

ON THE PAIR INTERACTION POTENTIALS IN LIQUID Al AND Sn

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Abstract: The pair interaction potentials for liquid aluminium and tin have been obtained from the structure factor measurements. The calculations are based on the approximation of the total correlation function. The result seems to reproduce the fact that for liquid metals the interaction potential strongly depends on the shape of the pair correlation function.

1. Introduction

One of the present most important open question is the knowledge of the pair interaction potential in liquid metals. Unfortunately, there is no general method so far for obtaining the reliable potentials from the experiment. The only approximate methods based on the structure factor data furnished by x-ray and neutron diffraction experiments are Born-Green, Percus-Yevick and hypernetted chain equations. Johnson and March¹⁾ and later Johnson et al.²⁾ were the first who used these methods. They have found the long range oscillatory behavior of the pair interaction potentials in liquid metals.

Because of their simplicity, Percus-Yevick and hypernetted chain equations have been used frequently³⁻⁵⁾, but the results are not always quantitatively correct. For example, Ruppertsberg and Wehr⁶⁾ on aluminium, North et al. on lead⁷⁾, Howells on rubidium⁸⁾, obtained potentials which do not possess the known negative minimum. Levesque and Verlet⁹⁾ pointed out by the computer simulation that the Percus-Yevick and HNC equations are not a reliable procedure. Recently,

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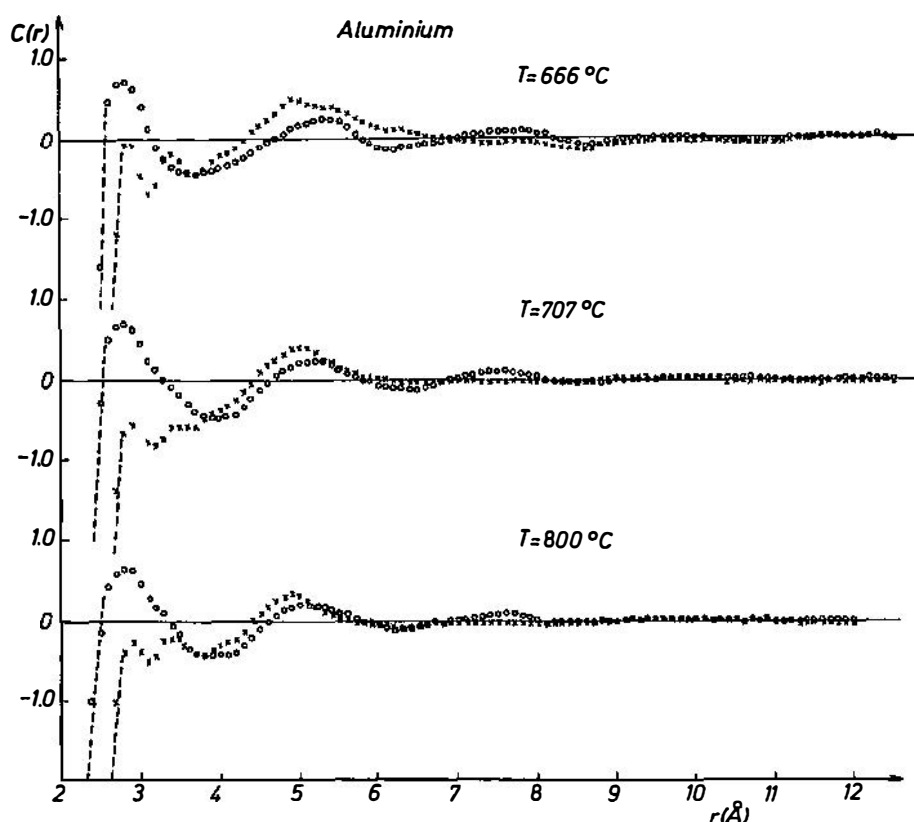


Fig. 1. Aluminium. Direct correlation functions $c(r)$ for the three temperatures calculated from the Fourier transform of $S(Q)$, Equ. (1) $\times \times \times$ and from the relation (3) $o o o$.

the Born-Green equation has been solved numerically using the method of linearized simultaneous equations¹⁰⁻¹²). This theory gives the relatively temperature independent potentials which is more appropriate for liquid metals. In the present paper an approximation of the total correlation function for the calculation of the pair interaction potential on liquid Al and Sn is suggested.

