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Relaxation-Time Representation and Dingle-Robinson Temperature Inversion*

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We extend our previous Fourier-series-representation schemes to include the representation of the relaxation time over the Fermi surface and to perform the inversion of the Dingle-Robinson temperature data. The scheme is applied to recent results of Miller, Poulsen, and Springford on Au : Cu alloys.

The anisotropy of the relaxation time over the Fermi surface, suggested by Ziman[1] to explain the results of transport experiments, may be studied experimentally in several ways. In relatively pure materials, techniques exist for determining local relaxation times $\tau(\vec{k})$ at points $\vec{k}$ of the surface.[2,3] Other methods, like cyclotron resonance[4] and de Haas–van Alphen[5] (dHvA) experiments, give only an orbitally averaged relaxation time τ. In dHvA work it is customary to introduce the Dingle-Robinson[6] temperature T_D defined by

$$\frac{1}{\tau} = \frac{2\pi k_B}{\hbar} T_D . \tag{1}$$

The problem therefore arises of inverting these data to obtain the local values $\tau(\vec{k})$.

Until recently, even for the noble metals and their alloys, only two or three values of $1/\tau$ were reported[4,7-12]; the appearance of the preliminary data of Lowndes *et al.*,[13] which sampled the Fermi surface in a more complete way, stimulated interest in inversion procedures.[13,14] The aim of this paper is to extend our Fourier-series schemes[15-17] by presenting a representation of $\tau(\vec{k})$ over the Fermi surface and developing and applying a simple inversion scheme for Dingle-Robinson temperature data. The method has already been discussed,[14] but at that time it was concluded that at least one or two more experimental data were necessary for a meaningful inversion; these data have now appeared.[18] Our scheme is similar to the procedure used by Miller *et al.*[18] to analyze their results; in view of its compactness and since it may be carried out at practically no extra cost during the inversion of dHvA-area data described in Ref. 17 (from now on referred to as I), we think it is worthwhile to make it more generally available.

As an ansatz it is natural to define the reciprocal of the orbital relaxation time τ as a time average of the reciprocal of the local relaxation time $\tau(\vec{k})$ over a cyclotron period $T = 2\pi m^* c/eH$. Thus we have

$$\frac{1}{\tau} = \frac{1}{T}\int_0^T \frac{1}{\tau(\vec{k})}\, dt . \tag{2}$$

To our knowledge this relation has never been fully justified but is commonly used in discussing orbital relaxation times with different scattering processes.[13,19] Kinetic-theory arguments suggest that it may be valid only in the limit $\tau/T \gg 1$. We may write Eq. (2) as a line integral $(1/T)\oint[1/\tau(\vec{k})]\, dk_\perp/\dot{k}_\perp$, where $k_\perp$ is the component of the Fermi momentum in the plane of the orbit (measured from some convenient center). Using the Lorentz-force

TABLE I. Coefficients C_j and C_j' of the Fermi-radii and Fermi-velocities representation and coefficients f_j found for the relaxation-time representation.

C	C'	$f(5)$	$f(6)$
1.000 000	0.000 0	−0.772 585	22.0525
4.028 360	0.000 0	−0.242 849	10.2821
−1.340 230	−82.458 60	−0.486 967	7.7038
−2.400 300	−70.848 50	−0.412 455	4.8954
−0.233 042	−16.891 50	−0.085 914	1.9234
−0.618 918	−14.724 80	...	0.9151
0.118 184	12.108 80	...	...
0.198 816	6.958 52	...	...

