Effect of Temperature on the Fermi Surface of Beryllium*

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By straightforward extension of the pseudopotential model which was originally developed for pure beryllium at 0°K, it is shown how to obtain the changes in the Fermi surface with temperature. Because of the very high Debye temperature of Be, the changes even at room temperature are not large. In particular, the calculations show that there are no changes in topology of the Fermi surface with rise in temperature and that the probability of breakdown between orbits in a magnetic field is not significantly enhanced.

INTRODUCTION

IN a previous paper[1] we have described in some detail the Fermi surface of Be and have shown how the experimental measurements can be accurately fitted by a nonlocal pseudopotential model. Since the calculation applies strictly only at 0°K, it is our aim here to extend the model to finite temperatures T. We confine our attention to two distinct effects of temperature on the Fermi surface: (a) the effect of the structure factors through the Debye-Waller factor, which is equivalent to altering the Fourier transform of the potential, and (b) the effect of lattice expansion. We shall not concern ourselves with thermal broadening of the Fermi-Dirac distribution, nor with the effect of temperature on the phonon spectrum and thus on the electron-phonon interaction. Our model then describes only certain geometric aspects of the Fermi surface and cannot, without additional assumptions, give direct information on transport properties and other scattering phenomena. Clearly, both thermal smearing and the scattering of electrons by phonons is a limiting factor in many methods of measuring the Fermi surface, so that this calculation which considers geometry alone will generally be useful only at low temperatures. This corresponds exactly to the situation in random-alloy calculations where a direct comparison of the theoretical Fermi surface with experiment can only be made at very low concentrations.

THERMAL MODEL

Keffer *et al.*[2] have shown how to introduce the temperature into a pseudopotential model of band structure by means of the Debye-Waller factor. If the structure factor for each reciprocal lattice vector $\mathbf{G}$ is expanded in powers of the ionic displacements $\mathbf{u}(\mathbf{R}_n,T)$, then to a first approximation the ideal structure factors are multiplied by e^{-W}, where W is the Debye-Waller factor given by $W=\frac{1}{2}G^2\langle u^2(T)\rangle$. $\mathbf{R}_n$ is a direct lattice vector and $\langle\ \rangle$ denotes an average over all phonon modes. Since the mean potential energy of an ion depends on $\mathbf{u}$ and equals the mean kinetic energy, $\langle u^2(T)\rangle$ can be estimated from the mean kinetic energy of the phonon gas, which in turn can be evaluated in certain cases, for example, the Debye model.

In the present pseudopotential model, the parameters of the pseudopotential were obtained by fitting to experimental measurements on pure Be at helium temperature, so that it is reasonable to assume that any effects of zero-point motion have already been incorporated. With this assumption, we have calculated the remaining part of the Debye-Waller factor as a function of T from a Debye model, using a value of 1250°K for Θ_D, the Debye temperature.[3] Because Θ_D is so high, at 10°K W is of the order of 10^{-8}, while even at room temperature e^{-W} has dropped only to about 0.99 for the G values of interest. To calculate changes in the Fermi surface due to thermal vibrations, then, we need only find $W(G,T)$ and scale the structure factors in the matrix elements accordingly.

The other temperature effect, thermal expansion, is very easily included in the model. Since the whole computation depends on the values of the c and a lattice spacings, it is simply a matter of taking values appropriate to the temperature from the literature.[4] The pseudopotential parameters are then adjusted according to the new lattice spacings as described in I, where we examined the pressure dependence of the Fermi surface.

These two modifications to the original calculation are incorporated into the programs and the only problem then is to find the new Fermi level. We are interested here in those features of the Fermi surface likely to show the largest percentage change with T, and these are also the features most sensitive to error in placing the Fermi level. Neglecting thermal broadening of the Fermi distribution, the Fermi level in Be is defined by equating the volumes of the hole and electron pieces of the Fermi surface. In the present work we have adopted a simple method of estimating the volume of an energy surface on the assumption that, for small perturbations, the surfaces remain similar to the 0°K case. Referring to Fig. 2 of I, we have taken the volume

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[1] J. H. Tripp, P. M. Everett, W. L. Gordon, and R. W. Stark, Phys. Rev. **180**, 669 (1969), to be referred to as I. The present notation is taken from this reference.

