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A Simple Approach to Calculation of the Phonon-Limited Electrical Resistivity in Metals

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Recently a considerable success was achieved in the numerical theory of superconductivity. Suffice it to note that up to date a good deal of numerical computations of the electron-phonon coupling constant λ is available for numerous metals. It is due not only to the recent development of computers but also to the fact that there is a simple Gaspari-Gyorffy formula for λ which expresses λ in terms of partial densities of state and phase shifts directly obtainable from band structure calculations. As it was mentioned by Allen /1/, the temperature-dependent part of electrical resistivity ϱ_{ph}, being closely related to the electron-phonon interaction, may be written in a form very similar to the basic equation of λ. In spite of this fact there are fewer ab initio calculations of ϱ_{ph} than those of λ. The object of our paper is to extend the well-known Gaspari-Gyorffy formula to the phonon-limited resistivity ϱ_{ph} in order to obtain a rather simple approximate expression which would allow to perform easily numerical calculations of this quantity for a large number of metals, as it has been done for λ. As an example we present the results for Mo and Pd.

We shall start from Allen's expression for $\varrho_{ph}(T)$ which is the lowest-order variational solution of the Boltzmann equation /6/:

$$\varrho_{ph}(T) = \frac{\pi k_B}{\hbar e^2}\,\lambda_{tr}\,B(T)\,T\Big/\sum_{\vec{k},\lambda}\delta(E_{\vec{k},\lambda} - E_F)\,v_z^2(\vec{k},\lambda)\,, \tag{1}$$

$$B(T) = \int \frac{d\omega}{\omega}\,\alpha_{tr}^2\,F(\omega)\left(\frac{\hbar\omega}{2k_BT}\Big/\operatorname{sh}\frac{\hbar\omega}{2k_BT}\right)^2\Big/\int\frac{d\omega}{\omega}\,\alpha_{tr}^2\,F(\omega)\,, \tag{2}$$

$$\lambda_{tr} = \eta_{tr}/M\langle\omega^2\rangle_{tr}\,, \tag{3}$$

$$\eta_{tr} = \frac{\sum_{\vec{k},\vec{k}',\lambda,\lambda'}\delta(E_{\vec{k},\lambda} - E_F)\,\delta(E_{\vec{k}',\lambda'} - E_F)\left|\langle\vec{k}',\lambda'|\vec{\nabla}V_{ei}|\vec{k},\lambda\rangle\right|^2\left(v_z(\vec{k},\lambda) - v_z(\vec{k}',\lambda')\right)^2}{2\sum_{\vec{k},\lambda}\delta(E_{\vec{k},\lambda} - E_F)\,v_z^2(\vec{k},\lambda)}\,, \tag{4}$$

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where $|\vec{k},\lambda\rangle$ is a one-electron state ($\vec{k}$ wave vector, λ band index) with the energy $E_{\vec{k},\lambda}$ and the velocity $v(\vec{k},\lambda) = \vec{\nabla}_{\vec{k}} E_{\vec{k},\lambda}/\hbar$, $\alpha^2_{tr} F(\omega)$ is the transport electron-phonon spectral function, $\vec{\nabla} V_{ei}$ is the screened gradient of the electron-ion potential. Equations (1) to (4) are written in a manner demonstrating the analogy with superconductivity. The quantities $\langle\omega^2\rangle_{tr}$ and B(T) are defined by a phonon spectrum and we shall assume them given. Further we shall deal only with the electron factor η_{tr}. Certainly such an approach does not allow to analyze $\varrho(T)$ at low temperatures ($T \lesssim 10$ K), but general trends and the value of resistivity at $T \approx 10^2$ K may be obtained with reasonable accuracy. We shall also use the rigid muffin-tin approximation.

