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ELECTRICAL RESISTIVITY OF LIQUID NOBLE METAL ALLOYS *

M. Anis Alam ** and M. Tomak ***
International Centre for Theoretical Physics, Trieste, Italy.

ABSTRACT

Calculations of the dependence of the electrical resistivity in liquid Ag-Au, Cu-Ag, Cu-Au binary alloys on composition are reported. The structure of the binary alloy is described as a hard sphere system. A one-parameter local pseudopotential, which incorporates s-d hybridization effects phenomenologically, is employed in the resistivity calculation. A reasonable agreement with experimental trends is observed in cases where experimental information is available.

MIRAMARE - TRIESTE
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** Permanent address: Physics Department, Punjab University, Lahore, Pakistan.

*** Permanent address: Physics Department, Middle East Technical University, Ankara, Turkey.

I. INTRODUCTION

The pseudopotential theory continues to provide a powerful tool for the study of electronic properties of simple liquid metals. Difficulties arise when the study involves noble, transition and rare-earth metals. In noble metals Cu, Ag and Au, narrow d-bands are filled and lie below the Fermi energy. Since the d-bands are not seriously affected by melting, as suggested by experimental studies, pseudopotential for noble metals have to be energy dependent and non-local if they are to explain fully all the structural and electronic properties. For simple transport properties such as electrical resistivity, however, local, energy independent pseudopotentials seem to give results in reasonable agreement with experiments. It is in this spirit that the present study has been undertaken to calculate the resistivity of noble metal alloys using a single parameter, energy independent local pseudopotential recently proposed by Idrees et al. [1].

Relatively few studies for liquid noble metal alloys have been undertaken, principally because of the non-availability of experimentally determined partial structure factors. These have therefore to be calculated using a theoretical model. In the present study a hard-sphere model has been used.

The plan of the present paper is as follows. In Sec.II, a brief discussion of the model pseudopotential, partial structure factors and the Faber-Ziman theory of electrical resistivity of liquid binary alloys is given. In the following section we present results on the composition dependence of electrical resistivity for Ag-Au, Cu-Ag and Cu-Au systems, with a brief summary of the conclusions.

II. THE ELECTRICAL RESISTIVITY OF NOBEL METAL BINARY ALLOYS

The Faber-Ziman [2] well-known formula for the electrical resistivity of a liquid binary alloy modified by Ashcroft and Langreth [3] can be written as

$$\rho = \frac{4\pi^3 \hbar Z^{*}}{e^2 k_F} \int_0^1 dy\, y^3 \left\{ x V_2^2(y) S_{22}(y) + 2\left[x(1-x)\right]^{1/2} V_1(y) V_2(y) S_{12}(y) + (1-x) V_1^2(y) S_{11}(y) \right\}, \tag{1}$$

where $y = q/2k_F$; x = concentration of species 2; Z^* = effective valence.

It requires a knowledge of the electron-ion pseudopotential V_i and the partial structure factor S_{ij}. In the following a brief discussion of each of these factors is given.

A. Model pseudopotentials

In their study of electrical resistivity of liquid noble metal binary alloys Ashcroft and Langreth [3] used the Ashcroft empty-core potential

$$V_i(y) = -\frac{\lambda^2 \cos(s_i y)}{\lambda^2 + \lambda^2 f(y)} , \qquad (2)$$

where $s_i = 2k_F R^i_{core}$, $\lambda^2 = (\pi a_0 k_F)^{-1}$ and f(y) is the Linhard dielectric function. In their calculation of the electrical resistivity, they have chosen R_{core} to fit the resistivity of the molten metal at both ends of the concentration. They claim reasonable agreement with the experimental results.

