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PHONON-LIMITED LIFETIMES OF ELECTRONS IN Pd.

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Quasiparticle lifetimes $1/\tau_k$ are calculated for electrons on the Fermi surface (FS) of Pd using the rigid muffin tin model. Results are presented for the Γ-centered and the open sheets.

Butler et al[1] predicted phonon line-widths in Nb and Pd, which subsequent experiments confirmed reasonably well. Butler has argued[2] that the rigid muffin tin (RMT) model used in ref. 1 might give a poor description of small $\underset{\sim}{Q}$ processes. To test this, we present predictions of the anisotropic low temperature (T) phonon-limited electron lifetimes τ_k in Pd. A measurement by radio-frequency size effect[3] or some other method will directly test the small-$\underset{\sim}{Q}$ RMT model.

The quasiparticle lifetime is given by the expression[3,4]

$$1/\tau(k,\omega) = 2\pi \int_0^\infty d\Omega\, \alpha^2F(k,\Omega)\{2N(\Omega)+f(\Omega+\omega)+f(\Omega-\omega)\} \quad (1)$$

$$\alpha^2F(k,\Omega) = \frac{1}{N}\sum_Q \sum_\nu |g^\nu_{k,k-Q}|^2 \delta(\Omega-\omega^\nu_Q)\delta(\epsilon_{k-Q}) \quad (2)$$

The notation is consistent with refs. 1,2,4. For $\omega=0$ and $T \ll \omega_D$ (ω_D is the Debye energy) only small values of Ω contribute to the integral in (1). In this regime we can use the form $\alpha^2F(k,\omega) = c_k\Omega^2$. Performing the integral gives[3,4]

$$1/\tau(k,0) = \alpha_k T^3, \quad \alpha_k = 14\pi\zeta(3)c_k \quad (T \ll \theta_D) \quad (3)$$

The experimental scattering rate $1/\tau_k{}^*$ differs from eq. (2) in two ways. First, at temperature T, electrons are sampled not just at the Fermi energy ($\omega=0$) but in a shell of thickness T. Averaging (1) by $-\partial f/\partial\omega$ enhances[3,4] $1/\tau_k$ by 12/7. Second, $1/\tau_k$ is reduced by $1+\lambda_k$, the mass enhancement factor. We have previously[1] calculated $\langle\lambda_k\rangle = \lambda = 0.4$, and expect anisotropy in λ_k to be fairly small. The present calculation uses an improved potential with little change in FS properties. We have not recalculated λ.

