

## $\alpha^2(\Omega)F(\Omega)$ in $V_3Si$ : Insight from the superconducting thermodynamic properties

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We calculate the superconducting thermodynamic properties on the basis of two model  $\alpha^2F$  spectra for  $V_3Si$  and compare them with recent experimental results. It is found that the spectrum obtained by scaling the measured phonon density of states in  $V_3Si$  in such a way that the resulting  $\lambda$  value is equal to 1 gives good agreement between the calculated and experimental values of thermodynamic quantities. On the other hand, an  $\alpha^2F$  spectrum set equal to  $\alpha^2F_{ir}$  which was deduced from far infrared measurements ( $\lambda=1.29$ ), implies thermodynamic properties of  $V_3Si$  which are not found experimentally.

### I. INTRODUCTION

$V_3Si$  is one of the most studied  $A15$  compounds with high superconducting critical temperature  $T_c \sim 17$  K. However, at present there is no detailed knowledge of the basic microscopic parameters determining the superconducting properties of  $V_3Si$ . So far it has not been possible to measure the electron-phonon spectral function  $\alpha^2(\Omega)F(\Omega)$  and the Coulomb pseudopotential  $\mu^*(\omega_c)$  (Ref. 1) for  $V_3Si$  by single-particle tunneling experiments.<sup>1</sup>

In the absence of a measured  $\alpha^2(\Omega)F(\Omega)$  for  $V_3Si$  there are several other experimental results which contain some information about the electron-phonon interaction:

(1) Measurements of the generalized phonon density of states  $G(\Omega)$  for  $V_3Si$  at  $T=297$ ,  $77$ , and  $4$  K by inelastic neutron scattering experiments.<sup>2</sup> Under the assumption  $G(\Omega) \propto \alpha^2(\Omega)F(\Omega)$ , which is a good approximation for simple polyvalent metals,<sup>3</sup>  $G(\Omega)$  gives the shape of  $\alpha^2(\Omega)F(\Omega)$  for  $V_3Si$  in the frequency region between  $\Omega_{min} \simeq 7$  meV and  $\Omega_{max} = 50$  meV. The scale of  $\alpha^2F$  can be fixed by using McMillian's formula<sup>4,5</sup> to fit the experimentally measured  $T_c$ , with some choice for  $\mu^* \equiv \mu^*(\Omega_{max})$  (usually between 0.1 and 0.13). Schweiss *et al.*<sup>2</sup> obtained in this way the value

$$\lambda = \int_0^{+\infty} d\Omega \alpha^2(\Omega)F(\Omega)/\Omega = 1.02$$

for  $V_3Si$ . The application of McMillian's formula is justified if  $\lambda$  is less than 1.4 (Refs. 6 and 7) (and

if the electronic density of states is constant in the range of a few times the maximum phonon frequency around the Fermi level<sup>8</sup>).

(2) Far-infrared-absorption measurements on  $V_3Si$  have been performed and  $\alpha_{ir}^2(\Omega)F(\Omega)$  has been extracted from these experiments<sup>9</sup> by using Allen's formulas.<sup>10</sup> The published<sup>9</sup> transport electron-phonon spectrum  $\alpha_{tr}^2(\Omega)F(\Omega)$  for  $V_3Si$  has

$$\lambda_{tr} \equiv 2 \int_0^{\infty} d\Omega \alpha_{tr}^2(\Omega)F(\Omega)/\Omega = 1.29$$

[usually  $\alpha_{tr}^2(\Omega)F(\Omega) \simeq \alpha^2(\Omega)F(\Omega)$  to reasonable approximation and  $\lambda_{tr}$  agrees with  $\lambda$  to within 10%]. Moreover, a new peak emerges around  $\sim 6$  meV (slightly below the range of the inelastic neutron scattering experiments) and considerable shift in weight under  $\alpha_{tr}^2(\Omega)F(\Omega)$  occurs towards the lower frequencies, as compared to  $G(\Omega)$  (Fig. 1). Also, there is a large shift in the position of the central peak in the phonon spectrum towards lower energy (Fig. 1). An analogous transfer of weight under the  $\alpha^2(\Omega)F(\Omega)$  to lower frequencies as compared to  $G(\Omega)$ , but with no changes in the position of the phonon peaks, has been observed for  $Nb_3Sn$  (Refs. 2, 11, and 12) and  $Nb_3Al$  (Ref. 13) when the tunneling experiments have been inverted conventionally<sup>11,14</sup> or including the proximity effect.<sup>12,13</sup> However, this analogy cannot be pushed too far, since there are indications that the features of the electron-phonon coupling in  $V_3Si$  are not the same as in other high- $T_c$   $A15$  compounds.<sup>15</sup> It should be noted that the fitting of far-infrared data in

