Vol. A56 (1979) *ACTA PHYSICA POLONICA* No 6

MONOVACANCY RESISTIVITY OF CUBIC METALS

By P. K. Sharma, Jai Prakash, K. N. Mehrotra and P. C. Sharma

Physics Department, University of Allahabad*

(Received March 6, 1978; Revised version received April 2, 1979)

The monovacancy resistivity of alkali, noble, aluminium and lead metals has been computed using various available pseudopotential models. A reasonably satisfactory agreement with the experimental data is obtained.

In recent years, the pseudopotential theory of metals [1, 2] has become an elegant and useful technique for calculating various physical properties of metals. A number of models have been developed to construct the form factors of pseudopotentials in simple metals in a semi-empirical way by fitting the parameters either to the dispersion curves [3] or to other experimental data [4, 5] and from first principles [6] using the results of atomic spectroscopy. Efforts [7–9] have also been made to extend and generalize the theory for noble metals by taking the overlapping conduction d-states separately from the remainder of the core. Cohen and Heine [10] have reviewed the technique and have summarized the empirical potentials which have been obtained for a large number of elements. In this communication, we report a theoretical computation of monovacancy resistivity of alkali metals, noble metals, aluminium and lead from various recently available pseudopotential form factors and compare them with available experimental values and other theoretical estimates.

Within the framework of pseudopotential formalism, the monovacancy resistivity ϱ_v of simple metals can be written as [1]

$$\varrho_v = \frac{3}{16\hbar n e^2 v_F^2 k_F^4} \int\limits_0^{2k_F} \int\limits_\Omega q^3 |W(q)|^2 dq d\Omega, \tag{1}$$

where n is the ion number density, $W(q)$ is the screened pseudopotential form factor of electron-ion interaction, v_F and k_F are the Fermi velocity and momentum, $\boldsymbol{q}$ is the momentum transfer vector and Ω is the solid angle in the scattering vector space.

---

* Address: Physics Department, University of Allahabad, Allahabad-211002, India.

TABLE I

Monovacancy resistivity of alkali metals for various model potentials (in units of μ ohm · cm/at. per cent)

Form factors	Monovacancy resistivity				
	Li	Na	K	Rb	Cs
Bardeen	0.49686	0.406260	0.805527	0.91404	1.15344
Schneoder–Stoll	0.592128	0.482355	0.3000	0.414522	0.383076
Animalu–Heine	2.72457	0.207050	0.534177	0.73259	0.288477
Ashcroft	0.99589	0.203742	0.45159	0.385776	0.71125
Lee–Heine	0.96471	0.491256	0.171882	0.893079	1.95579
Shaw	1.50489	0.25127	0.878265		
Sharma–Srivastava	0.88732	0.242262	0.562338	1.23525	1.14066
Bortolani–Calandra			0.32339	1.20087	1.51452
Giuliano–Ruggeri	1.20051	0.79798	0.397845	3.6261	5.23780
Appapillai–Williams	3.50629	0.16656	0.47379	1.88931	1.93097
Other theoretical calculations [a]	0.763	1.138	1.531		

[a] W. M. Shyu, J. H. Wehling, M. R. Cordes, G. D. Gaspari, *Phys. Rev.* **B4**, 1802 (1971).

TABLE II

Monovacancy resistivity of fcc metals for various model potentials (in units of μ ohm · cm/at. per cent)

Form factor	Monovacancy resistivity				
	Cu	Ag	Au	Al	Pb
Bardeen	0.3790	0.4610	1.5296	0.4645	0.9515
Ashcroft	1.03995	0.85535	2.34135	2.8209	
Borchi–deGennaro	2.0948	1.4611	3.2595		
Schneider–Stoll				0.982	0.419
Moriarty	3.2859	4.15863	8.50896		
Animalu–Heine				3.4156	0.1509
Jacobs	20.8555	7.0403	9.0691		
Appapillai–Williams				1.9400	0.4135
Animalu	3.3824	6.5453	19.1731		
Experimental values	1.2±0.6 [a]	1.3±0.7 [a] 1.6 [b]	1.5±0.3 [a] 2.4±0.4 [c] 1.8±0.4 [d] 1.8±0.6 [e]	3.00 [f] 2.2 [h]	0.19±0.02 [g]
Other theoretical calculations	1.28 [i]	1.45 [i]	1.45 [i]	0.673 [j] 0.8 [k]	