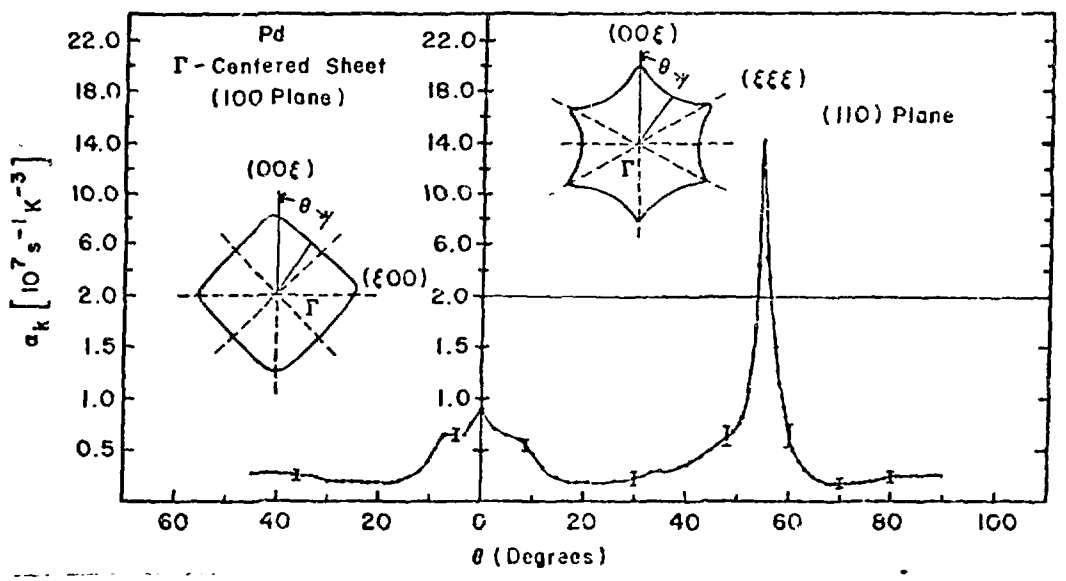

Fig. 1. α_k vs θ for the Γ-centered sheet of Pd

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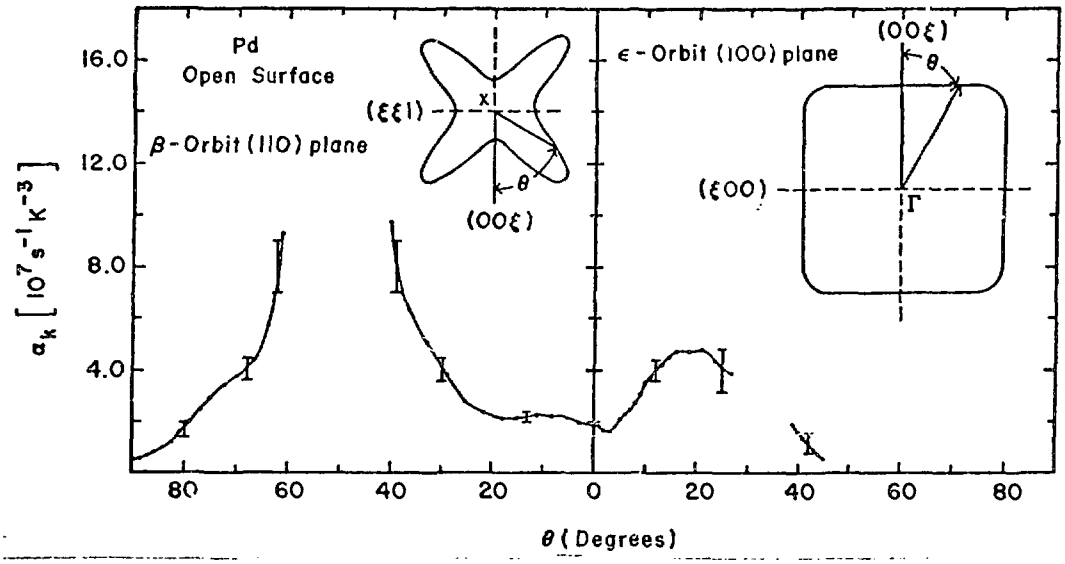

Fig. 2. α_k vs θ for the open surface of Pd. The missing points are points near glancing angles where convergence errors are large.

To calculate c_k, we need electron-phonon matrix elements $g^{\nu}_{k,k'}$. The details of the RMT model have been described previously.[5] Only small ω phonons are needed; sound velocities v^{ν}_{Q} and polarization vectors ϵ^{ν}_{Q} were derived from experimental elastic constants. The integral in eq.(2) is a surface integral over the points of FS lying very close to k. For small Q, $|g^{\nu}_{k,k+Q}|^2$ behaves as $G^{\nu}_{k}(\theta,\phi)Q$. (θ and φ give the direction of Q). Using the δ function to integrate over Q, the remaining integral is over directions of Q, where Q lies on a plane tangent to the FS at k. The integral contains $G^{\nu}_{k}(\theta,\phi)$, $\epsilon^{\nu}_{\theta,\phi}$ and $v^{\nu}_{\theta,\phi}$. Because of a finite mesh size, $G^{\nu}_{k}(\theta,\phi)$ is known only in some specific directions, and we interpolate linearly between these directions. Although $G^{\nu}_{k}(\theta,\phi)$ is a strong function of (θ,φ), we found that Q can be taken as large as 0.08(2π/a) giving typically 50 points in different directions for satisfactory convergence of c_k while still remaining in the regime where the matrix elements are linear in Q.

Results for the Γ-centered sheet and the open surface of Pd are shown in figs. 1 and 2. For a description of the FS of Pd see ref. 7. The mesh points on the FS are obtained as the points of intersection of the FS with a sampling ray originating from a search point. The mesh is coarsest in the region where there is a glancing angle of intersection, thus our results are not very accurate in these regions. We have included error bars in our figures to indicate the estimated errors from lack of convergence.

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