In the present study, a local, energy independent single parameter pseudopotential recently introduced by Idrees et al. [1] is employed. The potential has the form,

$$V^b(r) = \begin{cases} \dfrac{Ze^2(R_m^2 - R_w r)}{R_w^2 (R_w - R_m)} & 0 < r < R_m \\ -2\dfrac{Ze^2}{R_w} & R_m < r < R_w \\ -\dfrac{Ze^2}{r} & R_w < r \end{cases} \qquad (3)$$

and is repulsive in the region from r = 0 to $r = R_m^2/R_w = R_m$ (core radius), attractive and constant in the region $r = R_m$ to $r = R_w = (3\Omega/4\pi)^{1/3}$, the Wigner-Seitz radius and purely Coulombic beyond. The potential is claimed to give an improved account of the s-d mixing which has been introduced phenomenologically. The Fourier transform of Eq.(3) is given by

$$V^b(q) = \frac{4\pi}{\Omega q^3}\Big[(AR_m^2 + B - AR_w R_m)(\sin qR_m - qR_m \cos qR_m) - B(\sin qR_w - qR_w \cos qR_w) - \frac{AR_w}{q}(qR_m \sin qR_m + 2(\cos qR_m - 1)) - Ze^2 q \cos qR_w\Big] , \qquad (4)$$

where

$$A = \frac{Ze^2}{R_w(R_w - R_m)}$$

$$B = -\frac{Ze^2}{R_w} .$$

The parameter R_m is fixed by fitting the theoretical factor Eq.(4) to the experimental one or to a better calculation. The electron-ion pseudopotential to be used in Eq.(1) is the screened one. The screening has been done with the Vashista and Singwi [4] dielectric function.

B. Partial structure factors

For the partial structure factor of the binary alloys, the hard-sphere solution of the Percus-Yevick equation has been used. The analytic expression for these has been given by Ashcroft and Langreth [5].

III. NUMERICAL RESULTS AND CONCLUSIONS

The input parameters and the model pseudopotentials appropriate for Cu, Ag and Au are taken from Ref.1, since calculations based on these have been done for electrical resistivities, thermoelectric power and effective ion-ion interactions for liquid Cu, Ag and Au. The results seem to be somewhat better than those of other investigations. Thus, the present study may be considered as another test of the proposed pseudopotentials.

The concentration dependence of the calculated electrical resistivity for liquid Cu-Ag, Cu-Au and Ag-Au systems is shown in Figs.1, 2 and 3.

In the case of Ag-Au and Cu-Au systems, the experimental trend is well produced. At intermediate concentrations the model pseudopotential and the hard sphere structure factors used seem to be doing poorly as far as the absolute values of the resistivity are concerned. To get better numerical agreement with experimental resistivity values [6-8] one is forced to use hard sphere diameters which tend to result in structure factors that are in disagreement with the experimental one [9].

In the present calculation the atomic volume of the alloy is linearly interpolated between the values of the pure components. The Fermi wave number is calculated with this atomic volume. The packing function is taken to be 0.45 for all the three systems. Hard sphere diameter ratio for Cu-Ag, Cu-Au and Ag-Au has been taken to be 0.86, 0.86 and 0.99, respectively.

Results of the present study seem to confirm the generalization that the resistivity of binary alloys is a smooth function of concentration at constant temperature. The use of local, energy independent pseudo-potential even in the case of noble metals seems to be reasonable.

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FIGURE CAPTIONS

Fig.1 The concentration dependence of the calculated resistivity for liquid Cu-Ag binary alloy.

Fig.2 The concentration dependence of the calculated resistivity for liquid Cu-Au binary alloy.

Fig.3 The concentration dependence of the calculated resistivity for liquid Ag-Au binary alloy.

