# Thermodynamic and far-infrared properties of $V_3Si$ calculated from tunneling results for the Eliashberg function $\alpha^2F$ and Coulomb pseudopotential parameter $\mu^*$

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The superconducting thermodynamic properties of $V_3Si$ are calculated with the use of the tunneling results of Bangert, Geerk, and Schweiss ($\lambda=2.21$, $\mu^*=1.3$) and those of Kihlstrom ($\lambda=0.9$, $\mu^*=0.1$). It is found that Kihlstrom's result gives a good description of the thermodynamics, while the $\alpha^2F$ and the $\mu^*$ of Bangert *et al.* do not. This implies that $\mu^*$ is small and so spin fluctuations do not play a significant role. We also find that the tunneling $\alpha^2F$ with $0.8\leq\lambda\leq2.21$ does not describe well, within the standard theory, the observed far-infrared behavior of $V_3Si$.

Recently, Bangert, Geerk, and Schweiss[1] published the first tunneling results for the electron-phonon spectral function $\alpha^2(\Omega)F(\Omega)$ (Fig. 1) and the Coulomb pseudopotential $\mu^*$ in an $A15$ $V_3Si$ sample with superconducting $T_c$ equal to 14.0 K. Their spectrum had a $\lambda=2\int_0^{+\infty}d\Omega\,\alpha^2F/\Omega$ of 2.21 and $\mu^*$ was found to have an extremely high value of 1.3. This large value of $\mu^*$ was interpreted by Bangert *et al.*[1] as a possible indication for the presence of spin fluctuations (paramagnons) in $V_3Si$. However, in independent tunneling measurements on three $A15$ V-Si samples ($T_c=10.1$, 14.8, 15.4) Kihlstrom[2] obtained $\alpha^2F$ spectra with shapes similar to the one found in Ref. 1, but with much smaller $\lambda$'s ($\lambda=0.76\pm0.15$, $0.91\pm0.07$, $0.89\pm0.06$), and an order-of-magnitude smaller $\mu^*$'s ($\mu^*=0.14\pm0.07$, $0.14\pm0.06$, $0.11\pm0.04$). Such a large discrepancy between the two sets of tunneling results on $V_3Si$ is unsettling. Certainly, the correct $\alpha^2F$ and $\mu^*$ must yield the observed thermodynamic behavior. In this Brief Report we present the superconducting thermodynamic properties calculated from the two tunneling results for $\alpha^2F$ and $\mu^*$ in $V_3Si$, and compare them with the experimental results of Muto *et al.*[3] We also calculate, taking for the transport electron-phonon spectrum $\alpha^2_{tr}(\Omega)F(\Omega)$ the tunneling $\alpha^2F$'s, the far-infrared behavior of $V_3Si$ and compare it with recent experimental results of Perkowitz, Carr, Subramaniam, and Mitrovic.[4] The effects of paramagnons are discussed and we conclude that their role in determining the physical properties of $V_3Si$ is small. We also point out some effects of a sharp peak in the electronic band density of states $N(\epsilon)$ near the Fermi level, which has long been assumed to play an important role in $V_3Si$ (e.g., in the temperature dependence of magnetic susceptibility, in degradation of $T_c$ with disorder, etc.).

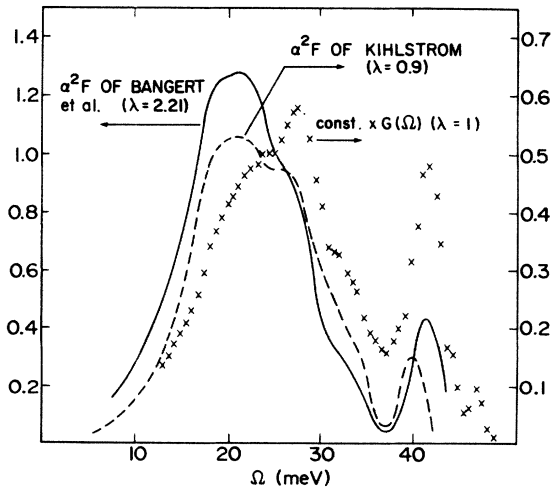


FIG. 1. Tunneling $\alpha^2F$'s of Bangert *et al.* (Ref. 1) (solid line) and of Kihlstrom (Ref. 2) (dashed line). The crosses give const$\times G(\Omega)$.

