A MODEL POTENTIAL FOR NOBLE METALS

By A. Kiejna

Institute of Experimental Physics, University of Wrocław*

(Received April 4, 1979; final version received June 11, 1979)

The validity of the model potential of Krasko-Gurskii has been tested for noble metals and used to calculate the form factor and liquid metal resistivity for copper. The results are in good agreement with experimental data.

In the recent decade a number of papers appeared concerning pseudopotentials of noble metals [1–6]. Moriarty [1] succesfully applied the generalized theory of the pseudopotential of *d*-band metals to calculate several properties of noble metals. This theory however is intricate in its applications. Because of this, a few local model potentials for these metals were proposed [2–6]. The main problem is to take into account the hybridization of *d*-states with the free-electron-like conduction band.

The purpose of this communication is to test the validity of the Krasko–Gurskii [7] model potential for noble metals. Compared to others [2–6], this pseudopotential, proposed originally for simple metals, has an advantage of being given by a smooth function in *r*-space. Thus, its Fourier transform does not demonstrate oscillations for larger values of wave vector and consequently ensures a good convergence of sums or integrals in the reciprocal space. In *r*-space this potential is given by

$$V_b(r) = \frac{Ze^2}{r}\left(e^{-r/r_c} - 1 + \frac{a}{r_c} re^{-r/r_c}\right), \tag{1}$$

where a and r_c are two unknown parameters and Z is the valence of the ion. The repulsive part of this potential arises form the tightly bound inner core states and the attractive part is due to *s–d* hybridization. To determine a and r_c we need a set of two independent equations. The first one follows from the requirement of equality of the ground state energy of an electron in the field of a pseudo-ion which generates the potential (1) and of

* Address: Instytut Fizyki Doświadczalnej, Uniwersytet Wrocławski, Cybulskiego 36, 50-205 Wrocław, Poland.

an electron in a real ion [7]. Consequently the model potential (1) should obey the radial Schrödinger equation

$$\left(\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - V_b(r) + E_i\right)\psi_0(r) = 0, \tag{2}$$

where E_i is the first ionization potential of a real ion with the valence $Z-1$, and $\psi_0(r)$ is a wave function of a ground state. The second parameter is determined by using the relation

$$v(h) = \frac{V_b(h)}{\mathscr{E}(h)} = v(h)_{exp}, \tag{3}$$

where $v(h)$ is the value of a screened form factor at a certain point of the Brillouin zone (in our case point L), and $v(h)_{exp}$ is the same quantity measured experimentally (one half of the s-p band gap at L). In a reciprocal space, the bare model potential is

$$V_b(q) = \frac{4\pi Ze^2}{\Omega_0 q^2}\,\frac{(2a-1)(qr_c)^2-1}{[(qr_c)^2+1]^2}, \tag{4}$$

where Ω_0 is the atomic volume. In Eq. (3), $\mathscr{E}(q)$ is the dielectric function of Geldart and Vosko [8] which describes the screening of the conduction electrons.

The set of Eqs. (2) and (3) was solved numerically for copper. First the value of a was found from Eq. (3), then the parametric solution for $V_b(r)$ was put into Eq. (2) to calculate r_c. In order to solve Eq. (2) a simple method described by Belenkii and Krasko [9] was adopted. The values of the ionization potential were taken from spectroscopic data for

TABLE I

Quantity	Z	Ω_0	k_F	a	r_c
Value	1	78.9	0.7163	54.195	0.097

All values in atomic units.

free ion [10]. The experimental values of the form factor $v(h)_{exp}$ were taken at point L of the Brillouin zone ($q = h\,(111)$) according to Pells and Shiga [11]. The parameters used in the computation (Ω_0 and k_F) and values of a and r_c are listed in Table I. A computed form factor along with that of Moriarty [1] is displayed in Fig. 1. As a test of the model potential determined in such a way, the resistivity of liquid copper has been calculated, using Ziman's well-known formula [12].

