Brief Reports

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Role of varying electronic density of states in the far-infrared behavior of V_3Si

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Far-infrared measurements in a thin film of V_3Si at 19 K are analyzed with new expressions for the ac conductivity for the case of a nonconstant electronic density of states $N(\epsilon)$. It is found that the infrared data can be fitted with a transport electron-phonon coupling function $\alpha^2_{tr}F$ which is proportional to the measured phonon density of states, and with an $N(\epsilon) \neq$ const. Thereby, the discrepancy between the neutron scattering results and the previous analysis of the infrared behavior is resolved.

Different experimental probes of the electron-phonon (EP) coupling function $\alpha^2(\Omega)F(\Omega)$ in the high superconducting T_c A-15 compound V_3Si give conflicting results. Inelastic neutron scattering experiments[1] on V_3Si at 4, 77, and 300 K give the phonon density of states $F(\Omega)$ with peaks at 25 and 42 meV (Fig. 1). In contrast, far-infrared data taken by McKnight, Perkowitz, Tanner, and Testardi[2] (hereafter referred to as MPTT), when analyzed by Allen's theory[3] of infrared absorption, give the transport EP coupling function $\alpha^2_{tr}(\Omega)F(\Omega)$ with peaks at 18 and 42 meV, and with entirely new structure at 6 meV (Fig. 1). Mitrović and Carbotte[4] have found that superconducting thermodynamic properties of V_3Si could be fitted with an α^2F set equal to const $\times F(\Omega)$, but not with the $\alpha^2_{tr}F$ deduced by MPTT. In general, the functions $F(\Omega)$, $\alpha^2(\Omega)F(\Omega)$ and $\alpha^2_{tr}(\Omega)F(\Omega)$ do not have the same shape, but the difference between F and $\alpha^2_{tr}F$ in Fig. 1 is too large to be explained by Ω dependence of α^2_{tr}. In this paper we show that a correction to Allen's original formulation, to include the effect of structure in the electronic density of states $N(\epsilon)$ very close to the chemical potential $\mu(=0)$, resolves the experimental discrepancy. Band-structure calculations,[5] the temperature dependence of magnetic susceptibility,[6] and the degradation of T_c with disorder[7,8] strongly suggest that $N(\epsilon)$ in V_3Si can vary on the scale of the maximum phonon frequency Ω_{max} (or smaller) near μ. A combination of

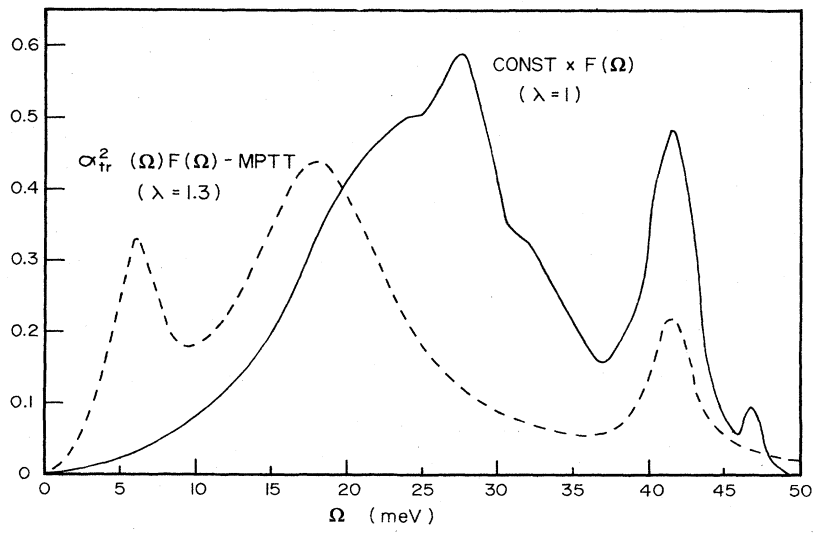

FIG. 1. Phonon density of states scaled by a constant factor (solid line) and $\alpha^2_{tr}F$ of McKnight *et al.* (Ref. 2) (dashed line).

