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ANHARMONICITY AS AN EXPLANATION FOR ANOMALOUS RESISTANCE OF HIGH- T_c SUPERCONDUCTORS

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Experimental evidence about the temperature dependence of phonon frequencies in V_3Si is used to demonstrate that anharmonicity is a major factor in causing the resistance anomalies recently observed in many high- T_c superconductors.

FISK and collaborators¹ have recently pointed out that the electrical resistance of high temperature superconductors (generally intermetallic compounds with both s - p and d -band constituents) deviates strongly from the Bloch–Gruneisen² behavior generally found in other metals. A typical example is V_3Si for which the data³ are shown in Fig. 1. Usually the Bloch–Gruneisen theory is interpreted to mean that the difference between the resistivity $\rho(T)$ for $T \gg \theta_D$ from the limiting (impurity dominated) resistivity for $T \rightarrow 0$ is linear in temperature, i.e.

$$\begin{aligned} \rho(T) - \rho_0 &= \rho_{e-p}(T) \\ &= (2\pi m k_B / ne^2 \hbar) \lambda_{tr} T, \quad \text{for } T \gg \theta_D, \quad (1) \end{aligned}$$

where (n/m) is the effective ratio of electron density to mass, and $\rho_{e-p}(T)$ is a complicated integral over the phonon distribution which simplifies at high temperatures to a linear power of T . The strength of the electron–phonon coupling is measured by the dimensionless number⁴ λ_{tr} which is closely related to the coupling constant λ of superconductivity theory.⁵ It is immediately clear that the data of Fig. 1 cannot satisfy equation (1) because the high temperature resistivity is not really linear. If we denote by $\rho^*(T)$ the extrapolated resistivity at zero temperature from the slope at

temperature T , $\rho^*(T) > \rho_0$ for $T \geq 150$ K. (For V_3Si $\theta_D \approx 300$ K.) The quantity $\zeta(300) \equiv [\rho^*(300) - \rho_0] / [\rho(300) - \rho_0]$ can be estimated from the data to be about 0.5. The data in Fig. 1 is taken from a published paper³ and the drawing of slopes is hazardous. We can be in error in estimating $\zeta(300)$ by as much as 50% in either direction.

Many possible explanations for this discrepancy have been given.⁶ In this note we present evidence for a particularly simple explanation, namely that λ_{tr} in equation (1) is temperature dependent because of an anomalously strong temperature dependence of the phonon frequencies. Following McMillan,⁵ we write λ_{tr} as

$$\lambda_{tr} = \frac{\eta_{tr}}{M \langle \omega^2 \rangle} \quad (2)$$

where η_{tr} is a purely electronic factor involving the electron density of states and matrix elements averaged over the Fermi surface, M is an averaged atomic mass, and $\langle \omega^2 \rangle$ is a mean square phonon frequency calculated with a weight factor $F(\omega)/\omega$ where $F(\omega)$ is the phonon density of states. (This involves an assumption that the coupling factor $\alpha_{tr}^2(\omega)$ is roughly independent of ω , an approximation which probably only fails at small ω .) If we assume the validity of equation (1) at high temperatures, then we can write

$$\begin{aligned} \zeta(T) &\equiv [\rho^*(T) - \rho_0] / [\rho(T) - \rho_0] \\ &= \frac{d \log \langle \omega^2 \rangle}{d \log T} - \frac{d \log (m/n) \eta_{tr}}{d \log T}. \end{aligned} \quad (3)$$

A close approximation to the phonon density of

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Table 1. Experimental mean squared phonon frequencies and interpolated value of $d \log \langle \omega^2 \rangle / d \log T$ compared with experimental resistance $\zeta(300) = [\rho^*(300) - \rho_0] / [\rho(300) - \rho_0]$ for four A-15 structure superconducting compounds

Compound	Superconductive T_c (K)	$\langle \omega^2 \rangle^a$ $T = 297$ K (meV ²)	$\langle \omega^2 \rangle^a$ low T (meV ²)	Fractional anharmonicity $1 - c$	$\frac{d \log \langle \omega^2 \rangle}{d \log T}$	$\zeta(300)$ Experimental
V ₃ Si	17	763	642 ^b	0.16	0.31	0.5, ^e 0.3 ^f
V ₃ Ga	15	456	408 ^c	0.072	0.17	0.45, ^g 0.3 ^f
V ₃ Ge	6	572	532 ^c	0.06	0.12	0.3 ^f
Nb ₃ Sn	18	331	287 ^d	0.072	0.21	0.6 ^h

^a Reference 7. ^b $T = 4.2$ K. ^c $T = 77$ K. ^d $T = 5.58$ K. ^e Reference 3.

^f SARACHIK M.P., SMITH G.E. & WERNICK J.H., *Can. J. Phys.* **41**, 1542 (1968).

^g FISK Z. Unpublished (1975).

^h WOODARD D.W. & CODY G.D., *Phys. Rev.* **136**, A166 (1964).