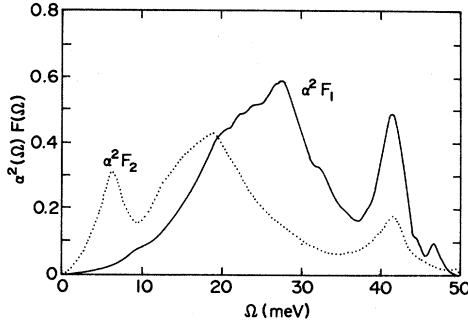


FIG. 1. Model  $\alpha^2 F$  spectra for  $V_3Si$ . The solid curve ( $\alpha^2 F_1$ ) has  $\lambda$  equal to 1 and is proportional (by a constant factor) to the phonon density of states  $G(\Omega)$  in  $V_3Si$  measured by Schweiss *et al.* (Ref. 2). Dotted curve ( $\alpha^2 F_2$ ) has  $\lambda = 1.29$  and is equal to  $\alpha^2 F_{tr}$  given in Ref. 9.

$V_3Si$  according to Allen's formulas is apparently not very sensitive to considerable changes in  $\alpha_{tr}^2(\Omega)F(\Omega)$ .<sup>9</sup>

(3) Recently, Muto *et al.*<sup>16</sup> performed a comprehensive experimental study of the thermodynamic properties of  $V_3Si$  in the superconducting state. From measurements of specific heat in both normal and superconducting states they obtained values for several parameters that depend on details of the electron-phonon interaction. Most importantly, they measured the superconducting thermodynamic critical field deviation function (Fig. 2),

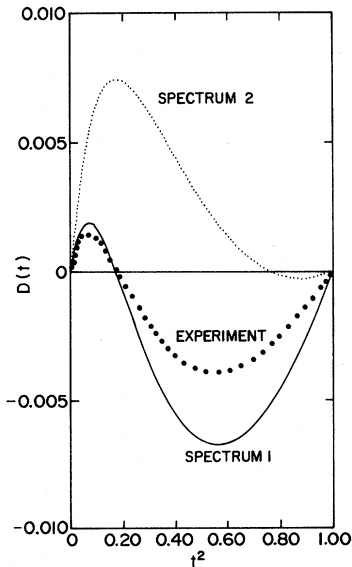


FIG. 2. Calculated and experimental (Ref. 16) values of  $D(t)$  in  $V_3Si$ . Solid curve was calculated from  $\alpha^2 F_1$  and dotted curve was calculated from  $\alpha^2 F_2$ .  $t = T/T_c$ .

$$D(t) = \frac{H_c(T)}{H_c(0)} - (1-t^2), \quad t = T/T_c.$$

The dependence of  $D(t)$  on details in  $\alpha^2 F$  is evident from the considerable structure in the functional derivative  $\delta D(t)/\delta \alpha^2(\Omega)F(\Omega)$ ,  $0 \leq t \leq 1$ , calculated for Pb by Daams and Carbotte.<sup>17</sup> Moreover, there is a simple empirical rule that relates the shape of  $D(t)$  to the electron-phonon renormalization parameter  $\lambda$ : For  $\lambda < 1$   $D(t)$  is negative, for  $\lambda > 1$   $D(t)$  is positive, and for  $\lambda \sim 1$   $D(t)$  has an S shape. Thus the experimental  $D(t)$  for  $V_3Si$  (Fig. 2) implies the value  $\lambda \simeq 1$  for  $V_3Si$ , which agrees with the finding of Schweiss *et al.*<sup>2</sup> and disagrees significantly with the result from the far-infrared-absorption experiments<sup>9</sup> [unless there is some reason for a large discrepancy between  $\alpha^2(\Omega)F(\Omega)$  and  $\alpha_{tr}^2(\Omega)F(\Omega)$  in  $V_3Si$ ].