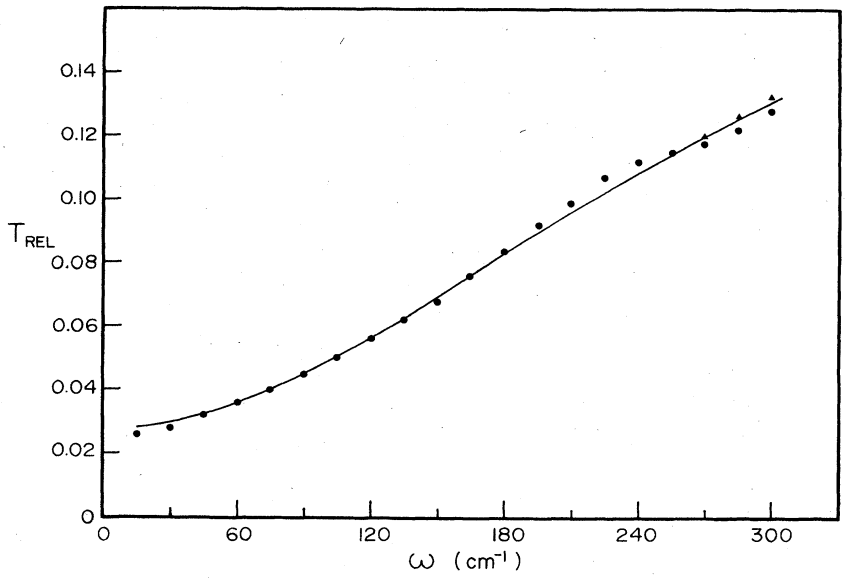

FIG. 2. Experimental values of T_{rel} (heavy dots) and theoretical fit (solid line). Triangles represent few points off the solid line which are calculated within the usual theory [$N(\epsilon)$ =const] from $\alpha_{tr}^2 F$ given by the dashed curve in Fig. 1.

an $\alpha_{tr}^2 F$ based on the neutron scattering data, and fine structure in $N(\epsilon)$ satisfactorily reproduces the infrared results on V_3Si without any need to invoke shifts in the peak positions or the existance of new peaks.

MPTT analyzed data between 0.6 and 37 meV, taken in transmission through a 20-nm film grown on a sapphire substrate. The measurement was made in the normal state at 19 K. The measured quantity was T_{rel}, the transmission of the film and substrate (ss) normalized to that of the substrate alone. It is given by

$$T_{rel} = T_{film+ss}/T_{ss} = \left[\left(1+\frac{y_1}{n+1}\right)^2 + \left(\frac{y_2}{n+1}\right)^2\right]^{-1} , \quad (1)$$

where

$$y_1 + iy_2 = \frac{4\pi}{c} d\sigma(\omega) . \quad (2)$$

Here $4\pi/c$ is the impedance of free space, $\sigma(\omega)$ the complex ac conductivity of the film, d the film thickness, and n the refractive index of the substrate. The ratio $T_{film+ss}/T_{ss}$ eliminates almost completely all absorptive effects in the substrate, although at higher frequencies, where the sapphire absorption increases, there is about a 5% error. The measured values of T_{rel} are given in Fig. 2.