We shall expand the one-electron wave function in terms of spherical harmonics ($L \equiv \{l, m\}$):

$$\Psi_{\vec{k},\lambda} = \sum_{\vec{R}} e^{i\vec{k}\vec{R}} \sum_{L} A_L(\vec{k},\lambda) Y_L(\widehat{\vec{r} - \vec{R}}) i^l R_l(|\vec{r} - \vec{R}|, E) . \tag{5}$$

Substituting (5) into (4) we have

$$\eta_{tr} \equiv \eta_{20} - \eta_{11} = \overline{\sum_{L, L_1, L_2, L_3}} V_{L, L_1} \left(T^{(2)}_{L_1 L_2} V_{L_2 L_3} T^{(o)}_{L_3 L} - T^{(1)}_{L_1 L_2} V_{L_2 L_3} T^{(1)}_{L_3 L} \right) \left(N(E_F) \langle v_z^2 \rangle \right)^{-1} , \tag{6}$$

$$V_{LL'} \equiv \langle L | \vec{\nabla} V_{ei} | L' \rangle = \sum_{\mu} e_\mu \, g^{l\,m}_{l'm',\,1\mu} \sqrt{\frac{4\pi}{3}} \, V_{ll'} , \tag{7}$$

$$T^{(i)}_{LL'} \equiv \sum_{\vec{k},\lambda} A^*_L(\vec{k},\lambda) A_{L'}(\vec{k},\lambda) (v_z(\vec{k},\lambda))^i \delta(E_{\vec{k},\lambda} - E_F) . \tag{8}$$

Here we have used spherical symmetry of the MT potential and have introduced cyclic orts $e_o = e_z$, $e_{\pm 1} = (\mp e_x + i e_y)/\sqrt{2}$, $g^{L}_{L', L''} = \int Y^*_L Y_{L'} Y_{L''} \, d\Omega$, $N(E_F)\langle v_z^2 \rangle = \sum_{\vec{k},\lambda} \delta(E_{\vec{k},\lambda} - E_F) v_z^2(\vec{k},\lambda)$. The matrix elements $V_{ll'} (l = l' \pm 1)$ may be easily expressed in terms of phase shifts /5/: $V_{ll+1} \equiv \int dr \, r^2 R_l(r, E_F) \times R_{l+1}(r, E_F) \partial V(r)/\partial r = \sin(\delta_l - \delta_{l+1})$. The matrix elements $T^{(i)}_{LL'}$ have more complicated selection rules determined by the symmetry of crystal lattice. In order to simplify selection rules, and following Gaspari-Gyorffy /5/, we shall use the so-called spherical approximation (SA), i.e. we shall consider selection

rules not for cubic but for spherical symmetry instead. Then the following selection rules may be obtained:

$$T^{(0)}_{LL'} = \delta_{LL'} t^{(0)}_l , \qquad T^{(2)}_{LL'} = \delta_{LL'} t^{(2)}_l , \qquad T^{(1)}_{LL'} = g^{L}_{L',\,1,\,0}\, t^{(1)}_{ll'} .$$

It has been shown /7/ that for cubic metals SA introduces an error of only $\approx 1\%$ even though at first sight SA seems rather questionable.

Direct calculations /7/ demonstrate that cubic symmetry is high enough for providing spherical selection rules. In our case one can expect SA to be less accurate for $T^{(1)}$, because it is obtained by averaging of vector quantities. However, computations show that η_{11} is usually comparatively small and the total error of SA seems to be insignificant. Within the frameworks of SA we can derive for η_{20} and η_{11} the following expressions:

$$\eta_{20} = \sum_l (l+1) V^2_{l,\,l+1} \left(t^{(0)}_l\, t^{(2)}_{l+1} + t^{(0)}_{l+1}\, t^{(2)}_l\right) / N(E_F) \langle v_z^2 \rangle , \tag{9}$$

$$\eta_{11} = \frac{2}{3} \sum_l \left\{ \frac{2(l+1)(l+2)}{2l+3} V_{l,\,l+1} V_{l+1,\,l+2} t^{(1)}_{l,\,l+1} t^{(1)}_{l+1,\,l+2} - \right.$$

$$\left. - \frac{l+1}{(2l+1)(2l+3)} V^2_{l,\,l+1}\, t^{(1)\,2}_{l,\,l+1} \right\} \Big/ N(E_F) \langle v_z^2 \rangle . \tag{10}$$