[a] R. O. Simmons, R. W. Balluffi, *Phys. Rev.* **129**, 1533 (1963). [b] L. J. Cuddy, E. S. Machlin, *Phil. Mag.* **7**, 745 (1962). [c] R. M. J. Cotterill, *Phil. Mag.* **6**, 1351 (1961). [d] R. W. Siegel, *Phil. Mag.* **13**, 359 (1966). [e] W. Desorbo, *Phys. Rev.* **117**, 444 (1960). [f] R. O. Simmons, R. W. Balluffi, *Phys. Rev.* **117**, 62 (1960). [g] A. J. Leadbetter, D. M. T. Newsham, N. H. Picton, *Phil. Mag.* **13**, 371 (1966). [h] J. Takamura, in Ref. [25], p. 521. [i] P. Jongenburger, *Appl. Sci. Res.* **3B**, 237 (1953); M. F. Abeles, *Compt. Rend.* **237**, 796 (1953). [j] Ref. [24]. [k] Ref. [1].

We have calculated the monovacancy resistivity of alkali metals (Li, Na, K, Rb, Cs), noble metals (Cu, Ag, Au), aluminium and lead from Eq. (1) by numerical integration. The form factors of the electron-ion coupling for alkali metals are taken from model potentials of Schneider and Stoll [3], Ashcroft [4], Sharma and Srivastava [5], Animalu and Heine [11], Shaw [12], Bortolani and Calandra [13], Giuliano and Ruggeri [14], Lee and Heine [15], Appapillai and Williams [16] and Bardeen [17]. In the case of noble metals, we have used the recently available pseudopotential form factors of Moriarty [9], Borchi and de Gennaro [18], Jacobs [19] and Animalu [20] as well as Ashcroft [4] and Bardeen [17] model potentials. For aluminium and lead, the electron-ion scattering form factors are obtained from pseudopotential models of Schneider and Stoll [3], Ashcroft [4], Animalu and Heine [11], Appapillai and Williams [16], and Bardeen [17].

The calculated values of the monovacancy resistivity of bcc and fcc metals from several pseudopotentials are given in Tables I and II, respectively, together with available experimental data and other theoretical estimates. From the theoretical point of view, earlier calculations for noble metals are due to Jongenburger [21] and Abeles [22]. These authors have employed a square-well potential whose height was adjusted such that the phase shift satisfied the Friedel rule. Ziman [23] has, however, pointed out that the Friedel rule does not determine the scattering with sufficient accuracy. For alkali metals and aluminium, Shyu et al. [24] have recently determined the residual resistivity due to vacancies using Shaw's [12] non local model potential. They have also studied the effects of exchange and correlation on the monovacancy resistivity. Harrison [1] has calculated ϱ_v of aluminium using the orthogonalized plane wave form factors. For comparison, the results of these authors are also shown in Tables I and II. Most of the experimental information on electrical resistivity of lattice vacancies in fcc metals have been obtained through quenching methods [25] but recently equilibrium techniques [26] have also been applied to measurements of monovacancy resistivity of metals. The most accurate values of the monovacancy resistivity of noble metals at melting point have been published by Simmons and Balluffi [27] by combining their measurements [28] of defect concentrations under equilibrium conditions with values of quenched-in resistivity increment obtained through quenching experiments by other authors [29, 30]. A somewhat larger value for the vacancy resistivity in gold, stated to be a lower limit, has been obtained by Cotterill [31] in a similar manner. His result is, however, subject to errors due to uncertainty in the knowledge of mechanism of annealing. These and other available experimental values are shown in Table II. No experimental determination of the vacancy resistivity has been reported for alkali metals.

It will be seen from Table II that the experimental data for noble metals show reasonably satisfactory agreement with the values deduced from form factors of Ashcroft [4], Borchi and de Gennaro [18], and Bardeen [17] potentials for Cu, Ag and Au, respectively. For gold correct value is found, but for other metals, in general, slightly higher values are obtained. Moriarty [9] and Jacobs' [19] potentials give considerably higher values for all the noble metals. It is due to the shape of the pseudopotential. In the case of aluminium and lead, Ashcroft [4] and Animalu and Heine [11] potentials give better agreement with experiments. On the whole, the agreement of the calculated values with experiments is better for Ashcroft [4] pseudopotentials for noble metals than those from other models.