[2] C. Keffer, T. M. Hayes, and A. Bienenstock, Phys. Rev. Letters **21**, 1676 (1968).

[3] G. Ahlers, Phys. Rev. **145**, 419 (1966). The value of the Debye temperature used here is taken as representative of the experimental values, which vary considerably with T.

[4] R. W. Meyerhoff and J. P. Smith, J. Appl. Phys. **33**, 219 (1962).

of the cigar surface to be proportional to its height Ke times its central cross section, given by α^1 with field along $\langle 0001 \rangle$. Similarly, the coronet has a volume proportional to its inner radius $\Gamma\bar{l}$ times a typical cross section, given by $\beta_2{}^2$ with field along $\langle 10\bar{1}0 \rangle$. The constants of proportionality are obtained from the known volume at 0°K and thus we can adjust the Fermi level to give exact compensation. The uncertainty in the Fermi level found this way depends on how much the Fermi surface has changed and for the highest temperature considered is of the order of 10^{-4} Ry.

As a rough check on the results, it is possible to treat the two temperature effects separately and to add the partial changes at given T. One advantage of this is that lattice expansion has already been treated in I. We are also able to see that for each quantity of interest, the partial changes have the same sign, which means that the variation with T will be always monotonic. Up to temperatures of 10°K or so, the changes are entirely negligible, but above 100°K, W begins to increase rapidly, roughly as $(T/\Theta_D)^4$, so that the influence of thermal vibrations becomes dominant at a few hundred °K.

RESULTS

Calculated values of some representative properties of the Fermi surface as a function of T are given in Table I. We have not given the uncertainty in each quantity, but the *changes* are generally accurate to 20% or better, so that Table I at least indicates the trend expected. In view of the difficulties of actually observing the Fermi surface at higher T, this is perhaps sufficient. It is emphasized that the greatest source of error lies in locating the Fermi level.

The thin horizontal connecting necks of the hole coronet grow in area, increasing about 12% by room temperature, so that any dismemberment of this monster by heating is ruled out. Both extremal sections of the cigars increase with T but the smaller central section increases faster, so that the observed beat frequency should drop. The distance between the hole and electron pieces, ak in the notation of I, decreases slightly so that magnetic breakdown across this gap will become somewhat easier as T rises. At 300 °K the breakdown field is calculated[5] to be about 110 kG, some 10 kG less than at 0°K. For field directions close to the c axis, however, the smallest breakdown orbit has an area far too high to be observable, so that we should expect just a loss of amplitude for the α^1 oscillations.

TABLE I. Variation with temperature of various quantities associated with the Fermi surface of Be. T in °K.

Quantity[a]	Units	$T=0$	100	200	300
$\gamma_1{}^1$ field along $\langle 11\bar{2}0 \rangle$	10^6 G	0.110	0.110(3)	0.114	0.123
α^1 field along $\langle 0001 \rangle$	10^6 G	9.48	9.48	9.50	9.55
α^2 field along $\langle 0001 \rangle$	10^6 G	9.75	9.75	9.75(6)	9.77
Cigar-coronet gap ak	a.u.	0.0098	0.0098	0.0096	0.0092
Neck diameter no	a.u.	0.0196	0.0196(2)	0.0199	0.0208

[a] See Ref. 1 for explanation of notation.

CONCLUSION

We have used a Debye model for the phonon gas in a metal to calculate the Debye-Waller factors required for a pseudopotential calculation. Using them in conjunction with experimental values for the lattice expansion, we have concluded that the effect of temperature on the geometry of the Fermi surface of Be is small because of the very high Debye temperature. Up to room temperature there is no change in topology of the Fermi surface. Even considering that the thermal smear of the Fermi-Dirac distribution at room temperature is about 2 mRy, there seems no chance of observing any effects of electron tunneling out of the semiclassical orbits. The energies required for this do not depend significantly on T. Near the thin necks or across the cigar-coronet gap the barrier is of the order of 10 mRy, while between the ends of two cigars it is about 30 mRy. Similarly, an electron would have to acquire some 30-mRy additional energy to move on to an incipient lens surface at Γ. From geometry alone, then, we do not anticipate any large variation in transport phenomena, such as the Hall effect, which are indirect reflections of the topology and shape of the Fermi surface.

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[5] R. G. Chambers, Proc. Phys. Soc. (London) 88, 701 (1966).