equation of motion

$$\dot{k}_\perp = (eH/\hbar c)\, v_\perp \tag{3}$$

and

$$dk_\perp = \frac{k_\perp\, d\theta}{\hat{k}_\perp \cdot \hat{v}_\perp}\ , \tag{4}$$

we obtain

$$\frac{1}{\tau_i} = \frac{\hbar}{2\pi m_i^*} \int \frac{d\theta}{\tau(\vec{k})}\, \frac{k_\perp^2}{\vec{v}\cdot\vec{k}_\perp}\ , \tag{5}$$

where the subscript i refers to the ith orbit. Using Eqs. (29), (30), and (31) of I, Eq. (5) becomes (in Rydberg-Bohr atomic units)

$$\frac{1}{\tau_i} = \frac{1}{\pi m_i^*} \sum_l C_l' \int_0^{2\pi} \frac{1}{\tau(\vec{k})}\, \frac{k_\perp^2}{\vec{k}_\perp \cdot \vec{\nabla} F}\ S_l(\vec{k})\, d\theta\ . \tag{6}$$

On the other hand, exploiting the symmetry properties of $\tau(\vec{k})$, we can write [note that we find it convenient to expand $1/\tau(\vec{k})$ rather than $\tau(\vec{k})$ [18]]

$$\frac{1}{\tau(\vec{k})} = \sum_{\vec{R}} f_{\vec{R}}\, e^{i\vec{k}\cdot\vec{R}} = \sum_j f_j S_j(\vec{k})\ . \tag{7}$$

Using Eq. (7), Eq. (6) becomes

$$\frac{1}{\tau_i} = -\frac{1}{\pi m_i^*} \sum_{jl} C_l' f_j \int_0^{2\pi} \frac{k_\perp^2}{\vec{k}_\perp \cdot \vec{\nabla} F}\ S_j(\vec{k})\, S_l(\vec{k})\, d\theta\ . \tag{8}$$

Defining now

$$M_{jl}^i = -\frac{1}{\pi m_i^*} \int_0^{2\pi} \frac{k_\perp^2}{\vec{k}_\perp \cdot \vec{\nabla} F}\ S_j(\vec{k})\, S_l(\vec{k})\, d\theta \tag{9}$$

and

$$X_j^i = \sum_l M_{jl}^i\, C_l'\ , \tag{10}$$

Eq. (8) assumes the simple form

$$\frac{1}{\tau_i} = \sum_j f_j X_j^i\ . \tag{11}$$

Now the coefficients C_l' have been obtained in I and therefore also the m_i^* are known [Eq. (33) of I]; the integral in (9) may be evaluated conveniently together with the integrals (8) of I, and the set of j coefficients X_j^i for any orbit i follows very directly. Once these are known, Eq. (11) is used to determine the coefficients f_j which minimize the function

$$\Delta^2 = \frac{1}{N} \sum_{i=1}^{N} \frac{(1/\tau_i - 1/\tau_i^e)^2}{1/\tau_i^{e\,2}}\ , \tag{12}$$

where the $1/\tau_i^e$ are the experimental results for a set of N orbits. [The minimization procedure, which results in a strictly linear set of equations, is completely analogous to the determination of the C_j''s from the values of m_i^*, in Ref. 1, Eqs. (33)–(39).] The set of f_j so obtained is a representation of the relaxation time, since it allows one to obtain $1/\tau$ for any orbit, through Eq. (11), and $\tau(\vec{k})$ at any point, through Eq. (7).

It may also be noted that, if one has a set of local relaxation times like those of Ref. 3, the f_j may be determined even more directly by using Eq. (7); the data of Koch and Doezema,[3] however, do not seem at present to sample the Fermi surface of copper in a sufficiently complete way to warrant such an attempt. We shall therefore limit ourselves to the application of our scheme to the new data[18] for the case of Au:Cu. Besides the $1/\tau^e$ for the main five orbits [B_{100}, B_{111}, N_{111}, R, and D; the notation is the same as in I] we have used the $1/\tau^e$ relative to the belly orbit at 20° from [001] and to the neck orbit at 7.5° from [111] in the (110) plane. (These data are the same as those used by Miller *et al.*[18] in their analysis.) If they had been available, data relative to the belly at 22° from [001] in the (110) plane and to the belly at 16.2° from [001] in the (100) plane would have been preferable since for them the factor F' (derivative of the area with respect to the angle[18]), which comes in the correction applied to the experimental value because of the effect caused by orientational inhomogeneity of the sample,[5] vanishes.