(4) The value of the ratio  $2\Delta_0/k_B T_c$ , where  $\Delta_0$  is the zero-temperature energy gap and  $k_B$  Boltzmann's constant, is also an excellent indicator of the electron-phonon coupling strength or, more precisely, the importance of the damping and retardation effects.<sup>18</sup> The experimental results for  $2\Delta_0/k_B T_c$  in  $V_3Si$  span the range from  $\sim 3.5$  (the BCS value) up to  $\sim 3.8$ , thus indicating that  $V_3Si$  is a weak- to medium-coupling superconductor, in agreement with the results of the thermodynamic measurements by Muto *et al.*

In this work we calculate the superconducting thermodynamic properties resulting from the two model spectra for  $\alpha^2(\Omega)F(\Omega)$  in  $V_3Si$  and compare them with experimental results. The first spectrum is  $\alpha^2 F_1(\Omega) = cG(\Omega)$ , where  $G(\Omega)$  is the measured<sup>2</sup> generalized phonon density of states in  $V_3Si$  (at  $T = 77$  K) and  $c$  is the normalization constant chosen in such a way that the corresponding  $\lambda$  value is equal to 1, following Schweiss *et al.* The second spectrum is  $\alpha^2 F_2(\Omega) = \alpha_{tr}^2(\Omega)F(\Omega)$ , with  $\alpha_{tr}^2 F$  determined from the far-infrared-absorption measurements,<sup>9</sup> and  $\lambda$  value equal to 1.29. Since various thermodynamic properties such as  $T_c$ ,  $2\Delta_0/k_B T_c$ ,  $D(t)$ ,  $-[dH_c(T)/dT]_{T_c} T_c/H_c(0)$ ,  $\gamma[T_c/H_c(0)]^2$ , and  $\Delta C_e/\gamma T_c$ , where  $H_c(T)$  is the thermodynamic critical field at temperature  $T$ ,  $\gamma$  the coefficient of the linear term in the specific heat, and  $\Delta C_e$  the jump in specific heat at  $T_c$ , put large constraints on the possible candidates for  $\alpha^2 F$ , one expects that such a calculation will provide some new information about  $\alpha^2 F$  in  $V_3Si$ .

The attractive feature of such a calculation is that none of the above listed quantities depends explicitly on the value for the band-structure electronic

density of states at the Fermi level (there is an implicit dependence via  $\alpha^2 F$ ).

We perform the calculation of thermodynamic properties within the Eliashberg theory of superconductivity.<sup>1,19</sup> A brief summary of necessary

theoretical background is given in Sec. II. In Sec. III we present the results of our numerical calculations, and Sec. IV contains the discussion and conclusions.

## II. FORMALISM

With a given electron-phonon spectral function  $\alpha^2(\Omega)F(\Omega)$  and the Coulomb pseudopotential  $[\omega_c, \mu^*(\omega_c)]$ , the thermodynamic properties of an isotropic superconductor can be calculated from the solutions of Eliashberg gap equations on the imaginary frequency axis<sup>19</sup>:

$$\Delta(i\omega_n)Z_s(i\omega_n) = \pi k_B T \sum_{m=-\infty}^{+\infty} [\lambda(n-m) - \mu^*(\omega_c)\theta(\omega_c - |\omega_m|)] \frac{\Delta(i\omega_m)}{[\omega_m^2 + \Delta^2(i\omega_m)]^{1/2}}, \quad (1)$$

$$\omega_n Z_s(i\omega_n) = \omega_n + \pi k_B T \sum_{m=-\infty}^{+\infty} \lambda(n-m) \frac{\omega_m}{[\omega_m^2 + \Delta^2(i\omega_m)]^{1/2}}, \quad (2)$$

$$\omega_n = \pi k_B T (2n - 1), \quad n = 0, \pm 1, \dots \quad (3)$$

$$\lambda(n-m) = \int_0^{+\infty} d\Omega \alpha^2(\Omega)F(\Omega) \frac{2\Omega}{\Omega^2 + (\omega_n - \omega_m)^2}. \quad (4)$$