2. Results and discussion

In a recent experiment¹³) the authors measured the structure factors of liquid Al and Sn as a function of temperature over a wide momentum transfer range by the neutron diffraction. The direct correlation function $c(r)$ was calculated taking the Fourier transform of the structure $S(Q)$ according to the equation

$$C(r) = (2\pi^2 n r)^{-1} \int_0^\infty \left[\frac{S(Q) - 1}{S(Q)} \right] Q \sin Qr dQ. \quad (1)$$

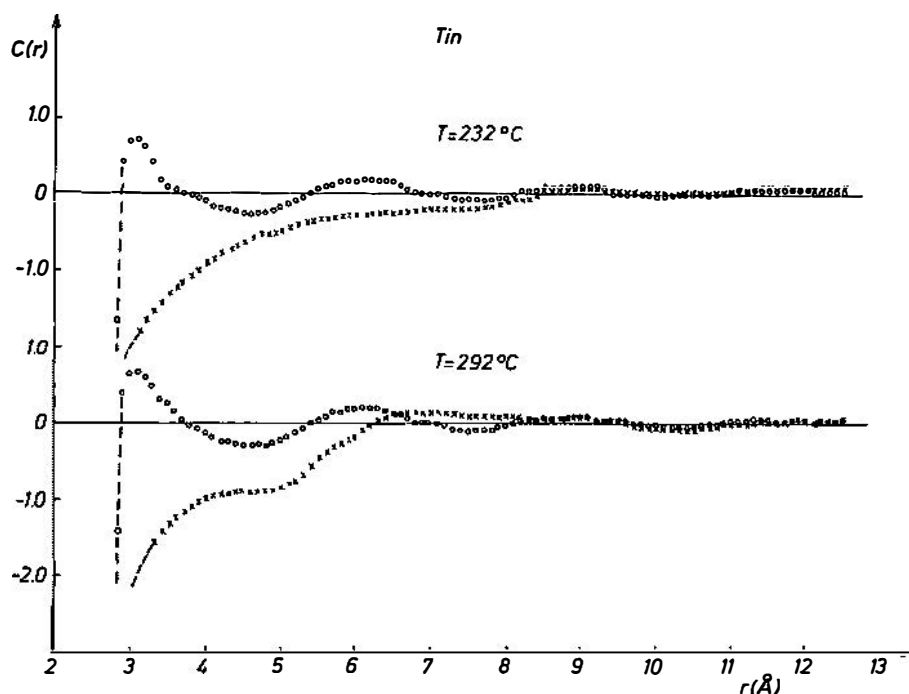


Fig. 2. Tin. Direct correlation functions $c(r)$ for the two temperatures calculated from the Fourier transform of $S(Q)$, Equ. (1) $\times \times \times$ and from the relation (3) $\circ \circ \circ$.

This means we cannot obtain the pair interaction potential in agreement with the pseudopotential theory from Percus Yevick and hypernetted chain theories. At the large distances the obtained potentials are of oscillatory nature, but the first main minimum is not negative. This could be due to the high sensitivity of $C(r)$ at very small errors of the structure factor at the small Q values¹⁴⁾. In order to avoid this, we propose to use the approximation of the total correlation function $h(r)$ according to the relation

$$h(r) = C(r) + h(r) C(r), \quad (2)$$

where the direct correlation function $C(r)$ is calculated from the equation

$$C(r) = \frac{(2\pi^2 n r)^{-1} \int_0^\infty [S(Q) - 1] Q \sin Q r dQ}{1 + (2\pi^2 n r)^{-1} \int_0^\infty [S(Q) - 1] Q \sin Q r dQ}. \quad (3)$$

For both Al and Sn, $C(r)$ was obtained from (3). The results are plotted in Figs. 1 and 2. It can be seen that the $C(r)$ values computed for Al from both the Fourier

transform of $S(Q)$ and the relation (3) are in rather good agreement at the distances larger than 3.5 \AA . The good agreement has also been obtained for the positions corresponding to the first maximum. However, the same cannot be said about the liquid Sn for which good agreement is observed only at distances larger than 7.5 \AA .

As Barker and Gaskell¹⁵⁾ have been pointed out for the distances larger than the core diameter, the more reliable information about the pair potential is obtained from the equation

$$\Phi(r) = -K_B T C(r). \quad (4)$$

Following this approach we have got $\Phi(r)$ for Al and Sn, Figs. 3 and 4, respectively. The numerical values obtained in this way for $\Phi(r)$ are given in Table I and 2. Applying a different method, namely, a linearized simultaneous equation method for the Born-Green equation, we have also plotted the potentials obtained for Al and Sn by Waseda and Suzuki⁵⁾ who used the structural data for these two metals from the x-ray measurements. However, they reported the numerical values only up to 4.4 \AA (Al) and 5.0 \AA (Sn). In this range, the agreement between the two results is quite good with respect to both the numerical values and the position of the maxima and minima. A characteristic feature of the results obtained in this way is the correlation between the r values for which $\Phi(r)$ vanishes and

