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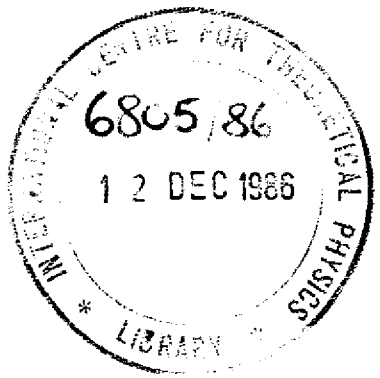

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

CALCULATION OF BINDING ENERGIES AND ELASTIC CONSTANTS OF Cu, Ag AND Au USING A ONE-PARAMETER MODEL POTENTIAL

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CALCULATION OF BINDING ENERGIES AND ELASTIC CONSTANTS OF Cu, Ag AND Au USING A ONE-PARAMETER MODEL POTENTIAL *

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ABSTRACT

The numerical calculations of binding energies and elastic constants for Cu, Ag and Au are carried out using a one-parameter model potential. A comparison of the results obtained in these calculations with experimental data and some previous theoretical results showed that the one-parameter model potential simulates the real electron-ion interaction of Cu, Ag and Au, and gives a much improved degree of agreement between theory and experiment for binding energies and elastic constants.

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1. INTRODUCTION

In a previous paper we proposed **a phenomenological one-parameter model** pseudopotential for the noble metals Cu, Ag, and Au [1]. This potential, which contains the s-d hybridization and core-core exchange contrications, was analyzed in some detail there and it was shown that its prediction on the liquid metal resistivity, thermoelectric power and band gaps were in better agreement with experiment than those of the other model potentials considered in **the literature.** Encouraged by this and a **number** of other successful calculations [2,3] based on our potential we undertook a computation of the binding energies and elastic constants for the three metals. In this report we present the results of our calculation and compare them with the experimental data as well as with the results of other calculations [4-6].

The one-parameter (bare) ion model potential proposed in [1] is given by

$$W^{b}(r) = \begin{cases} \dfrac{Ze^2(R_m^2 - rR_w)}{R_w^2(R_w - R_m)} & 0 < r < R_m \\ -2\dfrac{Ze^2}{R_w} & R_m < r < R_w \\ -\dfrac{Ze^2}{r} & R_w < r \end{cases} \qquad (1)$$

that is, the potential is repulsive from zero to $r = R_m^2/R_w$ (core radius), attractive and constant in the region $r = R_m$ to $r = R_w = (3\Omega/4\pi)^{1/3}$ (Wigner Seitz radius) and purely Coulombic beyond. The value of R_m for Cu, Ag and Au have been determined and tabulated in [1].

2. BINDING ENERGY AND ELASTIC CONSTANTS

2.1 Binding energy

Following Moriarity [4], the total energy (in ryd) per ion, or, what is the same thing, the binding energy of the metal, may be written as

$$E_{tot} = E_{fe} + E_{bs} + E_{es} + E_{ol} \qquad (2)$$

where the various pieces are

$$E_{fe} = 2.21 \frac{Z}{r_s^2} - Z\left(\frac{0.916}{r_s} + 0.115 - 0.031 \ln r_s\right) \qquad (3)$$

$$E_{bs} = -\frac{\Omega}{4\pi e^2} \sum_{q \neq 0} q^2 |S(q)|^2 |w(q)|^2 \frac{\varepsilon(q) - 1}{[1 - f(q)]\varepsilon(q)} \qquad (4)$$

$$E_{es} = \frac{AZ^2}{r_s} \qquad (5)$$

and E_{ol} is the overlap energy which has been calculated in an essentially model independent way by Moriarity and is given as [4].

$$E_{ol} = \alpha \left[1 + \ell\left(\frac{r}{r_m} - 1\right) + \beta \ell^2 \left(\frac{r}{r_m} - 1\right)^2\right] \times \exp\left\{-\gamma\left(\frac{r}{r_m} - 1\right)\right\} \qquad (6)$$

Here r_m is the nearest neighbour distance. The numerical values of α, β, γ and ℓ are given in [4]. Note that $r_s = (3\Omega/4\pi z)^{1/3}$ and A is the Madelung constant which equals - 1.792 for f.c.c. structures.