The superconducting properties were calculated within standard Eliashberg theory.[5] Our results for the reduced [and $N(0)$ independent] thermodynamic quantities are given in Table I, together with the experimental values. In Table I $H_c(T)$ is the thermodynamic critical field at temperature $T$, $\gamma$ is the coefficient of the linear term in the normal-state specific heat, $\Delta C$ is the jump in specific heat at $T_c$, and $\Delta_0$ is the zero-temperature gap edge. In Fig. 2 we show the calculated thermodynamic critical-field deviation function $D(t)=H_c(T)/H_c(0)-(1-t^2)$, $t=T/T_c$, for the two spectra together with the experimental result.[3]

Clearly, the $\alpha^2F$ and the $\mu^*$ obtained by Bangert *et al.* do not give the observed thermodynamics of $V_3Si$, while the tunneling results of Kihlstrom give a fairly good description with the remaining differences between the theory and the experiment possibly coming from the fact that the thermodynamic measurements[3] were done on a better sample [$T_c=16.7$ K, resistivity $\rho(T=17\text{ K})=5.74\,\mu\Omega\,\text{cm}\pm5\%$]. We wish to point out that a slightly better fit to thermodynamic properties was obtained by us in a previous publication,[5] with $\alpha^2F$ set equal to const$\times G(\Omega)$ ($\lambda=1$), where $G$ is the generalized phonon density of states obtained from the neutron scattering experiments on $V_3Si$ at $T=77$ K (Fig. 1), and with $\mu^*(\omega_c=250\text{ meV})=0.15$. Thus, there is a field of values for $(\alpha^2F,\mu^*)$ which can fit the thermodynamics of $V_3Si$, but the $\alpha^2F$ and $\mu^*$ from Ref. 1 certainly fall outside this range. One may erroneously argue that if pair-breaking spin fluctuations were explicitly included into the calculation of thermodynamics with the spectrum of

 

TABLE I. Calculated and experimental superconducting thermodynamic properties of $V_3Si$.

| | Bangert *et al.* (Ref. 1) | Kihlstrom (Ref. 2) | Experiment |
|---|---|---|---|
| $\lambda$ | 2.285[a] | 0.902[a] | |
| $A=\int_0^{+\infty} d\Omega\,\alpha^2(\Omega)F(\Omega)$ | 22.06 meV | 9.55 meV | |
| $\langle\omega\rangle=2A/\lambda$ | 9.65 meV | 10.59 meV | |
| $\Omega_{max}$ (maximum phonon energy) | 44.5 meV | 42.24 meV | |
| $\omega_c$ (cutoff energy in Matsubara sums) | 222.5 meV | 253.44 meV | |
| $\mu^*(\omega_c)$ | 1.3 | 0.1018 | |
| $T_c$ (calculated) | 18 K | 15.4 K | Maximum 17.1 K[b] |
| $-\frac{T_c}{H_c(0)}\left[\frac{dH_c(T)}{dT}\right]T_c$ (BCS value 1.74) | 2.11 | 1.93 | 1.97[c] |
| $\gamma\left[\frac{T_c}{H_c(0)}\right]^2$ (BCS value 0.168) | 0.141 | 0.151 | 0.153[c] |
| $\Delta C/\gamma T_c$ (BCS value 1.43) | 2.43 | 1.97 | 2.01[c] |
| $2\Delta_0/k_BT_c$ (BCS value 3.53) | 4.25 | 3.89 | $3.76\pm0.1$[d]<br>3.8[e]<br>3.8[f]<br>3.4–3.6[g]<br>3.3[h]<br>3.2–3.6[i] |

[a]Values read from graphs in Refs. 1 and 2.
[b]Reference 6.
[c]Reference 3.
[d]Reference 7.
[e]Reference 8.
[f]Reference 9.
[g]Reference 10.
[h]Reference 1.
[i]Reference 2.

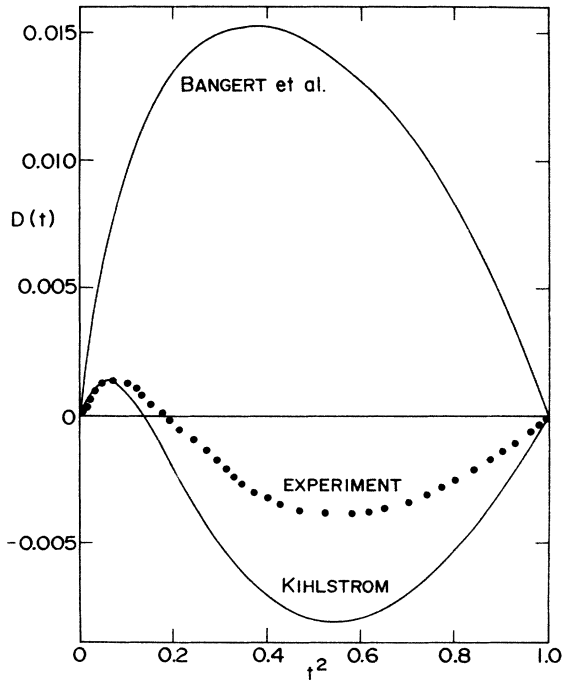


FIG. 2. Thermodynamic critical-field deviation function $D(t)$ calculated from $\alpha^2F$ and $\mu^*$ in Refs. 1 and 2. Heavy dots give the experimental values of Muto *et al.* (Ref. 3) $t=T/T_c$.