The superconducting critical temperature  $T_c$  is calculated from the linearized form of Eqs. (1) and (2) (i.e., the one obtained by setting  $\Delta^2=0$ ), according to the method proposed by Leavens.<sup>20</sup>

The free-energy difference per unit volume between the normal state and the superconducting state at temperature  $0 < T < T_c$  is given in terms of the solutions of Eqs. (1)–(4) by

$$\Delta F = -2\pi N(0)k_B T \sum_{n=1}^{\infty} \left[ \frac{\Delta^2(i\omega_n)Z_s(i\omega_n)}{[\omega_n^2 + \Delta^2(i\omega_n)]^{1/2}} - 2Z_s(i\omega_n)\{[\omega_n^2 + \Delta^2(i\omega_n)]^{1/2} - \omega_n\} - \omega_n [Z_s(i\omega_n) - Z_n(i\omega_n)] \left[ 1 - \frac{\omega_n}{[\omega_n^2 + \Delta^2(i\omega_n)]^{1/2}} \right] \right], \quad (5)$$

where  $N(0)$  is the single-spin electronic density of states per unit volume and  $Z_n(i\omega_n)$  is the normal-state renormalization function given by Eq. (2) with  $\Delta$  set equal to zero. Equation (5) is the Bardeen-Stephen<sup>21</sup> expression for the free-energy difference and is equivalent to the corresponding expression derived by Wada.<sup>22</sup> Once the  $\Delta F$  is known, various properties can be calculated using the well-known thermodynamic prescriptions [ $\Delta F(T) = H_c^2(T)/8\pi$ , etc.].

The low-temperature energy gap at the gap edge can be obtained by the analytic continuation of the imaginary axis solution  $[\Delta(i\omega_1), \Delta(i\omega_2), \dots]$  to the real frequency axis and then solving the equation

$$\Delta_0(T) = \text{Re}\Delta(T, \omega = \Delta_0(T)).$$

The  $N$ -point Padé approximant method proposed by Vidberg and Serene<sup>23</sup> is used for the numerical analytic continuation. Since  $\Delta_0(T)$  is practically

constant for  $T \lesssim 10\%T_c$ ,<sup>19</sup> one can calculate in this way the zero-temperature energy gap  $\Delta_0$ .

## III. NUMERICAL RESULTS

The two spectra used in calculations are shown in Fig. 1. The first spectrum was obtained by using  $G(\Omega)$  at  $T = 77$  K from the graph in Ref. 2, by continuing  $G(\Omega)$  below the lower-frequency bound of experimental results according to the quadratic law and by adjusting the constant  $c$  in  $\alpha^2 F_1(\Omega) = cG(\Omega)$  to get a  $\lambda$  value of 1. It should be noted that Schweiss *et al.* observed no change in  $G(\Omega)$  below  $T = 77$  K. The second spectrum was directly read from the graph in Ref. 9. Some typical parameters of the two spectra are given in the first five rows of Table I.

The cutoff  $\omega_c$  was chosen to be 250 meV

TABLE I. Summary of some typical parameters for the two model spectra of electron-phonon interaction in  $V_3Si$  and comparison of calculated values for several thermodynamic quantities with experimental results.

