [the $F(\nu)$ results in Fig. 1 are for $T = 300\,^\circ$K]. We are thus unable to make any definite statements regarding the accuracy of our calculated α^2F, except that the magnitude is ~50% too large.

III. MASS ENHANCEMENT

The local mass enhancement for electrons in a particular de Haas–van Alphen orbit can be obtained by taking the ratio of the measured cyclotron mass to the effective mass obtained from a band-structure calculation. There is, however, considerable uncertainty in both the experimental and theoretical effective masses, so that accurate values of λ are difficult to obtain by this procedure. In the discussion below the important aspect of these "measured" mass enhancements is the trends which are observed for orbits on different pieces of Fermi surface. Extensive experimental data for Nb have recently become available and have been compared with band-structure calculations.[25] These new results agree with previous de Haas–van Alphen experiments where data are available,[26,27] but generally give larger (~15%) masses than those originally obtained by magnetothermal oscillations.[28] The values of λ obtained for orbits on the N-centered ellipsoids and the multiply connected "jungle-gym" pieces of the Fermi surface follow the same trend reported earlier by Mattheiss[29] and by Anderson *et al.*[8]

In order to be specific, we will use the experimental effective masses reported by Karim and Ketterson[25] and the average values of the band-structure effective masses reported by Mattheiss[29] and by Elyashar and Koelling.[11,12] The values of λ for all the orbits on the ellipsoids are surprisingly uniform, the average λ being 0.97 with a rms deviation of 0.08. For the jungle-gym orbits, there is considerably more variation, with λ being about 1.2 for the Γ-centered orbits and increasing to ~1.8 for the jungle-gym arm minimum. The Γ-centered octahedron orbits were the most difficult to obtain because of the large masses; however, the results indicate λ is uniformally large and varies between ~1.5 and 2.0. We can summarize these results by noting that the largest effective mass and mass enhancements are associated with the Γ-centered octahedron; the jungle-gym orbits show more variation, but still have larger enhancements than the N-centered ellipsoids, which have very uniform and smaller enhancements. This relationship between the jungle-gym and ellipsoid enhancements has been observed previously.[8,29] We note that if these values of λ are taken as being

TABLE II. l decomposition (%) of ψ_k and mass enhancement.

Surface	$l=0$	$l=1$	$l=2$	$l=3$	λ_k
N-centered ellipse					
1	12	31	48	6	1.86
2	3	44	45	3	1.86
3	13	36	42	6	1.88
4	2	40	49	4	1.73
5	10	46	39	3	1.95
Jungle gym					
1	1	6	91	4	1.39
2	1	5	90	5	1.34
3	0	6	92	5	1.27
4	2	10	86	4	1.47
5	0	6	91	5	1.34
6	0	10	86	6	1.41
Γ-centered octahedron					
1	0	4	90	7	1.33
2	0	2	97	4	1.27
3	0	1	99	3	1.24

accurate, then the overall Fermi surface value for λ would be larger than 1.0, which is in disagreement with McMillan[1] or Allen and Dynes,[2] but is consistent with the mass enhancement derived from comparison of the bare band-structure density of states at E_F with the measured electronic contribution to the specific heat.[30]

In our calculations, the mass enhancements associated with the particular k points on the Fermi surface are obtained as an intermediate step in evaluating the total λ. Only the k' summation is performed in Eq. (1), so that λ_k can be evaluated at each step and then the total λ obtained from

$$\lambda = \frac{1}{N(E_F)} \frac{\Omega}{(2\pi)^3} \int \frac{dS}{|\nabla_k E|} \lambda_k . \tag{7}$$

The evaluation of each λ_k involved the summation of matrix elements between ψ_k and 11 087 different $\psi_{k'}$ on the Fermi surface. The results are summarized in Table II, in which we list a few representative λ_k's for each piece of the Fermi surface along with the l decomposition of the wave function ψ_k. The l decomposition was obtained by extrapolating the radial functions inside the muffin-tin sphere to the Wigner-Seitz sphere boundary. This is not exact (the reason some of the percents given in Table II do not sum to 100), but does give an excellent picture of the wave-function character. The weighted average [see Eq. (7)] of all the λ_k's was 1.56, so these values should not be considered accurate; however, the trend for the variation of λ on the different surfaces appears genuine within the rigid-ion approximation. In this regard, similar results were obtained by Yamashita and Asano,[18] except for their one k point on the Γ-centered octahedron.

The striking result apparent from Table II is that the theoretical trends are directly opposite the trends of the measured enhancements. Thus, we find the smallest λ_k's on the Γ-centered octahedron and the jungle gym, whereas the previously discussed de Haas–van Alphen experiments indicate that the smallest enhancements occur for the N-centered ellipsoids. The l decomposition suggests an explanation. The rigid-ion matrix elements contain an angular momentum selection rule allowing d states to couple only to p or f states. From Table II, it is evident that states with nearly pure $l=2$ character have the smallest values of λ, whereas the hybridized states with about equal $l=1$ and $l=2$ character have large λ's. The experiments indicate that another mechanism which would allow d-d coupling is probably important. Such a coupling is allowed if one goes beyond the rigid-ion approximation and includes screening. (See Ref. 5 for details of the formulation and a model calculation for Nb.) We postpone a thorough discussion of screening in Nb to a future publication, since the required calculations are considerably more difficult.

In addition to the screening matrix allowing d-d coupling, the part of the electron-phonon matrix elements outside the muffin-tin spheres can also give this coupling. Within the rigid-ion approximation the charge inside the muffin-tin sphere is displaced rigidly; however, the charge is not neutral, and there is thus a Coulomb tail extending throughout the crystal. This potential tail will certainly be screened and will thus have a very limited spatial extent; however, it does allow for d-like states located on the displaced site to couple to d-like states inside the surrounding muffin-tin spheres. We have made calculations using electron-phonon matrix elements which include the gradient of this potential screened by a Lindhard function with $k_F = 0.2\pi/a$ to prevent the matrix elements for small q from blowing up. We find that the λ_k's for the ellipsoids remain about constant, but the λ_k's on the jungle gym and octahedron are increased to about 2.0 and as in the experiments are now larger than the ellipsoid enhancements. However, the total λ is now ~1.9! These calculations are very suggestive, but until screening is correctly taken into account, it is impossible to make quantitative statements.

IV. CONCLUSION

First-principles calculations of relevant electron-phonon parameters are crucial for understanding the details governing superconductivity in high-T_c materials. These calculations are very involved and it is useful to make contact with several experimental results rather than just the single electron-phonon mass enhancement parameter λ. In this paper, we first considered the electron-phonon spectral function α^2F, but found the discrepancies between theory and experiment could be due to a number of experimental problems, so that it was difficult to assess the validity or limitations of the present calculations which used the rigid-ion approximation. The evaluation of the local mass enhancement for the different pieces of the Fermi surface gave surprising results in direct contradiction with experiment. This appears to be a very serious problem related to the use of rigid-ion matrix elements which apparently do not allow sufficient d-d coupling. The overall value of λ is also found to be quite large, although using a different potential or slightly different rigid-ion matrix elements would reduce the value. The problems of large λ and wrong orbital mass enhancements could easily be due to screening ef-

fects, and our results provide a strong motivation for undertaking the complicated but important task of including screening in calculations of the type described in this paper. We hope to report the results of such calculations in the near future.

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