Bangert *et al.*, one would come closer to the experiment, for example, $D(t)$ could be reduced to the observed weak to medium coupling shape. The point is that if paramagnons are present, the electron-phonon spectral function obtained from inversion of the tunneling data is an effective one, related to the true $\alpha^2F$ by $\alpha^2F/(1+\lambda_{sf})$,[11,12] where $\lambda_{sf}$ is the spin-fluctuation mass-renormalization parameter. This scaling relation is valid provided that the characteristic paramagnon energy $\Omega_{sf}$ is significantly larger than the characteristic phonon energy,[13] which should presumably be the case for $V_3Si$ considering its large value of $T_c$. Also, the Coulomb repulsion parameter $\mu^*(\omega_c)$ deduced from tunneling data contains information about spin fluctuations. It is approximately given by

$$\mu^*(\omega_c)=\frac{[\mu^*(\Omega_{sf})+\lambda_{sf}]/(1+\lambda_{sf})}{1+\{[\mu^*(\Omega_{sf})+\lambda_{sf}]/(1+\lambda_{sf})\}\ln(\Omega_{sf}/\omega_c)}\ .$$

Thus, if paramagnons were present in $V_3Si$, the $\alpha^2F$ and $\mu^*$ of Bangert *et al.* (and those of Kihlstrom) would already be dressed by the electron-paramagnon interaction. To include spin fluctuations in the calculation of thermodynamics with these $\alpha^2F$ and $\mu^*$ would be double counting. In fact, as demonstrated by Daams, Mitrović, and Carbotte[11] our results contain in full the contribution from paramagnons (if any), because they are based on the tunneling results for $\alpha^2F$ and $\mu^*$. Since the tunneling results of Kihlstrom give a good fit to thermodynamics of $V_3Si$, and since his $\mu^*$ has a

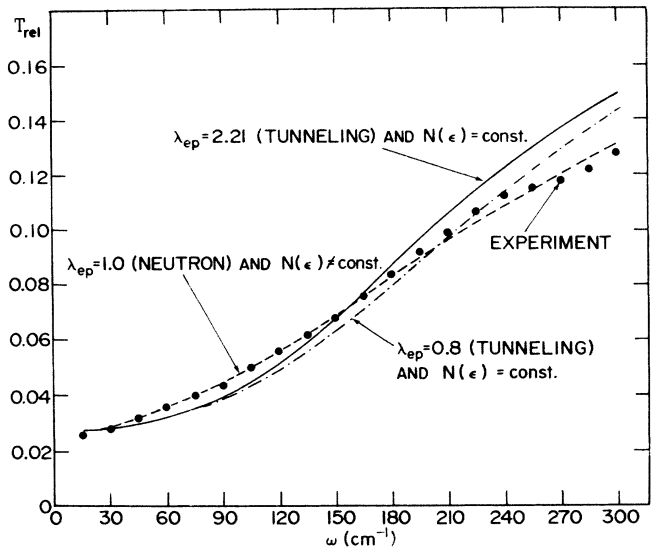


FIG. 3. Calculated and experimental relative transmission $T_{rel}(\omega)$ in the far infrared of a thin $V_3Si$ film. $\omega$ is the radiation frequency (in cm$^{-1}$).

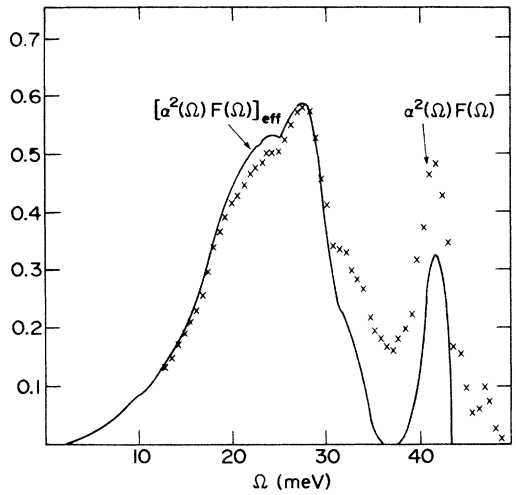


FIG. 4. The effective $\alpha^2F$ (negative tail not shown) and the actual input $\alpha^2F$.

usual value (0.1–0.15), we conclude that spin fluctuations play a minor role (if any) in determining the physical properties of $V_3Si$. Thus, the source of a large discrepancy (about a factor of 2) between the value of $N(0)$ obtained in the band-structure calculations and the one needed to account for the measured $\gamma$ (with $\lambda \cong 1$) has to be sought elsewhere. Perhaps the explanation of this discrepancy given by Testardi and Mattheiss[14] in terms of a rapid variation in $N(\epsilon)$ near the Fermi level is the correct one. They argue that the high $T_c$ samples correspond to the composition $V_{3-x}Si$ with small $x > 0$; then, in the rigid-band picture, the resulting shift of the Fermi level (about 35 meV for $V_{2.94}Si$) leads to a large increase in $N(0)$.