	Spectrum 1	Spectrum 2	Experiment
$\lambda = 2 \int_0^{+\infty} d\Omega \alpha^2(\Omega)F(\Omega)/\Omega$	1	1.29	
$A = \int_0^{+\infty} d\Omega \alpha^2(\Omega)F(\Omega)$	11.99 meV	8.63 meV	
$\langle \omega \rangle = 2A/\lambda$	23.96 meV	13.38 meV	
$\langle \omega^2 \rangle^{1/2} = \left[ 2 \int_0^{+\infty} d\Omega \Omega \alpha^2(\Omega)F(\Omega)/\lambda \right]^{1/2}$	25.78 meV	16.45 meV	
$\Omega_{\max}$ maximum phonon energy in $\alpha^2F$	50 meV	50 meV	
$\omega_c$ cutoff energy in Matsubara sums	250 meV	250 meV	
$\mu^*(\omega_c)$ Coulomb repulsion parameter	0.15	0.05	
$T_c$ superconducting critical temperature	17.1 K	16.63 K	14.5–17.1 K <sup>a</sup>
$-\frac{1}{H_c(0)} \left[ \frac{dH_c(T)}{dT} \right]_{T_c}$ $T_c$ parameter for which the BCS theory gives the value 1.74	1.95	2.44	1.97 <sup>b</sup>
$\gamma \left[ \frac{T_c}{H_c(0)} \right]^2$ parameter for which BCS theory gives the value 0.168	0.151	0.142	0.153 <sup>b</sup>
$\Delta C/\gamma T_c$ ratio of jump in specific heat at $T_c$ to the normal-state electronic specific heat at $T_c$ ; BCS value is 1.43	2.01	2.25	2.01 <sup>b</sup>
$2\Delta_0/k_B T_c$ BCS value is 3.53	3.85	4.33	3.76±0.1 <sup>c</sup> 3.8 <sup>d</sup> 3.8 <sup>e</sup> 3.4–3.6 <sup>f</sup>

<sup>a</sup>Reference 24.

<sup>b</sup>Reference 16.

<sup>c</sup>Reference 25.

<sup>d</sup>Reference 26.

<sup>e</sup>Reference 27.

<sup>f</sup>Reference 28.

( $=5\Omega_{\max}$ ) and the corresponding values of  $\mu^*(\omega_c)$  were fitted to the maximum experimental value<sup>24</sup> of  $T_c = 17.1$  K by solving the linearized Eliashberg equations. In the case of the second spectrum it turned out that  $\mu^*(\omega_c)$  had to be unusually small in order to get  $T_c > 16$  K. In the subsequent calculations the value  $\mu^*(\omega_c) = 0.05$  was taken for the

second  $\alpha^2F$  spectrum (see Table I).

In Fig. 2 we present the results of our calculation of the deviation functions  $D(t)$  for the two spectra together with the experimental results.<sup>16</sup> In Fig. 3 we plot  $C_{es}/\gamma T$  (the ratio of the electronic specific heat in the superconducting state to the low-temperature electronic specific heat in the nor-

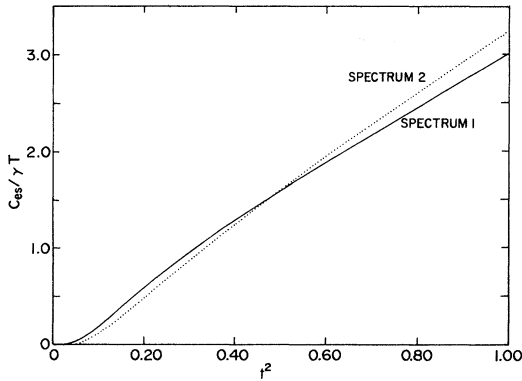


FIG. 3. Calculated values for the ratio of electronic specific heat in the superconducting state to that in the normal state.

mal state) vs  $t^2 = (T/T_c)^2$ , and in Fig. 4 we compare the calculated values of  $\ln(C_{es}/\gamma T_c)$  with the experimental results.<sup>16</sup> In Table I we give calculated and experimental values for some characteristic thermodynamic parameters.<sup>25-28</sup>

Obviously the results obtained from the spectrum based on the neutron experiments with  $\lambda = 1$  give a good fit to the experimental values of thermodynamic quantities. At the same time the thermodynamic properties calculated on the basis of the second spectrum ( $\lambda = 1.29$ ) would correspond to a superconductor that is considerably more strongly coupled than  $V_3Si$ . Also, the latter spectrum requires an unusually small Coulomb repulsion parameter, i.e.,  $\mu^*(\omega_c) = 0.05$ , in order to obtain the experimental value of  $T_c$ . Therefore, it can be safely ruled out as the possible candidate for  $\alpha^2F$  in  $V_3Si$ .

