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ELECTRICAL RESISTIVITY OF LIQUID METALS

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A general model pseudopotential is modified and applied to the calculation of electrical resistivity of twenty-two simple liquid metals on the basis of the Ziman formalism. The results are compared with the values known in literature. The agreement between the calculated resistivity and experimental data is very satisfactory.

1. Introduction

The resistivity of liquid metals is a usual object of investigation on the basis of pseudopotential method. It is a consequence of relatively simple calculations coming from the Ziman theory[1]. Theoretical relation for the electrical resistivity according to Ziman is given in the following form

$$\varrho = \frac{3\pi\, m\, \Omega_0}{8\hbar\, e^2\, E_F} \frac{1}{k_F^4} \int_0^{2k_F} |\langle \vec{k} + \vec{q}\, |w|\, \vec{k} \rangle|^2\, a(q)\, q^3\, \mathrm{d}q \qquad (1)$$

where Ω_0 is the atomic volume, m is the effective mass of electrons; E_F and k_F are the Fermi energy and Fermi momentum, respectively; $\langle \vec{k} + \vec{q} \,|w|\, \vec{k} \rangle$ is the form-factor of screened electron-ion potential for Fermi surface scattering from a single ion and a (q) is the structure factor of a liquid metal containing an interference of electronic waves scattered on all other ions of the metal.

Different forms of local or nonlocal potentials, theoretical and experimental structure factors and a variety of dielectric functions have been used for the electrical resistivity calculations based on expression (1). For that reason the calculated values are very different.

The general model pseudopotential[2] which is exclusively a function of the momentum transfer of the conducting electron and the valence number of the metal system studied, has given very good results for the calculations of the electrical resistivity of liquid metals[3]. One of the shortcomings of this pseudopotential is a weak convergence in the range of high values of the change of momentum, and owing to this its matrix elements for high q-values are characterised by unphysical oscillations. This shortcoming can be removed by including a factor $e^{-\beta_3 q/2k_F}$ into the potential. Along with the improvement of the precision of the potential near the point $q = 2k_F$, essentialy defining the values of the resistivity of liquid metals (integral (1)), this correction at the same time provides a better convergence of the potential in the range of high q-values. A calculation of the electric resistivity on the basis of such a modified general model potential with the theoretical and experimental structure factors is given here.

2. *Electrical resistivity of liquid metals*

In order to calculate the electrical resistivity of liquid metals on the basis of Eq. (1), we must know the electron-ion potential and liquid structure factor.

A modified form factor of the general model pseudopotential, which is used in the calculation, has a simple form

$$\langle \vec{k} + \vec{q} \,|w|\, \vec{k} \rangle = \beta_1 \beta_2 \frac{\sin 2\pi \beta_2 q/2k_F}{2\pi\beta_2 q/2k_F} e^{-\beta_3 q/2k_F} \tag{2}$$

where the values of the parameters β_2 and β_3 are obtained by fitting the Animalu and Heine data[4], based on the Heine-Abarenkov model potential[5]. The errors are about 0.01 Ry for $q \leq 2\ k_F$. As the limit value of every local potential which includes Coulomb potential, when the wave number tends to zero is equal $-2/3$ E_F, can be calculated. The pseudopotential (2) includes screening with free electrons. Along with the Hartree (*HAR*) dielectric function, we have used a dielectric function of Thomas — Fermi (*TF*) and Sham (*SH*)[8]. The calculations of the electrical resistivity with potential (2) are listed in Table 1. We have taken the experimental values for E_F[6] in expression (2), and effective mass is assumed to be unity for all metals.

The resistivity values obtained with potential (2) are designated by $\varrho^{(1)}$ for theoretical and $\varrho^{(2)}$ for experimental structure factor, respectively. The dielectric function used is given in the index. There we have used that structure factors

TABLE 1.