In the case of nonconstant $N(\epsilon)$ ac conductivity in the local approximation and in the weak-coupling limit is given by

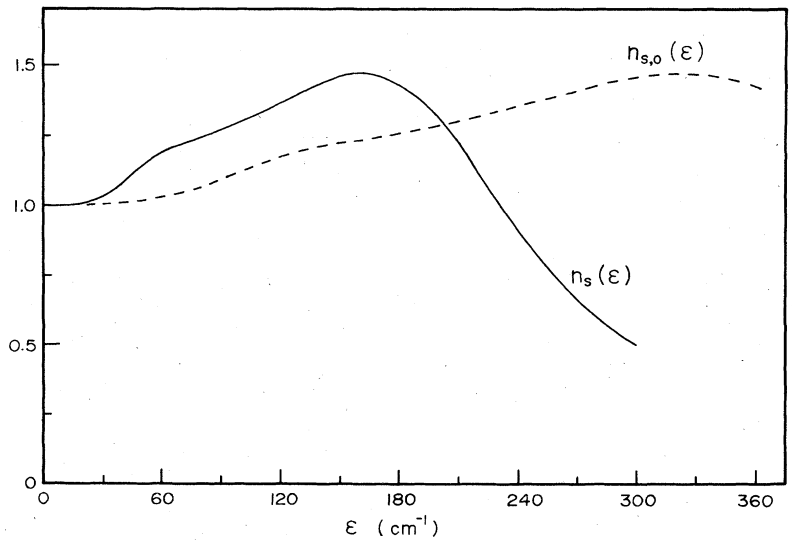

FIG. 3. $n_s(\epsilon)$ which gives the fit in Fig. 2. $n_{s,0}$ is obtained from n_s by eliminating the energy renormalization.

($\hbar = 1$)

$$\sigma(\omega) = \frac{\Omega_p^2}{4\pi} \frac{\tau^*(\omega)}{1+\bar{\lambda}(\omega)} \frac{1}{1-i\omega\tau^*(\omega)} \quad , \tag{3}$$

where

$$1/\tau^*(\omega) = [1/\bar{\tau}_{ep}(\omega) + 1/\bar{\tau}_i(\omega)]/[1+\bar{\lambda}(\omega)] \quad , \tag{4}$$

$$1/\bar{\tau}_{ep}(\omega) = \frac{2\pi}{\omega} \int_0^{\omega} d\Omega \alpha_{\rm tr}^2(\Omega) F(\Omega) \int_0^{\omega-\Omega} d\epsilon n_s(\epsilon) \quad , \tag{5}$$

$$1/\bar{\tau}_i(\omega) = \frac{1}{\tau_i} \frac{1}{\omega} \int_0^{\omega} d\epsilon n_s(\epsilon) \quad , \tag{6}$$

$$\bar{\lambda}(\omega) = \bar{\lambda}_{ep}(\omega) + \bar{\lambda}_i(\omega) \quad , \tag{7}$$

$$\bar{\lambda}_{ep}(\omega) = \frac{2}{\omega^2} \int_0^{\Omega_{\max}} d\Omega \alpha_{\rm tr}^2(\Omega) F(\Omega) \times \int_0^{+\infty} d\epsilon n_s(\epsilon) \ln \left| \frac{(\epsilon+\Omega)^2}{(\epsilon+\Omega)^2-\omega^2} \right| \quad , \tag{8}$$

$$\bar{\lambda}_i(\omega) = \frac{1}{\pi\tau_i\omega} \int_0^{+\infty} d\epsilon n_s(\epsilon) \ln \left| \frac{\epsilon^2}{\epsilon^2-\omega^2} \right| \quad , \tag{9}$$

$$n_s(\epsilon) = [N(\epsilon)/N(0) + N(-\epsilon)/N(0)]/2 \quad , \tag{10}$$

$$\tau_i = \tau_i(\omega=0) \quad . \tag{11}$$

Equations (3)–(11) can be derived[9] by using Allen's golden rule treatment[3] of EP and electron-impurity (EI) scattering plus the requirement that the conductivity satisfies the f-sum rule.[10,11] Also, it is assumed that the ϵ dependence of the Drude plasma frequency $\Omega_p(\epsilon)$ can be ignored. This approximation is justified by the band-structure calculations[5,8] for A-15 materials. It also underlies the analysis of the upper crtitical field data which yields the dependence of $N(0)$ on disorder.[7] In the case of $N(\epsilon) = \text{const}$ Eqs. (3)–(11) reduce to Allen's expression.[3] We point out that Eqs. (3)–(11) can also be obtained[9] from Holstein's theory[12] in the weak-coupling limit and in the local approximation. This approach indicates[9] that $N(\epsilon)$ should be interpreted as the quasiparticle density of states[13]

