RESISTIVITY CALCULATIONS FOR LIQUID Na-K, K-RB, Na-Rb, Na-Cs and K-Cs ALLOY SYSTEMS

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The aim of the present work is the resistivity calculations for liquid alloy systems on the basis of general model pseudopotential (GMP) /1/ and recent experimental and theoretical information about the structure factors /2-5/.

The electrical resistivity $\rho(c)$, as a function of concentracion c of heavier component , may be written as:

$$\rho(c) = \frac{3\pi m^2 \Omega_0}{4e^2\hbar^3 k_F^2} \int_0^{2k_F} \left\{(1-c)\left[W_q^{(1)}(k_F)\right]^2 a_{11}(q) + c\left[W_q^{(2)}(k_F)\right]^2 a_{22}(q) + 2\left[c(1-c)\right]^{1/2} W_q^{(1)}(k_F) W_q^{(2)}(k_F) a_{12}(q)\right\} q^3 dq \qquad (1)$$

where Ω_0 is the atomic volume of the system, m is the effective mass of the electrons, $W_q^{(1)}(K_F)$ and $W_q^{(2)}(K_F)$ are the matrix elements of the screened electron-ion potential, and $a_{11}(q)$, $a_{22}(q)$, and $a_{12}(q)$ are the partial structure factors of the liquid.

The GMP, obtained by fitting form-factor data based on the Heine-Abarenkov model potential has the form:

$$\langle \vec{k}+\vec{q}|W|\vec{k}\rangle = -\frac{1}{3} E_F \cdot \frac{\sin(2\pi\beta_2 \cdot q/2k_F)}{2\pi\beta_2 \cdot q/2k_F} \qquad (2)$$

The screening effect of free electrons (Hartree dielectric function)is also included in (2).

Since there are no accurate experimental structure factors available for mentioned alloy systems,we are forced to use the results obtained from solution of Percus-Yevick equation for a model liquid consisting of hard spheres /3,6/.

In order to get partial structure factors we have used the modification suggested in the work /2/. For pure components one can get the best agreement with available experimental structure factors in this case.

The hard sphere diameters and packing densities of elements for which experimental structure factors are not

known well,(Rb and Cs), are obtained by scailing procedure applied in /4/.

Using the partial structure factors /6/ with the above mentioned modifications and GMP (2), we have calculated electrical resistivities as a function of concentracion c of heavier component for liquid Na-K, K-Rb, Na-Rb, Na-Cs and K-Cs alloy systems at 100°C. The results for two K systems are compared with the experimental /7,8/ and the theoretical results /4,5/ in figures 1 and 2. The agreement of our results with experiments is good. The maximal deviations (30%) are obtained for limiting concentrations (c=0 and c=1).

Such a comparison for sodium alloys gives greater differences (about 60%).

We would like to point out that our results are obtained without the use of any free parameters which could be selected so to give the best agreement with experiment. For pure metals structure-factor parameters η and σ where chosen for the Na and K in such a way to achieve the best agreement with experimental structure-factors, rather than to obtain the best agreement with resistivity values.

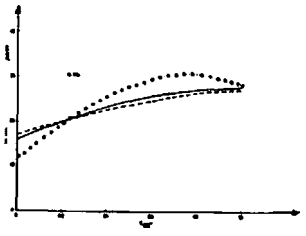

Fig. 1 The resistivity of K-Rb alloy as a function of Rb concentration at 100°C.
—— experimental results /8/
- - calculated values /4/
••• our results

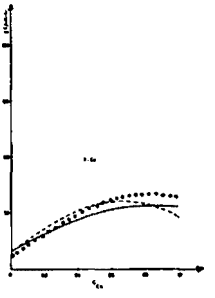

Fig. 2 The resistivity of K-Cs alloy as a function of Cs concentration at 100°C.
- - experimental results /7/
—— calculated values /5/
••• our results

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