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W. Ruesink, J. de Wilde, R. Griessen, M. Lee. AN EXPERIMENTAL TEST OF THE RIGID-MUFFIN-TIN APPROXIMATION USED IN THE THEORY OF ELECTRON-PHONON INTERACTION. Journal de Physique Colloques, 1978, 39 (C6), pp.C6-1097-C6-1098. 10.1051/jphyscol:19786486 . jpa-00217968

HAL Id: jpa-00217968

<https://hal.science/jpa-00217968>

Submitted on 4 Feb 2008

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AN EXPERIMENTAL TEST OF THE RIGID-MUFFIN-TIN APPROXIMATION USED IN THE THEORY OF ELECTRON-PHONON INTERACTION

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Résumé.- La validité de l'approximation du potentiel rigide est analysée à l'aide de mesures de l'influence d'un cisaillement pur sur la surface de Fermi du palladium. Les valeurs expérimentales sont environ 30 % plus petites que les valeurs obtenues à l'aide de la méthode KKR. Quelques implications relatives au couplage electron-phonon et à T_c sont présentées.

Abstract.- The validity of the rigid-muffin-tin approximation is discussed on the basis of measurements of the response of the Fermi surface of palladium to homogeneous volume conserving strains. The experimental strain derivatives are found to be consistently 30 % smaller than theoretical values obtained from a KKR band structure calculations. Implications of this result are discussed for the electron-phonon λ and the superconducting T_c .

According to the McMillan theory /1,2/ the superconducting transition temperature T_c of a metal depends on the electron-phonon enhancement factor λ through the following relation

$$T_c = (1.2)^{-1} \omega_{\log} \exp \{-1.04(1+\lambda)/\lambda - \mu^x(1+0.62\lambda)\} \quad (1)$$

where μ^x is a constant (assumed to be 0.13) and ω_{\log} is an average over the phonon frequencies. The parameter λ can be expressed as a product of a purely electronic factor η and an essentially phononic factor so that : $\lambda \approx \eta/M\langle\omega^2\rangle$ (2)

Here M is the mass of the ions ; $\langle\omega^2\rangle$ depends only weakly on the electronic properties and is determined by the phonon spectrum of the metal under consideration. The central problem is the calculation of η which is proportional /1/ to the gradient of the potential V . Most of the recent theoretical work on electron-phonon interaction in transition metals makes use of the rigid-muffin-tin (RMT) approximation of Gaspari and Gyorffy /3/. In this approximation one assumes that the self-consistent muffin-tin potential around an ion moves rigidly with the ion when a phonon is propagating through the lattice. The validity of this approximation is difficult to test by means of superconducting T_c data, because of the uncertainties in ω_{\log} , $\langle\omega^2\rangle$ and μ^x . In this paper we present a direct method to test the validity of the RMT approximation based on measurements of the strain response of the Fermi surface (FS) of transition metals to homogeneous volume conserving strains (shears).

In order to show which role the RMT approximation plays in the shear response of the FS of a

metal we write the KKR secular equation as

$$\chi(\vec{k}, E, \delta_\ell, e_j) = 0 \quad (3)$$

where δ_ℓ are scattering phase shifts of the muffin-tin potential and e_j is the j -th component of the strain tensor. The strain dependence of the area A of an extremal cross-section of the FS is obtained by solving the implicit equation (3) with respect to \vec{k} at an energy equal to E_F . As shown by Shaw, Ketterson and Windmiller /4/ and by Griessen, Stanley and Lee /5/, the strain derivative $D_j = d\ln A/de_j$ can be calculated from an integral along the orbit containing the term $D\chi/De_j$, where $D\chi/De_j$

$$= \frac{\partial \chi}{\partial E} \frac{dE_F}{de_j} + \sum_\ell \frac{\partial \chi}{\partial \delta_\ell} \frac{d\delta_\ell}{de_j} + \frac{\partial \chi}{\partial e_j} \quad (4)$$

