

The samples are believed to be representative of an ideal covalent disordered material.¹⁴ As a matter of fact, conductance changes associated with inelastic tunneling yields a tunneling density of states which is clearly reminiscent of the phonon density of states of crystalline germanium, considerably broadened however. This is related to the short phonon correlation length to be expected in a disordered material.

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Scattering of Quasiparticles by Thermal Phonons in Copper*

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We present an augmented-plane-wave pseudopotential calculation of the scattering of quasiparticle excitations by thermal phonons in symmetry zones of the Fermi surface of copper. The results provide an interpretation of recent experimental data.

Low-temperature experiments¹⁻³ have yielded for the first time measurements of the relaxation time for quasiparticle excitations averaged over small regions of the Fermi surface. It is convenient to express the experimental relaxation times in the form

$$1/\tau = \Gamma_0 + \gamma T^3,$$

where the coefficient γ measures the rate of scattering of quasiparticles by thermally excited phonons. The data for copper show that γ is strongly anisotropic, varying by factors as large as 30 between different regions of the Fermi surface. In this Letter we report some results of a calculation of the anisotropy of the coefficient γ in copper, based on an augmented-plane-wave (APW) formulation of the matrix element of the electron-phonon interaction.

In the rigid-ion approximation, the matrix element of the electron-phonon interaction in a metal can be expressed in terms of pseudoatom phase shifts⁴ that are determined by an analysis

of experimental Fermi-surface data. Screening by conduction electrons is treated approximately by choosing the phase shifts so that the Fermi-surface average of the low- q limit of the pseudopotential is consistent with the known response to a long-wavelength density fluctuation.⁵ Such a model has proved quite successful in predicting the phonon resistivities and renormalization factors for metals of the alkali series.⁴ As a further and more rigorous test of the model, we have carried out a calculation of the anisotropy of the scattering of quasiparticles by thermal phonons in copper, evaluating the matrix elements of the electron-phonon interaction from an empirical phase-shift pseudopotential.

In the low-temperature limit $T \ll \Theta$, the phonon scattering rate is given by⁶

$$\frac{\hbar}{\tau(\vec{k})} = \frac{1.31\Omega k_B^3 T^3}{M V_{\vec{k}} \hbar^3} \sum_{\sigma} \left\langle \frac{|V_{\sigma}(0, \vec{k})|^2}{C_{\sigma}^4} \right\rangle,$$

where Ω is the volume of the primitive unit cell, M is the ion mass, $V_{\vec{k}}$ is the Fermi velocity of

the state \vec{k} , $V_{\sigma}(0, \vec{k})$ is the small-angle scattering limit of the pseudopotential, and C_{σ} is the velocity associated with the phonon mode of polarization σ . This expression has been evaluated numerically,⁶ taking into account the known anisotropies of the Fermi surface⁷ and the phonon spectrum of copper.⁸ The wave functions for states on the Fermi surface were determined by solving an APW secular equation involving empirical phase shifts. The matrix element of the electron-phonon interaction was calculated by a procedure that has been discussed elsewhere,⁴ but generalized to take into account the nonspherical Fermi surface of copper. In a spherical approximation the matrix elements of the APW pseudopotential closely resemble the orthogonalized-plane-wave form factors of Harrison⁹ and Moriarty.¹⁰

At sufficiently low temperatures, the scattering of quasiparticles by thermally excited phonons is dominated by small-angle processes. On the belly of the Fermi surface of copper only scattering by longitudinal phonons can contribute to such processes, whereas on the necks coupling by transverse phonons is possible and must be taken into account. Our results for the anisotropy of γ are shown in Fig. 1, where they are compared with the experimental data of Koch and Doezema.² The variation of γ over the belly correlates with variations in the long-wavelength limit of the APW pseudopotential, and the large increase in the scattering rate close to the necks is caused primarily by interaction with transverse phonons. The overall agreement with the experimental anisotropy and absolute scattering rate is satisfactory, although our calculation underestimates the absolute scattering rate close to (100).

Thus, the principal features of the variation of γ over the Fermi surface of copper can be explained by combining realistic models of the Fermi surface and phonon spectrum with a phase-shift pseudopotential calculation of the matrix elements of the electron-phonon interaction. A complete discussion of the scattering calculations, together with an analysis of the anisotropy of the renormalization of the energy bands in

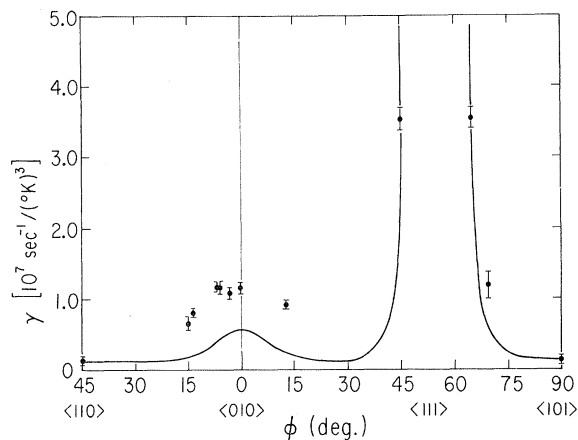


FIG. 1. APW pseudopotential calculation of the anisotropy of the rate of scattering of quasiparticles by thermal phonons in copper, and comparison with the experimental data of Koch and Doezema (Ref. 2). The experimental points represent averages over an angular range of about $\pm 6^\circ$.

copper by the electron-phonon interaction, will be published elsewhere.

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