$$\varrho = \frac{3\pi m\Omega_0}{2\hbar e^2 E_F}\langle a(q)\,|v(q)|^2\rangle, \tag{5}$$

where E_F is the Fermi energy and

$$\langle a(q)\,|v(q)|^2\rangle = \frac{1}{4k_F^4}\int_0^{2k_F} a(q)\,|v(q)|^2 q^3 dq, \tag{6}$$

where k_F is the Fermi wave vector and $a(q)$ is the expectation value of $|S(q)|^2$, $S(q)$ being the structure factor. The structure factor data for copper were taken from Wagner et al. [12]. The calculated value of the resistivity of liquid copper is found to be 22.37 $\mu\Omega \cdot$ cm in

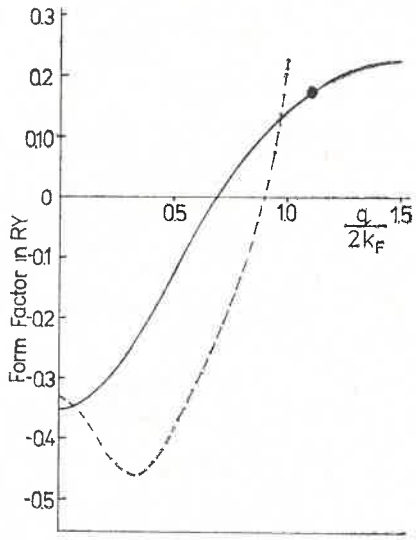

Fig. 1. Model potential form factor of Cu; solid line proposed model, dashed line Moriarty [1]. Circle represents the experimental value [11]

a good agreement with the experimental (21.5 $\mu\Omega \cdot$ cm [14]) and calculated values (Moriarty [1] — 21.6 $\mu\Omega \cdot$ cm, Leoni et al. [3] — 23.6 $\mu\Omega \cdot$ cm).

In conclusion, the model potential of the form (1) seems to be a reasonable approximation of the electron-ion interaction in noble metals. Of course, this conclusion should be confirmed by calculation of other quantities such as, e.g. elastic constants, the density of states, or phonon spectra. Only then it will be possible to estimate fully the validity of this approximation.

The author wishes to thank Professor K. F. Wojciechowski and J. Peisert for helpful discussions.

REFERENCES

[1] J. A. Moriarty, *Phys. Rev.* **B1** 1363 (1970); **B6**, 1239 (1972).
[2] B. Borchi, De Gennaro, *Phys. Lett.* **32A**, 301 (1970).
[3] F. Leoni, S. Lal, A. Paskin, *Lett. Nuovo Cimento* **8**, 1036 (1973).
[4] S. Lal, A. Paskin, F. Leoni, *J. Phys. F* **5**, 697 (1975).

[5] O. P. Kulshretha, H. C. Gupta, J. C. Upadhyaya, *Solid State Commun.* **17**, 291 (1975); *Physica* **84B**, 236 (1976).
[6] M. Kumar, M. P. Hemkar, *Phys. Lett.* **65A**, 49 (1978).
[7] G. L. Krasko, Z. A. Gurskii, *Zh. Eksp. Teor. Fiz. Pis'ma* **9**, 596 (1969).
[8] D. J. W. Geldart, S. H. Vosko, *Can. J. Phys.* **44**, 2137 (1966).
[9] A. Ya. Belenkii, G. L. Krasko, *Dokl. Akad. Nauk SSSR* **213**, 1280 (1973).
[10] C. E. Moore, *Atomic Energy Levels*, NBS Circular 467 (1949).
[11] G. P. Pells, M. Shiga, *J. Phys. C* **2**, 1835 (1969).
[12] J. M. Ziman, *Phil. Mag.* **6**, 1013 (1961).
[13] C. N. J. Wagner, H. Ocken, M. L. Joshi, *Z. Naturforsch.* **20A**, 325 (1965).
[14] N. E. Cusack, *Rep. Progr. Phys.* **26**, 361 (1963).