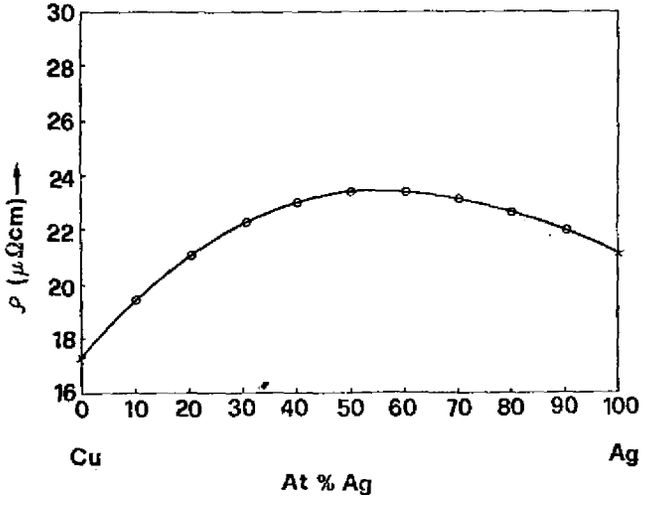

Fig.1

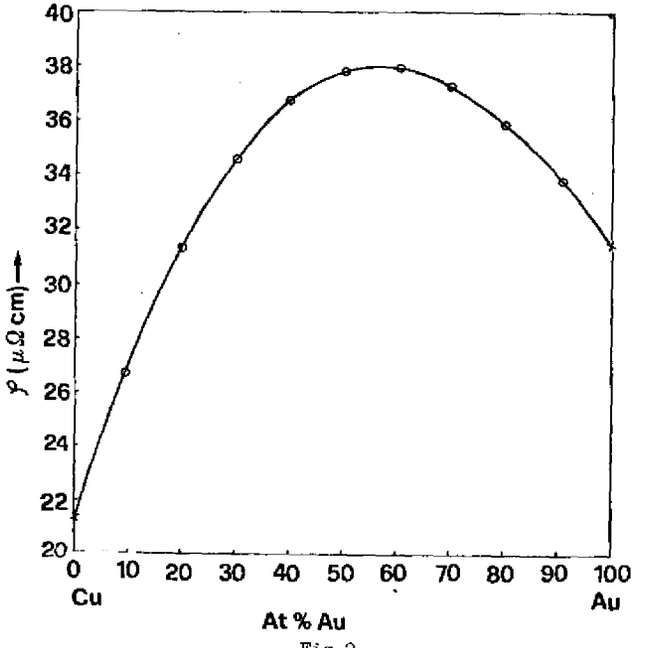

Fig.2

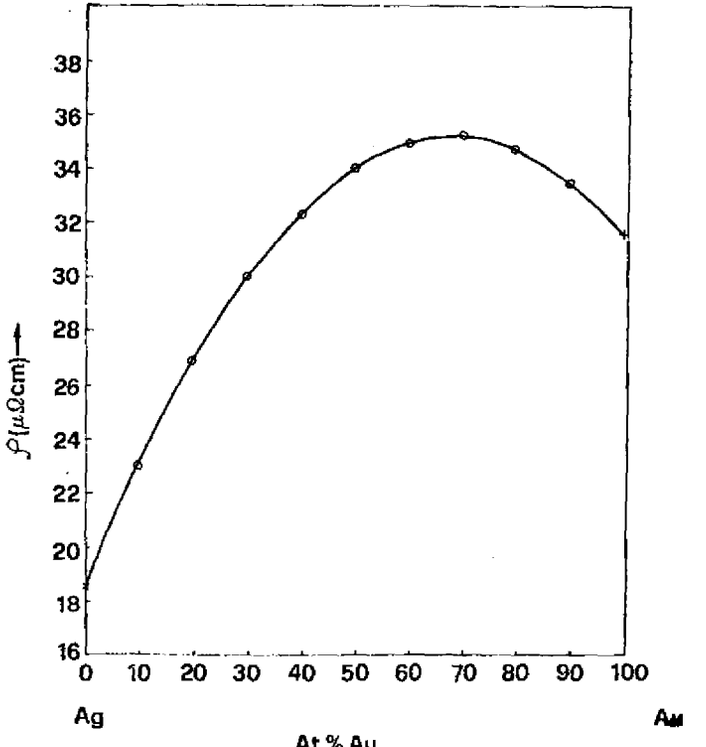

Fig.3