

authors express the length of the wave vector to the Fermi surface by:

$$k = k_0 [1 + AY_4(\theta, \phi) + A_1 Y_6(\theta, \phi)] \quad (IV-1)$$

The Kubic harmonics $Y_4(\theta, \phi)$ and $Y_6(\theta, \phi)$ are combinations of spherical harmonics having cubic symmetry; they are given by [4]

$$Y_4(\theta, \phi) = 5/2 [x^4 + y^4 + z^4 - 3/5] \quad (IV-2)$$

and

$$Y_6(\theta, \phi) = 231/2 [x^2 y^2 z^2 - Y_4(\theta, \phi)/55 - 1/105] \quad (IV-3)$$

where $x = \sin \theta \cos \phi$, $y = \sin \theta \sin \phi$ and $z = \cos \theta$. In the principal directions the values of the Kubic harmonics are:

$$\begin{array}{lll} Y_4(100) = 1 & Y_4(110) = -1/4 & Y_4(111) = -2/3 \\ Y_6(100) = 1 & Y_6(110) = -13/8 & Y_6(111) = 16/9 \end{array}$$

Similarly they write

$$\left(\frac{\partial k}{\partial E}\right)_{E_F} = k_0' [1 + BY_4(\theta, \phi) + B_1 Y_6(\theta, \phi)]; \quad (IV-4)$$

the derivative is taken at the Fermi energy E_F . The scattering time is also expanded in Kubic harmonics;

$$\tau = \tau_0 [1 + CY_4(\theta, \phi) + C_1 Y_6(\theta, \phi)] \quad (IV-5)$$

The expression for n^* may be obtained from Eq. (8) of Ref. [3]:

$$\begin{aligned} n^* = 1 + 4/21 [9A^2 - 18A(C - B) - (C - B)^2] \\ + 8/13 [20A_1^2 - 40A_1(C_1 - B_1) - (C_1 - B_1)^2] \end{aligned} \quad (IV-6)$$

The expression is correct to second-order in the coefficients of Y_4 and Y_6 . We note that the value of n^* depends on the anisotropy of the scattering time, but not on its magnitude. As we expect, $n^* = 1$ for spherical surfaces

and isotropic scattering times. Furthermore, we see that the terms in AC and $A_1 C_1$ can give a decrease of n^* as the warping, ($|A|$ and $|A_1|$), increases, provided A , A_1 , C , and C_1 have the proper sign. Once an anisotropic scattering time is introduced, increased warping of the Fermi surface does not necessarily increase n^* .

The expression of the warping in this manner has introduced two more coefficients, B and B_1 , which did not appear when the energy was expanded in Kubic harmonics as in Eq. (I-4). However, B and B_1 are not independent of A and A_1 . In Appendix 1 we derive the relations between B , B_1 and A , A_1 on the assumption that the warping is small.

B. Calculation of the Warping Parameters

We obtained the warping parameters A and A_1 from the computations of Ham [5] for the alkali metals. Ham's data give electron energy vs. $ka/2\pi$, where a is the lattice constant, for the 100, 110 and 111 directions. If the Fermi energy is known, we can use these curves to obtain the length of the k vector at the Fermi surface for the three principal directions. Equation (IV-1) can then be used to obtain three equations, from which k_0 , A and A_1 can be computed.

The Fermi level can be obtained by a simple procedure. The Fermi surface must enclose a volume in k space which contains all the electronic states of the valence electrons. The density of states in k space per unit volume of crystal is $1/4\pi^3$ and a b.c.c. crystal with lattice constant a and one valence electron/atom has $2/a^3$ valence electrons/unit volume. For a spherical Fermi surface the radius, k_s , is given by

$$\frac{1}{4\pi^3} k_s^3 4\pi/3 = 2/a^3 \quad (\text{IV-7})$$

or

$$a k_s / 2\pi = .62 \quad (\text{IV-8})$$