The results presented so far do not depend on the numerical value for  $N(0)$ , but only on  $\alpha^2(\Omega)F(\Omega)$  and  $(\omega_c, \mu^*(\omega_c))$ . Since the results based on the first spectrum give good agreement with the experiments one is encouraged to fit the value of  $N(0)$  to the experimental value of some particular thermodynamic quantity which depends explicitly on  $N(0)$  and then compare the calculated values of other quantities, which also depend on  $N(0)$ , with the experiment. The value of  $N(0)$  extracted in such a way can then be compared with the values inferred from other experiments or obtained in band-structure calculations.

We have fitted  $N(0)$  to the zero-temperature thermodynamic critical field  $H_c(0) = 6.43$  kOe.<sup>16</sup> The obtained value was  $N(0) = 13.64 \times 10^{19}$  states/(meV cm<sup>3</sup> spin). In Table II we compare some calculated thermodynamic parameters for the

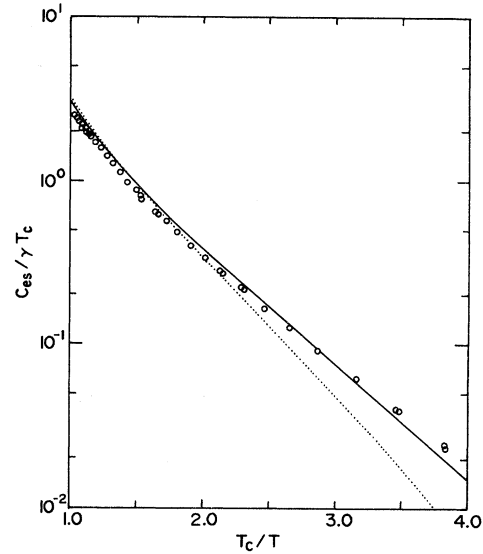


FIG. 4. Calculated and experimental (Ref. 16) values of  $\ln(C_{es}/\gamma T_c)$ . Solid curve was calculated from  $\alpha^2F_1$  and dotted curve was calculated from  $\alpha^2F_2$ . Circles denote experimental points.

above value of  $N(0)$  with the experimental results.<sup>29,30</sup> The agreement is within a few percent.

#### IV. DISCUSSION AND CONCLUSIONS

The results presented in the previous section clearly suggest that the  $\alpha^2F$  spectrum, based on the measured<sup>2</sup>  $G(\Omega)$  at  $T = 77$  K and with  $\lambda = 1$ , is able to account for the thermodynamic properties of  $V_3Si$  within the usual Eliashberg theory of superconductivity.<sup>19</sup> At the same time the  $\alpha_{tr}^2(\Omega)F(\Omega)$  inferred from the far-infrared-absorption measurements<sup>9</sup> cannot be taken as the  $\alpha^2F$  spectrum in  $V_3Si$ . In the following discussion we will not refer to the results obtained on the basis of the latter spectrum.

Considering the crudeness of our approximation  $\alpha^2(\Omega) = \text{const}$ , as well as the fact that experimental points should have error bars, we find that the calculated  $D(t)$  agrees surprisingly well with experiment. As mentioned in the introduction, the considerable structure in  $\delta D(t)/\delta \alpha^2(\Omega)F(\Omega)$  (Ref. 17) shows that the critical field deviation function is fairly sensitive to the details in  $\alpha^2(\Omega)F(\Omega)$ . Thus we expect that the true  $\alpha^2(\Omega)F(\Omega)$  in  $V_3Si$  is not too different from our guess (Fig. 1). This statement is supported by the fact that calculated quantities,  $-[dH_c(T)/dT]_{T=T_c} T_c/H_c(0)$  (BCS value

TABLE II. Comparison of calculated and experimental values for several thermodynamic quantities which depend explicitly on  $N(0)$ .