$$N(\epsilon) = -\frac{1}{\pi} \operatorname{Im} \sum_k G(k, \epsilon + i0^+) \quad , \tag{12}$$

where G is the Green's function, i.e., as the density of states which includes the self-energy effects (lifetime broadening plus the energy renormalization). The derivation is lengthy and will be presented elsewhere.[9] Note that in the case of $N(\epsilon) \neq \text{const}$ the impurity contribution to $1/\bar{\tau}(\omega)$ becomes frequency dependent, and thus impurities start contributing to the renormalization parameter $\bar{\lambda}(\omega)$. This fact was first pointed out by Pickett and Allen.[11]

In fitting the experimental data on $T_{\rm rel}$ we have used $\alpha_{\rm tr}^2(\Omega)F(\Omega) = CF(\Omega)$, where $F(\Omega)$ is the measured phonon density of states and the constant C was chosen so that $\bar{\lambda}_{ep}(0) = 1$ (Fig. 1). The $n_s(\epsilon)$ which gives the best fit to the data in Fig. 2 is shown in Fig. 3. The corresponding value of $1/\tau_i$ was 296 cm^{-1} (i.e., 37 meV). Ω_p^2 was absorbed into the experimental value of $\sigma(0)d$ (Ref. 2). The overall shape of $n_s(\epsilon)$ does not depend much on the detailed shape of $\alpha_{\rm tr}^2F$ provided that the positions of the peaks in this function coincide with the positions of the peaks in $F(\Omega)$. [For example, an $\alpha_{\rm tr}^2F$ obtained by multiplying the solid curve in Fig. 1 with a factor which varies smoothly from 2 at $\omega = 0$ to 0.5 at $\omega = 42$ meV yields an $n_s(\epsilon)$ which has the same overall shape as the n_s in Fig. 3.] We particularly note that the fit in Fig. 2 is identical to that obtained by MPTT with their modified $\alpha_{\rm tr}^2F$ (dashed line in Fig. 1) and $N(\epsilon) = \text{const}$. As pointed out by MPTT, the measured $T_{\rm rel}$ for V_3Si can be fitted within the usual formalism [$N(\epsilon) = \text{const}$] only with an $\alpha_{\rm tr}^2F$ which is exhausted by 25 meV, i.e., with a major peak below this energy. Since the neutron scattering experiments down to 4 K do not give any significant shift of the broadest peak at 25 meV, such an $\alpha_{\rm tr}^2F$ is very unlikely. We emphasize that the most important effect of nonconstant $N(\epsilon)$ on infrared behavior comes via EI scattering [$1/\bar{\tau}_i(\omega)$ and $\bar{\lambda}_i(\omega)$]. In Fig. 4 we show