The quantity $\varepsilon(q)$ in equation (4) is the Hartree dielectric function, modified to include the exchange and correlation corrections through the function f(q) to provide screening of the bare potential. As for the structure factor $S(\vec{q})$, it is unity at the reciprocal lattice vectors $\vec{H}$ and zero elsewhere, so that the right-hand side of equation (4) simplifies in an obvious way.

2.2 Elastic constants

By the method of homogeneous deformation, the three independent elastic constants of the cubic crystal can be obtained as the second order derivative of the total energy with respect to certain deformation parameters. The elastic constants C_{11}, C_{12} and C_{44} can be determined from the bulk and shear modulus B, C and C' respectively:

$$B = \frac{1}{3}\left(C_{11} + 2C_{12}\right) = \frac{1}{\Omega}\frac{d^2 E_{tot}}{d\delta^2}$$

$$C = C_{44} = \frac{1}{\Omega}\frac{d^2 E_{tot}}{d\gamma_1^2}$$

$$C' = \frac{1}{2}\left(C_{11} - C_{12}\right) = \frac{1}{4\Omega}\frac{d^2 E_{tot}}{d\xi_1^2} \qquad (7)$$

where δ, γ_1 and ξ are parameters of bulk deformation, shear deformation in one plane and compression in one direction respectively.

3. RESULTS AND DISCUSSION

To calculate the binding energies of the three noble metals, we have summed over 512 reciprocal lattice vectors in equation (4) in order to obtain proper convergence. The calculated values of binding energies are given in Table I, where we also give the corresponding experimental numbers [7-9]. For comparison, the values calculated by Moriarity are also shown.

While the Moriarity predictions do not satisfy even the experimental inequalities

$$\left| E_{tot}(Au) \right| > \left| E_{tot}(Cu) \right| > \left| E_{tot}(Ag) \right|$$

the prediction of our one-parameter model pseudopotential shows detailed agreement with experiment for all the three metals.

The computed values of the elastic constants are given in Table II together with the observed data [9,10] as well as the results of some previous calculations.

It is seen that while the agreement between theory and experiment for C_{11} and C_{12} is at least as good as that in Kulshrestha et al. and Khanna's calculations, we have achieved a much better agreement for C_{44} than Kulshrestha et al. for all the three metals Cu, Ag and Au.

These results together with those presented in [1,3] lead us to believe that the model potential (1) simulates the real electron-ion potentials of Cu, Ag and Au closely enough to correctly predict in any of their electronic and transport properties.

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Table I

Binding Energy of noble metals (in Ryd)

Element	Present Calculation	Moriarity [4]	Expt [7-9]
Cu	- 0.855	- 0.800	- 0.826
Ag	- 0.785	- 0.649	- 0.775
Au	- 0.915	- 0.652	- 0.957

Table II

Elastic constants of Cu, Ag and Au in units of 10^{11} dyne Cm^{-2}

Cu		C_{11}	C_{12}	C_{44}
Present Calculation		16.105	11.821	7.700
Kulshrestha et al.	[5]	15.497	13.331	4.174
Fuchs	[7]	17.500	12.400	8.900
Khanna	[6]	15.126	11.680	7.932
Observed	[9,10]	16.84	12.14	7.54
Ag				
Present Calculation		11.824	10.210	4.989
Kulshrestha et al.	[5]	10.162	9.105	2.936
Fuchs	[7]			
Khanna	[6]	12.929	11.149	4.969
Observed	[9,10]	12.400	9.34	4.6
Au				
Present Calculation		18.875	16.342	4.848
Kulshrestha et al.	[5]	19.970	19.018	2.431
Observed	[9,10]	18.600	15.700	4.200