It appears that with the proper choice of pseudopotential, one can expect to get very good agreement with experiments.

One of the authors (P.K.S.) is thankful to the University Grants Commission for financial support.

Editioral note. This article was proofread by the editors only, not by the authors.

REFERENCES

[1] W. A. Harrison, *Pseudopotentials in the Theory of Metals*, W. A. Benjamin, Inc., New York 1965.
[2] V. Heine, D. Weaire, *Solid State Phys.* **24**, 249 (1970).
[3] T. Schneider, E. Stoll, *Phys. Kondens. Mater.* **5**, 331, 364 (1966); **8**, 58 (1968).
[4] N. W. Ashcroft, *Phys. Lett.* **23**, 48 (1966); *J. Phys. C* **1**, 232 (1968).
[5] P. K. Sharma, S. K. Srivastava, *J. Phys. Chem. Solids* **33**, 1979 (1972).
[6] W. A. Harrison, *Phys. Rev.* **129**, 2503, 2512 (1963); **131**, 2433 (1963).
[7] V. Heine, *Phys. Rev.* **153**, 673 (1967).
[8] W. A. Harrison, *Phys. Rev.* **181**, 1036 (1969).
[9] J. A. Moriarty, *Phys. Rev.* **B1**, 1363 (1970).
[10] M. L. Cohen, V. Heine, *Solid State Phys.* **24**, 37 (1970).
[11] A. O. E. Animalu, V. Heine, *Phil. Mag.* **12**, 1249 (1965).
[12] R. W. Shaw, *Phys. Rev.* **174**, 769 (1968).
[13] V. Bortolani, C. Calandra, *Phys. Rev.* **B1**, 2405 (1970).
[14] E. S. Giuliano, R. Ruggeri, *Nuovo Cimento* **61B**, 53 (1969); *Lett. Nuovo Cimento* **2**, 817 (1969).
[15] M. J. G. Lee, V. Heine, private communication; M. J. G. Lee, *Phys. Rev.* **178**, 953 (1969).
[16] M. Appapillai, A. R. Williams, *J. Phys. F* **3**, 759 (1973).
[17] J. Bardeen, *Phys. Rev.* **52**, 688 (1937).
[18] E. Borchi, S. de Gennaro, *Phys. Lett.* **32A**, 301 (1970).
[19] R. Jacobs, *J. Phys. C* **1**, 1296, 1307 (1968).
[20] A. O. E. Animalu, *Phys. Rev.* **B8**, 3542 (1973); **B8**, 3555 (1973).
[21] P. Jongenburger, *Appl. Sci. Res.* **3B**, 237 (1953).
[22] M. F. Abeles, *Compt. Rend.* **237**, 796 (1953).
[23] J. M. Ziman, *Adv. Phys.* **13**, 89 (1964).
[24] W. M. Shyu, J. H. Wehling, M. R. Cordes, G. D. Gaspari, *Phys. Rev.* **B4**, 1802 (1971).
[25] *Lattice Defects in Quenched Metals*, Ed. R. M. J. Cotterill, M. Doyama, J. J. Jackson, M. Meshii, Academic Press, New York 1965.
[26] A. Ascoli, G. Guarini, G. T. Queirolo, *Cryst. Lattice Defects* **1**, 159 (1970).
[27] R. O. Simmons, R. W. Balluffi, *Phys. Rev.* **129**, 1533 (1963).
[28] R. O. Simmons, R. W. Balluffi, *Phys. Rev.* **119**, 600 (1960); **125**, 862 (1962).
[29] M. Doyama, J. S. Koehler, *Phys. Rev.* **119**, 939 (1960); **127**, 21 (1962).
[30] J. E. Bauerle, J. S. Koehler, *Phys. Rev.* **107**, 1493 (1957).
[31] R. M. J. Cotterill, *Phil. Mag.* **6**, 1351 (1961).