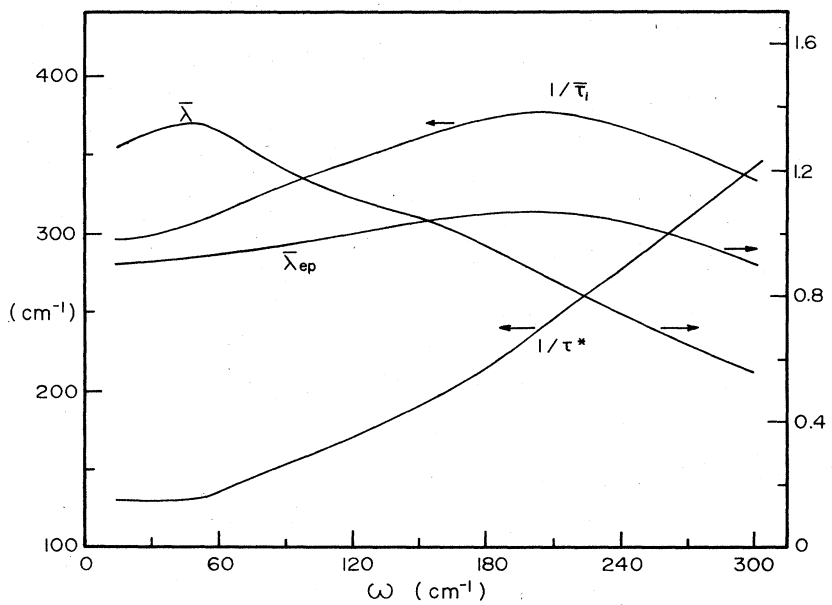

FIG. 4. Calculated renormalization parameters and scattering times.

$1/\tau^*$, $1/\bar{\tau}_i$, $\bar{\lambda}_{ep}$, and $\bar{\lambda}$ calculated with $n_s(\epsilon)$ from Fig. 3. Note that with our input $\alpha^2_{\rm tr}F$ (solid curve in Fig. 1) $\bar{\lambda}_{ep}$ is almost constant, whereas $\bar{\lambda}_i$ is rapidly decreasing, giving a rapidly decreasing $\bar{\lambda}$. The original $\alpha^2_{\rm tr}F$ of MPTT (dashed curve in Fig. 1) would yield an $\bar{\lambda}_{ep}$ very similar to $\bar{\lambda}$ in Fig. 4.

The question arises as to whether the impurity scattering parameter $1/\tau_i = 37$ meV is compatible with the structure in $n_s(\epsilon)$ in Fig. 3. First, the lifetime broadening due to EI scattering is given by[13]

$$\Gamma_i(\epsilon) = \frac{1}{2\tau_i}\frac{N(\epsilon)}{N(0)} ,$$

where N is defined by Eq. (12). Thus, Γ_i is about a factor of 2 smaller than $1/\tau_i$. Second, the quasiparticle density of states [Eq. (12)] includes the energy renormalization due to interactions and thus displays a sharper structure within $\pm\Omega_{\rm max}$ of μ than its bare band-electron counterpart.[13] Roughly speaking, $N(\epsilon) = N_0[\epsilon(1+\lambda)]$, where N_0 is the band-electron density of states broadened by the lifetime effects and λ is the (energy-dependent) electron mass renormalization parameter.[13] In Fig. 3 we also show $n_{s,0}(\epsilon) = n_s[\epsilon/(1+\lambda)]$. The structure in $n_{s,0}(\epsilon)$ is not incompatible with Γ_i of about 20 meV. We also point out that with $\Omega_p = 3.1$ eV (Ref. 7) and $1/\tau_i = 37$ meV we get the residual resistivity of $\rho_0 = 29\ \mu\Omega$ cm for this sample of V_3Si. This value of ρ_0 correlates well[7] with the measured $T_c = 15 \pm 0.5$ K.

Finally, we comment that the study of effects of nonconstant $N(\epsilon)$ on superconducting thermodynamic properties[14] indicates that an $n_{s,0}(\epsilon)$ from Fig. 3 does not have to be accounted for in the calculation of thermodynamics. Therefore, the results obtained in Ref. 4 remain valid. In contrast, the analysis of the effects of $N(\epsilon) \neq$ const on superconducting tunneling[15] indicates that an $n_{s,0}$ from Fig. 3 would influence the α^2F obtained from the tunneling. At the moment, there is no information about α^2F in V_3Si from the tunneling experiments. We predict that even if the tunneling junction is free of the proximity effect, the inverted α^2F for a high T_c V_3Si sample would contain a negative tail for $\Omega \gtrsim \Omega_{\rm max}$,[15] provided that no constraint is imposed on the upper cutoff in α^2F during the inversion procedure.

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