

## Part II

In the previous report of the same title, we have calculated, on the basis of the two species model of Rapoport, the volume decreases of the liquid cesium and the liquid tellurium along their melting curves, the condition of a melting curve maximum, and the pressures at which the entropy changes during melting take maxima. But any criticisms have not been made to the two species model in that report. We shall re-examine the several assumptions of Rapoport in the present report. Then we shall determine the forms of the radial distribution function and the pair-potential corresponding to the two species model to satisfy the Rapoport's assumptions simultaneously.

### The Assumptions of Rapoport for Molten Cesium

There are two main assumptions in Rapoport's<sup>1) 2)</sup> report they are

- i) the assumption for the electrical resistance

$$R = (1 - \chi) R_I + \chi R_{III},$$

- ii) the assumption for the property of the liquid that "the liquid consists of two species, in the broad sense of the word, the one corresponding to the low pressure phase and the other to the high pressure phase. A species therefore is characterized by coordination number, nearest neighbor distance and bond type. The liquid is looked upon as a quasilattice with an average coordination number and can be treated by statistical mechanical methods by use of Bragg-Williams and Quasichemical approximations."

We think that there is an inconsistency in the assumption ii). If a species is defined as ii), the all ions must be equivalent to each other and there are not any pairs between different ions in the liquid, hence the quasichemical approach loses its physical meanings. In fact, there may not be any pairs between different ions in a liquid consisting of equivalent atoms. Nevertheless the treatments have given the good results. Therefore it may be concluded that even if the two species model is ambiguous and includes the inconsistency in the physical sense, it has the correctness as a result of the mathematical treatments.

### Radial Distribution Function and Pair Potential

We shall derive the forms of the radial distribution function and the pair-potential corresponding to the two species model, on the basis of its correctness as the results.

At first we consider the equation

$$g(r) = \alpha g_{AA}(r) + \beta g_{BB}(r), \quad (1)$$

where  $g(r)$  is the radial distribution function for the liquid under consideration which can be observed,  $g_{AA}(r)$ ,  $g_{BB}(r)$  and  $\alpha$ ,  $\beta$  are proper functions of distance  $r$  and proper coefficients respectively. It is obvious that the transformation such as (1) of  $g(r)$  is always possible mathematically. But, here, we look at the eq.(1) in the physical sense. The eq.(1) means that the observed feature of the distribution of the ions (i.e.g) consists of the superposition of the two different features of the distributions of the ions (i.e.  $g_{AA}$  and  $g_{BB}$ ). Of course

the all ions must be equivalent to each other and the eq. (1) satisfies this physical demand. Then we look upon anew  $g_{AA}$ ,  $g_{BB}$  as the species A and B respectively.

Now we consider the corresponding form of the pair-potential. It should be noted that arbitral two ions in the liquid form the species A or the species B, that is, the correlation between the two ions is shown by  $g_{AA}$  or  $g_{BB}$ . Therefore it may be reasonable to consider that the pair-potential consists of two different features too and the number of the features is restricted to two. The form of the pair-potential is then

$$\phi(r) = \alpha \phi_{AA}(r) + \beta \phi_{BB}(r), \quad (2)$$

$\phi(r)$  is the total pair-potential,  $\phi_{AA}$  and  $\phi_{BB}$  are corresponding to the species A and B respectively. It has not been established that the approximation by a pair-potential is reasonable for molten metal, but we proceed our discussion under the assumption that the approximation is reasonable.

#### Verification of Rapoport's Treatments

Ziman<sup>3)</sup> has given an electrical resistivity of molten metal by

$$\rho = \frac{m v_F}{n e^2 \Lambda}, \quad (3)$$

Hereafter we use the notations of Ziman. The mean free path  $\Lambda$  of an electron in the liquid is written from Born approximation as

$$\frac{1}{\Lambda} = \frac{3\pi \epsilon_F^{1/2}}{2\sqrt{2}} \cdot \frac{\langle a \rangle \cdot |u|}{\epsilon_F^2}, \quad (4)$$

where

$$\langle a \rangle |u|^2 = \frac{1}{4k_F^4} \int_0^{2k_F} |u|^2 a(k) \cdot k^3 dk. \quad (5)$$

$U_K$  is the Fourier transform of the pseudo potential of an ion in the liquid and  $a(k)$  is the Fourier transform of the radial distribution function. Since all ions are equivalent to each other,  $U_K$  is equivalent for all ions.  $a(k)$  is written as

$$a(k) = 1 + \frac{N}{V} \int (g-1) \frac{\sin kr}{kr} 4\pi r^2 dr. \quad (6)$$

Substituting the eq.(1) into the eq.(6) and pursuing the eq.'s (6), (5), (4) and (3) in this order, we have

$$\rho = \alpha \rho_{AA} + \beta \rho_{BB} \quad (7)$$

where

$$\rho_{AA} = \frac{m v_F}{n e^2 \Lambda_A},$$

$$\frac{1}{\Lambda_A} = \frac{3\pi \epsilon_F^{1/2}}{2\sqrt{2}} \cdot \frac{\langle a_{AA} \rangle |u|^2}{\epsilon_F^2},$$

$$\langle a_{AA} \rangle |u|^2 = \frac{1}{4k_F^4} \int_0^{2k_F} |u_k|^2 a_{AA}(k) \cdot k^3 dk,$$

and

$$a_{AA}(k) = 1 + \frac{N}{V} \int (g_{AA} - 1) \cdot \frac{\sin kr}{kr} 4\pi r^2 dr.$$

$\rho_{BB}$  is given similarly. The eq.(7) corresponds to Rapoport's assumption i).