Table I lists the coefficients C_j and C_j' which we have used to represent the Fermi surface of gold,

TABLE II. Experimental Dingle-Robinson temperatures (K) used in the fit and corresponding values calculated with the f_j coefficients of Table I.

Orbit	Experimental T_D (Ref. 18)	Calculated T_D $f(5)$	Calculated T_D $f(6)$
B_{100}	2.58	2.6134	2.5799
$B_{20°}$	2.10	2.0386	2.0998
B_{111}	2.30	2.5394	2.3006
R_{100}	2.33	2.1112	2.3297
D_{110}	1.90	1.8928	1.9002
N_{111}	1.26	1.3012	1.2817
$N_{7.5°}$	1.32	1.3191	1.2976
Error (%)		5.57	0.91

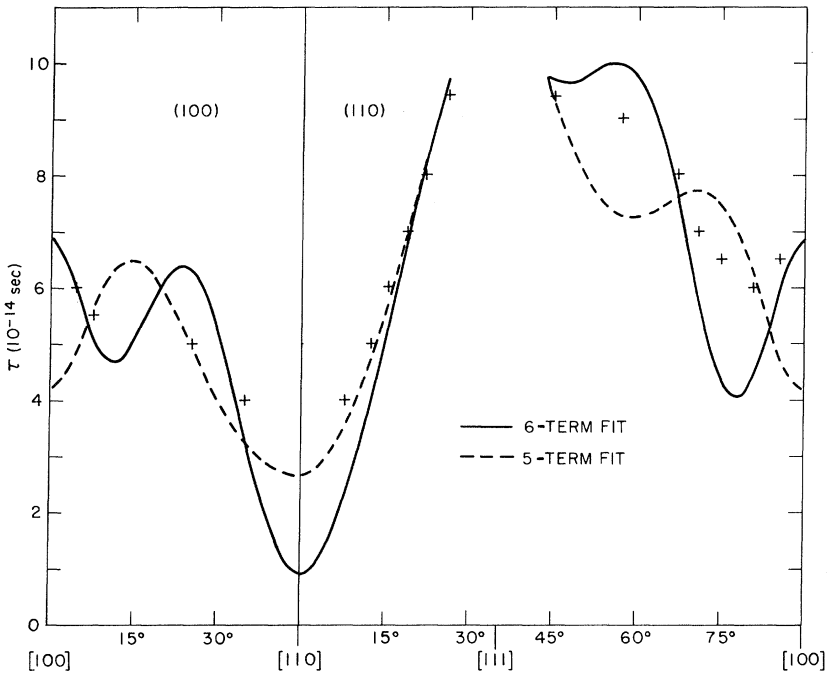

FIG. 1. Angular dependence of $\tau(\vec{k})$ for the (100) and (110) planes in the two representations [dashed curve, $f(5)$; continuous curve, $f(6)$].

and the coefficients f_j obtained with the above inversion by using five and six coefficients [$f(5)$ and $f(6)$ representations, respectively]. Table II shows the experimental Dingle-Robinson temperatures[18] used in the fits and the corresponding values calculated with the above two sets of f_j coefficients; the global error, defined as in (12), is 5.57% for $f(5)$ and 0.91% for $f(6)$. The angular dependence of $\tau(\vec{k})$ in the (100) and (110) planes is reported in Fig. 1 [dashed curve for $f(5)$ and continuous curve for $f(6)$]; it may be noted that the small wiggles near [100] would probably disappear by adding more experimental data, whereas the over-all anisotropy is real. The results are in reasonable agreement with those of Ref. 18, Fig. 5, which are shown as crosses in our figure.

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