	Spectrum 1 with $N(0)=13.64 \times 10^{19}$ states/(meV cm <sup>3</sup> spin) chosen to fit experimental $H_c(0)=6.43$ kOe	Experiment
$\gamma$ [mJ/(mol K <sup>2</sup> )]	67.7 [calculated as $2\pi^2 k_B^2 N(0)(1+\lambda)/3$ ]	72.1 <sup>a</sup> 67.3 <sup>b</sup> 66.8 <sup>c</sup>
$-\left[\frac{dH_c(T)}{dT}\right]_{T=T_c}$ (kOe/K)	0.734	0.76 <sup>a</sup>
$\Delta C_e = (C_{es} - C_{en})_{T_c}$ Jump in electronic specific heat at $T_c$ [J/(mol K)]	2.32	2.42 <sup>a</sup>
$(C_{en})_{T_c} = \gamma T_c$ Normal-state electronic specific heat at $T_c$ [J/(mol K)]	1.16	1.20 <sup>a</sup>

<sup>a</sup>Reference 16.

<sup>b</sup>Reference 29.

<sup>c</sup>Reference 30.

1.74),  $\gamma[T_c/H_c(0)]^2$  (BCS value 0.168), and  $\Delta C_e/\gamma T_c$  (BCS value 1.43), agree with experimental results to within 1% (Table I).

The calculated value for the ratio  $2\Delta_0/k_B T_c$  is in excellent agreement with the value  $\sim 3.8$  obtained in the recent far-infrared measurements<sup>25</sup> as well as in the older tunneling results.<sup>26,27</sup> More recent tunneling experiments<sup>28</sup> give the value  $2\Delta_0/k_B T_c \sim 3.5$ , but there were indications that the bulk value for  $\Delta_0$  was underestimated.<sup>28</sup> On the basis of the functional derivatives  $\delta T_c/\delta\alpha^2(\Omega)F(\Omega)$ ,<sup>31,32</sup>  $\delta\Delta_0/\delta\alpha^2(\Omega)F(\Omega)$ , and  $\delta(2\Delta_0/k_B T_c)/\delta\alpha^2(\Omega)F(\Omega)$ ,<sup>32</sup> which are non-negative peaked functions with the peak frequencies  $\Omega^*(T_c) \sim 8k_B T_c$ ,  $\Omega^*(\Delta_0) \sim 2\Delta_0$ , and  $\Omega^*(2\Delta_0/k_B T_c) \sim \Delta_0/3$ , respectively, we can conclude that  $\alpha^2(\Omega)F(\Omega)$  in  $V_3Si$  cannot have considerably more weight at lower frequencies and less at higher frequencies than our guess (solid curve in Fig. 1) since that would increase the value of the ratio  $2\Delta_0/k_B T_c$  above the observed upper limit 3.8.

It is instructive to compare the value of  $N(0) = 13.64 \times 10^{19}$  states/(spin meV cm<sup>3</sup>), obtained by fitting the calculated zero-temperature thermodynamic critical field to the experimental value, with the values for  $N(0)$  in  $V_3Si$  available in the

literature. We note that our choice for  $N(0)$  leads to excellent agreement with experiment for calculated values of several thermodynamic quantities which explicitly depend on  $N(0)$  (Table II).

Muto *et al.*<sup>16</sup> have obtained from their experiments the value of 7.6 states/(eV atom), i.e.,  $28.27 \times 10^{19}$  states/(meV cm<sup>3</sup> spin) for the fully dressed electronic density of states  $N^*(0) = N(0)(1+\lambda)$ , where we assume that  $N(0)$  contains the renormalization by the Coulomb interactions.<sup>33</sup> If we take  $\lambda=1$  this would give  $N(0) = 14.44 \times 10^{19}$  states/(meV cm<sup>3</sup> spin) in good agreement ( $\sim 5\%$ ) with our value.

Testardi and Mattheis<sup>34</sup> give the experimental value  $N(0) = 2.5$  states/(eV spin V atom), i.e.,  $14.25 \times 10^{19}$  states/(spin meV cm<sup>3</sup>) for nearly perfect  $V_3Si$ , again in excellent agreement with our value for  $N(0)$ . [In conversion of various units for  $N(0)$  we have always used  $a = 4.722$  Å for the lattice parameter of  $V_3Si$ .]