Reducing (8) to the irreducible part of the Brillouin zone (IBZ), we obtain final equations for $t^{(i)}$ (for cubic crystals):

$$t^{(0)}_l = 48 \frac{\Omega}{(2\pi)^3} \sum_\lambda \int_{IBZ} d\vec{k}\, \delta(E_{\vec{k},\lambda} - E_F) \sum_m \left| A_{lm}(\vec{k},\lambda) \right|^2 \Big/ (2l+1) , \tag{11}$$

$$t^{(2)}_l = 48 \frac{\Omega}{(2\pi)^3} \sum_\lambda \int_{IBZ} d\vec{k}\, \delta(E_{\vec{k},\lambda} - E_F) \sum_m v^2(\vec{k},\lambda) \left| A_{lm}(\vec{k},\lambda) \right|^2 \Big/ 3(2l+1) , \tag{12}$$

$$t^{(1)}_{l,\,l+1} = \frac{48}{\sqrt{(2l+1)(l+1)}} \frac{\Omega}{(2\pi)^3} \sum_\lambda \int_{IBZ} d\vec{k}\, \delta(E_{\vec{k},\lambda} - E_F) \times$$

$$\times \sum_{m,\,m',\,\mu} C^{lm}_{l'm',\,1\mu} A^*_{lm}(\vec{k},\lambda) A_{l'm'}(\vec{k},\lambda) v_\mu(\vec{k},\lambda) , \tag{13}$$

where $C^{L}_{L',\,L''}$ are Clebsch-Gordan coefficients and $v(\vec{k},\lambda) = \Sigma\, v_\mu(\vec{k},\lambda) e_\mu$. Equations (9) to (13) allow to compute η_{tr} and then $\varrho_{ph}(T)$ by formulae (1) to

Table 1

Mo	$N(E_F)\langle v^2\rangle$ at. units	5.64	T(K)	100	200	273	400	500
	η_{11} at. units	0.3×10^{-5}	ϱ_{exp} ($\mu\Omega$cm)	0.92	3.18	4.90	8.00	10.49
	η_{20} at. units	0.126						
	Θ_D(K)	400	ϱ_{calc} ($\mu\Omega$cm)	0.95	3.35	5.03	7.84	10.00
Pd	$N(E_F)\langle v^2\rangle$ at. units	3.15	T(K)	73	173	273	373	473
	η_{11} at. units	-3.2×10^{-6}	ϱ_{exp} ($\mu\Omega$cm)	2.14	6.12	10.2	14.0	17.4
	η_{20} at. units	0.067						
	Θ_D(K)	275	ϱ_{calc} ($\mu\Omega$cm)	1.38	5.73	9.79	13.73	17.45

(3) assuming $\alpha^2_{tr}F(\omega)$ is given.

As an example we have calculated the electrical resistivity of Mo and Pd. Electron energies and wave functions have been obtained from LMTO band-structure calculations with self-consistent crystal potential taken from the book /9/. Brillouin zone integrations were performed by the tetrahedron method over 1024 (Mo) and 1536 (Pd) tetrahedra in IBZ. The results are displayed in Table 1. Phonon spectra used in computation were approximated by the Debye model giving rise to the Bloch-Grüneisen formula for the temperature dependence of resistivity. As such a temperature dependence is well-known we present only results for a few values of temperature 100 K $\lesssim$ T $\lesssim$ 500 K. In Table 1 we have used experimental values for Pd compiled by Savitsky et al. /10/ and those for Mo compiled by Peletskii and Belskaya /11/.

We think this method to be efficient for calculations of the resistivity of metals and to be accurate at least to 10 to 15%. It is rather good for the rigid-

muffin-tin approximation, taking into account the fact that the experimental values have often a discrepancy of the order of 10%.

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