Phonon density of states of superconducting lead*

B. Farnworth and T. Timusk
Department of Physics, McMaster University, Hamilton, Ontario, Canada
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Far-infrared reflectivity data, containing phonon-induced structure, have been inverted to give a phonon density of states, $\alpha_{tr}^2 F(\omega)$, for superconducting lead.

We previously reported measurements of the far-infrared reflectivity of lead which clearly showed structure associated with the phonon spectrum.[1] Except for a shift in the positions of the phonon peaks, the derivative of the measured spectrum,

$$S(\omega) = \frac{d}{d\omega}\left[A_S(\omega) - A_N(\omega)\right], \tag{1}$$

where A_S and A_N are the absorptivities of the superconducting and normal metals, was in good agreement with a calculation based on the tunneling-derived density of states[2] and a simple theory for the phonon-induced absorption due to Allen.[3] Our spectrum, however, contained fine structure that was missing in the tunneling experiments, but that was generally in good agreement with the phonon spectrum derived from inelastic-neutron-scattering experiments.[4] In this note we would like to present additional analysis of our data which allows a more direct comparison between the tunneling and far-infrared results.

The derivatives of Allen's expressions for the phonon contribution to the absorptivity are, for the superconductor,

$$\frac{d}{d\omega}A_S(\omega) = \frac{4\pi^2\Delta}{\omega\omega_p}\phi_S(\omega)\alpha_{tr}^2 F(\omega - 2\Delta) + \frac{4\pi}{\omega^2\omega_p}\phi_S(\omega)\int_0^{\omega-2\Delta} d\Omega\,\alpha_{tr}^2 F(\Omega)\left(\Omega E(k) + \frac{\omega(1-k^2)}{k^2}\left[E(k) - K(k)\right]\right) \tag{2}$$

and for the normal metal,

$$\frac{d}{d\omega}A_N(\omega) = \frac{4\pi}{\omega^2\omega_p}\phi_N(\omega)\int_0^{\omega} d\Omega\,\Omega\alpha_{tr}^2(\Omega). \tag{3}$$

Here Δ is the superconducting energy gap, ω_p is the plasma frequency, and $E(k)$ and $K(k)$ are complete elliptic integrals with

$$k^2 = 1 - [2\Delta]/(\omega - \Omega)^2.$$

The quantity $\alpha_{tr}^2 F(\omega)$ is a weighted phonon density of states, similar to the $\alpha^2 F$ in the theory of strong coupling superconductivity, but with additional weight given to large-angle scattering as is appropriate to transport properties. The quantities $\phi_S(\omega)$ and $\phi_N(\omega)$ are expected to be of order 1 and slowly varying with frequency. In our analysis they are assumed to be constant and equal.

Combining Eqs. (1)–(3) gives an integral equation relating the experimental spectrum to the phonon density of states. We have solved this equation numerically to give $\alpha_{tr}^2 F(\omega)$ for lead.

In the analysis, we have used a value for the energy gap, $2\Delta = 21.5\ \text{cm}^{-1}$, determined from the onset of the absorption in measurements by a direct absorption technique.[5] This value is somewhat lower than that quoted previously ($23.5\ \text{cm}^{-1}$) which was taken from the point of steepest slope on the absorption edge in the reflectivity experiments. Since the absorption edge is more easily discernible in the direct absorption experiment we feel that the lower value is more reliable. Additional imput to the inversion routine is the assumption that $\alpha_{tr}^2 F(\omega)$ is proportional to ω^2 at low frequencies. This is necessary since the experiment and calculations do not agree for $\hbar\Omega \lesssim 4\Delta$ ($\hbar$ phonon $\lesssim 2\Delta$) where other processes give significant contributions to $dA_S(\omega)/d\omega$.

The results of the inversion are shown in Fig. 1 and are compared to $\alpha^2 F(\omega)$ derived from tunneling experiments.[2] In making the comparison we have shifted the far-infrared curve down in frequency (by $5.5\ \text{cm}^{-1}$) and scaled so that the transverse peak C agrees in intensity and position with tunneling. The origin of this discrepancy is not clear but appears to be related to our use of the simple theory in our inversion routines. We have evaluated the derivative of the calculated spectrum of Swihart and Shaw[6] and found that it gives excellent agreement ($\pm 1\ \text{cm}^{-1}$) with our results, that is without the need for any shift. Since the Swihart-Shaw calculation uses the same tunneling data as a starting point as our com-

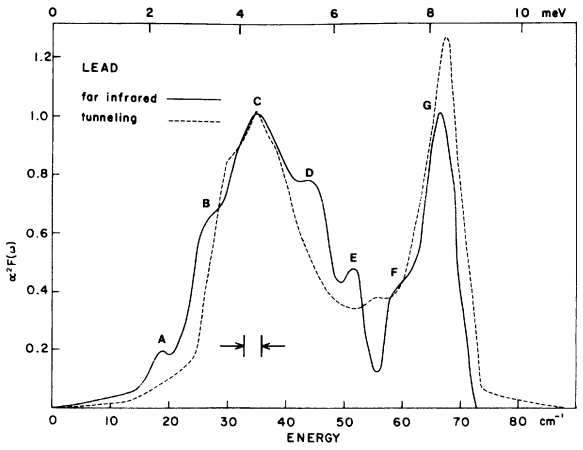

FIG. 1. Weighted phonon density of states obtained from far-infrared reflectivity measurements (solid curve) using an inversion routine based on Allen's theory (Ref. 3). The dotted curve is the tunneling result fitted at point C to our curve. The peaks B, D, and F are in good agreement with corresponding features in the neutron density of states of lead and the peak A, we suggest, is due to phonon life time effects at 2Δ.

parison above, we are led to conclude that the 5.5 cm^{-1} shift is related to the approximations in the simple theory. This agreement with the Swihart-Shaw derivative refers to the position of the gross broad structure only; the fine structure we observe is of course absent from the theoretical curves since it is absent from the starting tunneling results. In addition, the grid used in the theory is too coarse to reveal much fine detail. Ideally, we should use the more complete theory in our inversions, but the complexity of the more complete theory makes this approach unpractical. A simpler approach could be the use of our shifted version of $\alpha^2F(\omega)$ as a starting point in a fine-grid Swihart-Shaw type of calculation of the far-infrared absorption. The derivative of this, we feel, would agree in all detail with experimental derivative of Ref. 1.

The main differences between the two spectra obtained from tunneling and the far-infrared are the width of the main transverse peak, the relative height of the longitudinal peak C, and the appearance of fine structure A, B, D, E, and F in the far-infrared data. The experimental uncertainties, about 2% of the peak heights, are much less than these differences. Calculations by Tomlinson and Carbotte[7] do not predict any significant difference between $\alpha^2F(\omega)$ and $\alpha^2_{tr}F(\omega)$ so that the major difference between the two curves may be attributed to the simplifying assumptions of Allen's theory. The fine structure, as we previously pointed out, agrees well with structure in the neutron-derived phonon spectrum, except for peak A which we attributed to phonon lifetime effects associated with the superconducting energy gap.

We suggest that these data, and preliminary results on indium and niobium,[5] indicate that far-infrared absorption can provide an alternative to tunneling for the determination of α^2F in superconductors.

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