Metal	T (K)	ϱ_{exp}	$\varrho^{(1)}_{HAR}$	$\varrho^{(2)}_{HAR}$	$\varrho^{(1)}_{TP}$	$\varrho^{(2)}_{TP}$	$\varrho^{(1)}_{SH}$	$\varrho^{(2)}_{SH}$
Li	453	25	2.81	3.44	2.12	2.61	3.35	4.11
Na	373	9.6	11.7	14.21	8.31	10.15	14.07	17.04
	598	18.3	—	17.16	—	12.17	—	20.71
K	338	13	12.85	10.3	9.87	7.97	16.23	12.97
	408	16.8	—	12.72	—	9.85	—	16.02
Rb	313	22	17.83	22.45	13.38	16.58	22.56	28.39
	513	40.5	—	26.92	—	20.10	—	34.13
Cs	303	36	27.5	18.95	19.95	13.58	34.88	23.94
	573	67.8	—	29.78	—	21.43	—	33.7
Mg	923	27.4	17.34	—	14.27	—	21.12	—
Ca	1123	33	20.29	—	16.51	—	25.22	—
Ba	1003	306	22.4	—	17.02	—	27.4	—
Zn	693	33.4	38.25	—	30.14	—	44.46	—
	723	37	—	37.85	—	29.98	—	44.08
Cd	603	33.7	34	—	28.02	—	41.61	—
Hg	253	91	97.8	—	78.49	—	119	—
	293	98	—	105.22	—	84.22	—	128.2
	353	108.5	—	115.57	—	93.12	—	141
Al	933	24.2	23.84	—	20.31	—	28.7	—
	943	24.5	—	26.19	—	22.52	—	31.79
	1025	27.3	—	26.7	—	22.95	—	32.4
Ga	303	25.8	28.39	—	24.16	—	34.52	—
	325	—	—	74.72	—	65.99	—	91.56
In	429	33.1	44.41	—	37.57	—	54.77	—
	443	—	—	35.69	—	29.84	—	44.03
Tl	576	73.1	147.54	—	122.2	—	181.4	—
	588	75	—	157.4	—	130.57	—	193.94
Si	1683	71	69.33	—	60.13	—	84.89	—
Ge	1210	73	98.95	—	85.35	—	121.6	—
Sn	523	—	—	92.47	—	79.57	—	114.47
	573	—	—	98.3	—	84.51	—	121.61
	683	48	87	—	74.73	—	107.4	—
Pb	613	96.5	—	104.64	—	89.43	—	129.54
	673	99	106.87	—	91.47	—	132.38	—
Sb	913	113.5	124.17	—	107.6	—	153.42	—
Bi	573	128.9	160.16	151.13	137.64	130	198.48	187.4
Be	1557	—	15.88	—	13.11	—	18.27	—

Electrical resistivity of simple liquid metals (in units of $\mu\Omega$cm).

for one-component liquids, in the region of first diffraction maximum, could be well represented by solving the Percus-Yevick equation for a model liquid consisting of hard spheres. The least departures of the theoretical structure factor compared with the experimental values in the melting point were obtained for a packing density of 45%[7]. For the calculation of the resistivity ϱ_l[2] we used the experimental structure factors values according to Refs. 9 and 10. The change in the results of the resistivity as a consequence of using different dielectric functions with theo-

retically calculated structure factor, or the factor taken from the experiment, is between 15% and 25% as can be seen from Table 2.

3. *Conclusion*

The obtained results agree very well with experimental results, except for a few metals (Li, Ba, Tl) where it could be the consequence of fitting procedure for the potential. It shows that the proposed potential could be successfully used for the calculations of other electronic features of simple metals.

TABLE 2.

Metal	T (K)	$\frac{\varrho_m^{(1)} - \varrho_{SH}^{(1)}}{\varrho_m^{(1)}}$	$\frac{\varrho_m^{(2)} - \varrho_{SQ}^{(2)}}{\varrho_m^{(2)}}$
Li	453	21	21
Na	373	24	24
	598	—	24
Ca	338	25	25
	408	—	25
Rb	313	26	26
	513	—	26
Cs	303	27	27
	573	—	27
Mg	923	20	—
Ca	1123	22	—
Ba	1003	23	—
Zn	693	18	—
	723	—	18
Cd	603	21	—
Hg	253	21	—
	293	—	17
	353	—	21
Al	933	18	—
	943	—	18
	1025	—	18
Ga	303	19	18
	323	—	18
In	429	20	—
	443	—	21
Tl	573	21	—
	588	—	21
Si	1683	19	—
Ge	1210	18	—
Sn	523	—	20
	573	—	20
	683	16	—
Pb	613	—	20
	673	20	—
Sb	913	19	—
Bi	573	20	20
Be	1557	16	—

Maximal error in relation to average value ϱ_m for theoretical and experimental structure factor, respectively.

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ELEKTRIČNI OTPOR TEČNIH METALA

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Opšti modelni pseudopotencijal modifikovan je i primijenjen za izračunavanje električkog otpora 22 jednostavna tečna metala na osnovu Zimanovog formalizma. Rezultati su upoređeni sa poznatim vrijednostima iz literature. Slaganje između izračunatih otpora i eksperimentalnih podataka je vrlo dobro.