We have also calculated the relative transmission $T_{rel}(\omega)$ in the far infrared of a thin $V_3Si$ film, using for $\alpha^2_{tr}F$ the spectrum of Bangert *et al.* with two values of $\lambda$: $\lambda = 2.21$ (solid line in Fig. 3) and $\lambda = 0.8$ (dash-dot line in Fig. 3). The calculations were performed within Allen's theory (as described in Ref. 15) assuming a constant $N(\epsilon)$, and the impurity scattering rates were adjusted to achieve the experimental values[4,16] of $T_{rel}$ in the zero-frequency limit. We do not find that the two calculated curves give a good fit to the experimental results of Perkowitz *et al.*[4,16] (heavy dots in Fig. 3). Reducing $\lambda$ from 2.21 to 0.8 (the lowest value found by Kihlstrom) slightly improves the fit at high frequencies, where the experimental accuracy is about 5%, but makes it worse in the range of low and intermediate $\omega$'s. Thus, either $\alpha^2_{tr}F$ in $V_3Si$ has more weight at low $\Omega$'s than the tunneling $\alpha^2F$'s,[16] or one ought to include the energy dependence in $N(\epsilon)$ when trying to account for the observed $T_{rel}(\omega)$.[15] In Fig. 3 we also show the fit to $T_{rel}(\omega)$ from Ref. 15 (dashed line) with $\alpha^2_{tr}F$ set equal to const $\times G(\Omega)$ (see Fig. 1) and with a suitably chosen $n_s(\epsilon) = [N(\epsilon) + N(-\epsilon)]/2$.

It was suggested in Ref. 15 that tunneling experiments should look for a negative tail in the inverted $\alpha^2F$ in the multiphonon region (i.e., for $\Omega \gtrsim \Omega_{max}$) to decide whether or not a peak in $N(\epsilon)$ near the Fermi level plays an important role in $V_3Si$. If negative tails are found, then the inverted $\alpha^2F$ is only an effective spectrum, distorted from its actual shape due to neglect of variation in $N(\epsilon)$ during the inversion procedure.[17,18] This is illustrated in Fig. 4. The solid line is the effective $\alpha^2F$ (the negative tail is not shown) obtained by inverting, within $N(\epsilon) = \text{const}$ theory, the normalized tunneling conductance calculated with $\alpha^2F = \text{const} \times G(\Omega)$ (crosses in Fig. 4) and with a peak in $N(\epsilon)$. For $N(\epsilon)$ we used a triangular shape symmetric about the chemical potential superimposed on a constant background. The base of the triangle was 60 meV and the height twice the background. Note that $(\alpha^2F)_{eff}$ has a more relative weight at low $\Omega$'s than the true input $\alpha^2F$. Of course, if we included the assumed shape of $N(\epsilon)$ into the inversion procedure, we would get back our input $\alpha^2F$. The relation between $(\alpha^2F)_{eff}$ and $\alpha^2F$ in Fig. 4 is similar to the relation between the tunneling $\alpha^2F$'s and const $\times G(\Omega)$. Thus, a part of the observed decrease in $\alpha^2(\Omega)$ with increasing $\Omega$ may be due to the neglect of a peak in $N(\epsilon)$ during inversion. Unfortunately, the $\alpha^2F$ of Bangert *et al.* does not even extend to $\Omega_{max}$ (reasons for this were not given in Ref. 1), and Kihlstrom[2] found that the inversion program could not be made to converge when the extra energies (above $\Omega_{max}$) were included. Hopefully, future tunneling experiments will be made to probe the multiphonon region and shed more light onto the effects of nonconstant $N(\epsilon)$.

In conclusion, we have found that the tunneling results of Kihlstrom describe well the thermodynamics of superconducting $V_3Si$, while those by Bangert *et al.* do not. The values of $\mu^*$ obtained in Ref. 2 suggest that the paramagnons do not play an important role in $V_3Si$. We found that the tunneling $\alpha^2F$'s do not explain, within the standard theory, the detailed shape of the relative transmission $T_{rel}(\omega)$ in the far infrared of a thin $V_3Si$ film. This is in contrast to the better fit obtained previously with an energy-dependent electronic density of state.

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