For a general strain ξ , the derivative $d\ln A/d\xi$ depends explicitly on the strain dependence of E_F and the scattering phase shifts. For volume conserving strains γ it is however easy to show that in a cubic crystal :

$$d\ln A/d\gamma = \sum_{j=1}^6 \left. \frac{\partial \ln A}{\partial e_j} \right|_{\delta_\ell, E_F} de_j/d\gamma \quad (5)$$

where $de_j/d\gamma$ is entirely determined by the strain state of the crystal. Eq.(5) shows explicitly that the response of the FS to a shear depends on the perturbation of the electronic band structure by the lattice deformation at constant values of δ_ℓ and E_F . Therefore the shear response can be calculated from a KKR model using zero-pressure values for E_F and δ_ℓ and the validity of the RMT-approximation can be tested by comparing measured $d\ln A/d\gamma$ with calculated derivatives. Experimental values for D_j were obtained

ned by simultaneously measuring the amplitude of quantum oscillations in the magnetization (\tilde{M}) and the sound velocity (\tilde{v}_s). As shown by Testardi and Condon/7/ the strain dependence of the FS can be calculated from :

$$\{D_i D_j\} = \tilde{v}_s C_{eff} / \pi F \tilde{M} \quad (6)$$

where C_{eff} is the effective elastic constant corresponding to the ultrasonic configuration, F is the de Haas-van Alphen frequency and $\{D_i D_j\}$ is a combination of derivatives D_j .

The measurements were done on palladium single crystals of 4N purity in magnetic fields up to 6.5 tesla. The oscillations in M were detected by means of a fluxgate probe coupled to a superconducting flux transformer /8,9/ and the oscillations in v_s were measured with a continuous wave set-up. From the D_j measured in several ultrasonic configurations we determined the response to tetragonal shear $\gamma_z (e_1=e_2=-\frac{1}{2}e_3)$ and angular shear γ_{xy} of the hole-ellipsoids at point X and L of the Brillouin zone, listed in table I.

The experimental numbers are found to be 30 % smaller than the theoretical values from the relativistic KKR calculation. This is also true for the tetragonal shear derivative of the belly orbit $\Gamma|100|$ determined from the uniaxial stress measurements of Joss and Van der Mark /6/. This information may be used to estimate the error introduced in η by the use of the RMT approximation as in the deformation potential approximation /10/ η is proportional to $(D\chi/D\xi)^2$, whereas $d\ln A/d\gamma$ is /5/ proportional to $D\chi/D\xi$. As a consequence of this quadratic dependence we expect the RMT approximation to give values approximately 1.7 too high for η . This tendency has also been found by Butler /11/ in Y,Zr,Tc and Rh, while Gyorffy /12/ pointed out that the experimental value of η from measurements of T_c in niobium is about 1.6 times lower than the calculated value of Butler /11/. It is interesting to point out that the T_c of palladium obtained with a "scaled" value of $\eta = \eta_{RMT}/1.7$ is essentially zero ($T_c \sim 10^{-18}$ mK) while the value calculated by Butler /11/ with the RMT leads to 5.5 mK.

TABLE I

Experimental and theoretical shear derivatives of the area of extremal cross-sections of the FS of palladium. γ_z is a tetragonal shear in the $|001|$ direction and γ_{xy} is equal to the decrease of the angle between $|100|$ and $|010|$ axes of the real space lattice induced by the shear. The parameters entering the KKR bandstructure calculations are :

$$E_F = 0.4816 \text{ a.u.}, \delta_0 = -0.09887 \text{ rad}, \delta_{1,1/2} = -0.00205 \text{ rad}, \\ \delta_{1,3/2} = -0.04170 \text{ rad}, \delta_{2,3/2} = -0.23918 \text{ rad}, \delta_{2,5/2} = -0.29095 \text{ rad}$$

orbit center	direction of \vec{H}	F(tesla)	$\frac{d\ln A}{d\gamma_z} \Big _{\text{exp}}$	$\frac{d\ln A}{d\gamma_z} \Big _{\text{Theor}}$	$\frac{d\ln A}{d\gamma_{xy}} \Big _{\text{exp}}$	$\frac{d\ln A}{d\gamma_{xy}} \Big _{\text{Theor}}$
X(001)	$ 001 $	572	-8.7 ± 0.7	-10.3	0	0
X(100)	$ 001 $	890	9.2 ± 1.4	12.1	0	0
X(100)	$ 110 $	692	-	-	-1.18 ± 0.06	-1.48
X(111)	$ 001 $	224	3.2 ± 0.6	5.3	-	-
$\Gamma(000)$	$ 001 $	27315	0.13^a	0.21	0	0

a) Obtained from uniaxial stress data /6/

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