Fig. 1. Experimental values of electrical resistance ρ as a function of temperature T for V₃Si (from reference 3). The value $\rho^*(296) - \rho_0 = 35 \mu\Omega\text{-cm}$ found by linear extrapolation deviates significantly from the Bloch–Grüneisen value of 0.

Fig. 2. Experimental values of $\log \langle \omega^2 \rangle$ (calculated from the phonon densities of states of reference 7) plotted vs $\log T$. The solid line is an empirical fit using equation (6).

states $F(\omega)$ of V₃Si has been measured at $T = 4.2$, 77, and 296 K by Schweiss⁷ by the technique of incoherent inelastic neutron scattering. We have used these data to calculate $\langle \omega^2 \rangle$ at these three temperatures, the results being 641, 654, and 758 meV², respectively. The results are plotted in Fig. 2. We need to estimate the slope ($d \log \langle \omega^2 \rangle / d \log T$) at $T = 296$ K, the highest temperature at which data are available. For this purpose we make a simple model to fit the temperature dependence of $\langle \omega^2 \rangle$. The model considers the shift in phonon frequencies due to anharmonicity from their value ω_h in a harmonic crystal:

$$\omega^2(T) = \omega_h^2 + \omega_{ah}^2, \quad (4)$$

$$\omega_{ah}^2 = V_{3-4} \langle u^2 \rangle_T \quad (5)$$

where V_{3-4} schematically denotes the dependence on the cubic and quartic anharmonicity and $\langle u^2 \rangle_T$ is the mean square displacement at a temperature T . Notice that to $O(\langle u^2 \rangle)$ the contribution of the cubic anharmonicity would be such as to decrease the phonon frequencies and of the quartic anharmonicity to increase them. The experimental results lead one to conclude that the quartic anharmonicity is dominant in V₃Si (and we suspect also in other transition metal compounds). The physical origin of the strong quartic anharmonicity probably lies in the strong short range repulsion of tightly bound d shells.

We may put for $\langle u^2 \rangle_T$ the expression for a harmonic crystal and obtain from (4)

$$\langle \omega^2(T) \rangle / \langle \omega^2(0) \rangle = c + (1 - c) \coth(\theta/2T) \quad (6)$$

where we determine c by fitting to the data of Fig. 2. Choosing $\theta \approx \langle \omega^2(0) \rangle^{1/2} \approx 296$ K, we find that a value $c = 0.84$ fits the available data. The resulting curve is shown as the solid line in Fig. 2, and yields a value ($d \log \langle \omega^2 \rangle / d \log T$) = 0.31. Inserting in (3) this gives us

only about 60% of the effect we are looking for. However, as already mentioned our deduction of $\zeta(300)$ from the data is quite uncertain. So is the deduction of $(d \log \langle \omega^2 \rangle / d \log T)$ at room temperature from the data which extends only to room temperature. More precise knowledge of resistivity as well as measurements of $\langle \omega^2 \rangle$ at higher temperatures are required to see whether mechanisms other than the one discussed here contribute significantly to the resistivity anomaly.

Reichardt and collaborators at Karlsruhe have also sent us unpublished data for $F(\omega)$ in V_3Ga , V_3Ge , and Nb_3Sn at two different temperature each. The moments $\langle \omega^2 \rangle$ are shown in Table 1. For the vanadium compounds, an incoherent scattering method was used, while for Nb_3Sn , an average of several scattering angles was taken with a polycrystalline target. The interpolated values of $d \log \langle \omega^2 \rangle / d \log T$ are smaller than in V_3Si , but still fairly large, and tend to scale with T_c , in agreement with Fisk's observations¹ about resistance anomalies. As can be seen from Table 1, anharmonic effects can account for 30% of the anomaly in Nb_3Sn .

Previous attempts⁸⁻¹⁰ to explain the resistivity anomaly have mainly invoked a temperature dependence of $(m/n)\eta_{tr}$ which arises from having the electronic density of states vary rapidly with energy over a range kT . It is hard to estimate the magnitude of this effect since no reliable knowledge of the density of states near the Fermi surface to this accuracy is available.

Our mechanism is based on the experimental results on $\langle \omega^2(T) \rangle$ which can only be understood if the anharmonic forces in V_3Si are anomalously large. Independent evidence that this is so are provided by the extraordinary harmonic generation observed by Testardi¹¹ in V_3Si . The confirmation of strong anharmonicity in other high temperature superconductors discussed in reference 1 must await determination of $\langle \omega^2(T) \rangle$ for them. The reason for the relatively strong anharmonicity of high temperature superconductors is that the harmonic force constants in these materials as measured, say, by the low temperature sound velocities, are relatively small. This leads to a larger mean square displacement and effectively a larger anharmonic contribution to the phonon frequencies.

In the A-15 structure extraordinary anharmonicity has earlier been inferred by Testardi and Bateman,¹² who also speculated on its effect on the resistivity. Testardi's¹³ heuristic model for the interatomic potential in A-15 compounds also leads to temperature dependence of phonon frequencies of the form given by equation (6).

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