Multiple-Plane-Wave Theory of Gap Anisotropy in Al*

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(Received October 20, 1975)

The variation over the Fermi surface of the superconducting gap edge \( \Delta_0(\mathbf{k}) \) has been calculated for Al. We include in the computations a realistic Fermi surface, multiple-plane-wave electron–phonon matrix elements, and realistic phonons. The computations proceed from directional electron–phonon spectral weights which contain the information on the phonon-mediated electron–electron interaction for a given electron \(|\mathbf{k}\rangle\). To relate the microscopic parameters to the gaps, we use the equations due to Leavens and Carbotte. They are an approximate version of the Eliashberg equations valid for the gap edge in the weak coupling limit. The results are used to compute the pure single-crystal transition temperature.

1. INTRODUCTION

Realistic microscopic calculations of gap anisotropy in Al were first attempted by Dynes and Carbotte and extended by Leavens and Carbotte. In their work the Fermi surface is a sphere and a single plane wave is used to describe the electronic structure. This paper presents results of calculations that involve several improvements over previous work.

For the Fermi surface the realistic four-plane-wave pseudopotential model of Ashcroft is used. The electron–phonon matrix elements are computed with 15 plane waves included in the description of initial and final electronic states. For the lattice dynamics we use a Born–von Karman model derived from inelastic neutron scattering data on the phonon dispersion curves.

To calculate the gap at position \(|\mathbf{k}\rangle\) on the Fermi surface we require a directional electron–phonon spectral weight \( \alpha^2(\omega)F_k(\omega) \) describing the

*Research supported in part by the National Research Council of Canada.
electron–phonon interaction and a parameter $\mu^*$ related to the Coulomb repulsions between electrons. The directional electron–phonon function $\alpha_k^2(\omega)F_k(\omega)$ contains all of the information on the electronic structure, the phonon spectrum, and the coupling between electrons and phonons that is needed in considerations of the superconducting state. From this information a formula due to Leavens and Carbotte $^2$ can be used to calculate the anisotropic gap edge in Al.

The paper is structured as follows. In Section 2 we specify the expression for $\alpha_k^2(\omega)F_k(\omega)$, which we use in Section 3 to calculate the anisotropic gap. In Section 4 we discuss the average gap for a pure single crystal and compare it with the dirty isotropic case. The critical temperature is also discussed and conclusions are drawn.

### 2. ELECTRON–PHONON FUNCTION $\alpha_k^2(\omega)F_k(\omega)$

The quantities central to this work are directional electron–phonon distribution functions $\alpha_k^2(\omega)F_k(\omega)$, which contain all of the information on the electron–phonon interaction as it enters superconductivity. For a given electronic state $|k\rangle$ on the Fermi surface we have

$$
\alpha_k^2(\omega)F_k(\omega) = \int \frac{dS_k}{\hbar |V(k')|} \frac{1}{(2\pi)^3} \sum_\lambda |g_k k \lambda|^2 \delta(\omega - \omega_\lambda (k' - k))
$$

(1)

with $dS_k$ an element of the Al Fermi surface, $V(k')$ the Fermi velocity, and $\hbar$ Planck's constant divided by $2\pi$. In (1), $\omega_\lambda (k' - k)$ denotes a phonon frequency for the $\lambda$th branch and $g_k k \lambda$ is the electron–phonon vertex describing the scattering of an electron from $|k\rangle$ to $|k'\rangle$ due to the emission or absorption of a phonon. The delta function in (1) has the effect of generating a direction phonon frequency distribution for a given state $|k\rangle$ in which each mode is properly weighted by the strength of the electron–phonon interaction.

The details of the electronic structure of Al enter (1) not only through the Fermi surface integral over final states but also in the electron–phonon vertex $g_k k \lambda$. It can be written as

$$
g_k k \lambda = \frac{-ie_\lambda (k' - k)}{[2M N\omega_\lambda (k' - k)]^{1/2}} \left\{ \sum_{k' k n'} (k' + k' n - k - k_n) (k' + k' n W k + k_n) \right\}
$$

(2)

where $N$ is the number of ions of mass $M$ and the $k_n$ are the reciprocal lattice vectors. In (2), $\langle f | W | f' \rangle$ stands for the electron–ion pseudopotential form factor between plane waves $|f\rangle$ and $|f'\rangle$ and the $a_k (k_n)$ are the expansion coefficients of the electronic wave functions in terms of plane waves. Finally