However, the band-structure calculations give for  $N(0)$  in perfect  $V_3Si$  a value which is about one half of the above-quoted numbers. Mattheis *et al.*<sup>35</sup> calculated  $N(0) = 1.00$  states/(eV spin V atom), i.e.,  $5.70 \times 10^{19}$  states/(meV cm<sup>3</sup> spin). As the result of self-consistent augmented plane wave

(APW) calculations Klein *et al.*<sup>36</sup> have obtained the similar result  $N(0) = 200.2$  states/(Ry unit cell), that is  $6.99 \times 10^{19}$  states/(meV cm<sup>3</sup> spin). By using linear combination of muffin-tin orbital self-consistent band-structure calculations Arbman and Jarlborg<sup>37,38</sup> have calculated an even smaller value  $N(0) \sim 120$  states/(Ry unit cell) that is  $\sim 4.2 \times 10^{19}$  states/(meV cm<sup>3</sup> spin).

Note that if the calculated band-structure electronic density of states  $N(0) \leq 7 \times 10^{19}$  states/(meV cm<sup>3</sup> spin) is to account for the coefficient  $\gamma \sim 70$  mJ/(mol K<sup>2</sup>) in the linear term in specific heat of V<sub>3</sub>Si determined in the recent measurements,<sup>16,29,38</sup> the total renormalization term  $\lambda_T$  in  $\gamma = 2\pi^2 k_B^2 N(0)(1 + \lambda_T)/3$  has to be  $\geq 3$ . Such a large  $\lambda_T$  cannot be understood even if one invokes the existence of paramagnons (spin fluctuations) in V<sub>3</sub>Si.<sup>38</sup>

Testardi and Mattheiss<sup>34</sup> have offered an explanation for the large discrepancy in the values of calculated  $N(0)$  and the one inferred from the experiments on V<sub>3</sub>Si in terms of the rapid variation in  $N(E)$  around the Fermi level. They assume that actual samples correspond to V<sub>3-x</sub>Si with small  $x > 0$ . Then by assuming the rigid-band model they conclude that the resulting shift (of about 35 meV) in the position of the Fermi level in V<sub>2.94</sub>Si compared to its value in V<sub>3</sub>Si leads to a large increase in  $N(0)$ . Although this explanation cannot be ruled out, such sharp peaks in  $N(E)$  around the Fermi level require modification of the standard Migdal-Eliashberg theory to account for rapidly varying  $N(E)$ .<sup>39</sup> We have shown<sup>40</sup> that sharp peaks in  $N(E)$  with the half-width  $\leq \Omega_{\max}$  ( $\Omega_{\max} \sim 50$  meV in V<sub>3</sub>Si) lead to considerable changes in the values of calculated thermodynamic properties in the superconducting state. However, here we were able to account for the experimental-

ly observed superconducting thermodynamic properties of V<sub>3</sub>Si within the usual Eliashberg theory [constant  $N(E)$ ] by using  $\alpha^2(\Omega)F(\Omega)$  based on the measured phonon density of states. The latter two quantities are usually proportional to one another by a weakly varying factor.<sup>3</sup>

It should be mentioned that the experimental  $\gamma$  values listed in Table II have been obtained by analyzing the normal-state specific heat according to the formula  $C(T) = \gamma T + \beta T^3 + \alpha T^5$  (plus the requirement that at  $T_c$  the entropy in the normal state is equal to that in the superconducting state). The above-mentioned formula is more appropriate for the specific heat of solids such as V<sub>3</sub>Si, which cannot be described by Debye's model. An analysis of the specific-heat data on the basis of  $C(T) = \gamma T + \beta T^3$  usually gives smaller value for  $\gamma$ , between 55 and 62 mJ/mol K<sup>2</sup>) (see Ref. 16).

In conclusion, we have found on the basis of neutron scattering experiments an  $\alpha^2 F$  spectrum in V<sub>3</sub>Si, which accounts, within the usual Eliashberg theory, for all experimentally measured thermodynamic properties in superconducting state of V<sub>3</sub>Si. Nevertheless, the final test of the correctness of the above spectrum in V<sub>3</sub>Si should come from single-particle tunneling experiments.

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