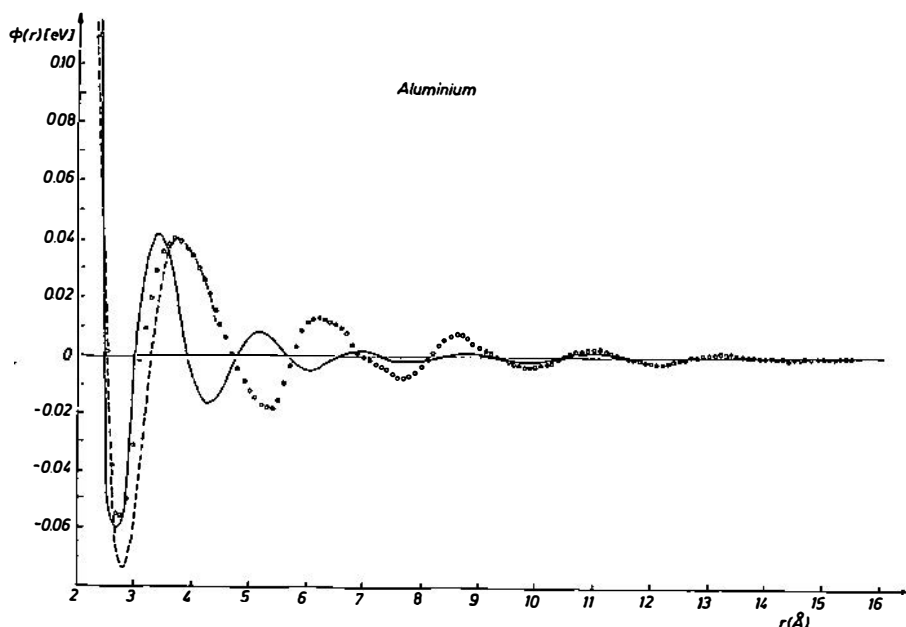


Fig. 3. Aluminium. The pair interaction potential $\Phi(r)$, calculated from the relation (4) ---, Waseda and Suzuki - - -, Schiff —.

those for which $g(r)$ is equal to unity. In other words, the structure of the pair correlation function is reflected in the shape of $\Phi(r)$.

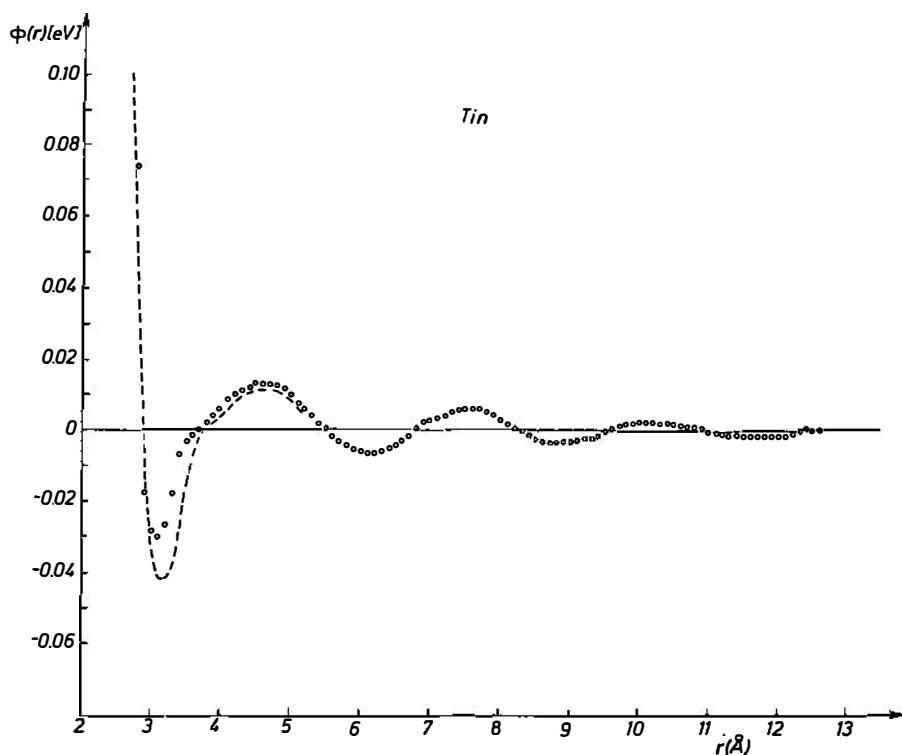


Fig. 4 Tin. The pair interaction potential $\Phi(r)$. ooo, calculated from the relation (4) ---, Waseda and Suzuki

TABLE 1
PAIR INTERACTION POTENTIAL IN LIQUID Al $\Phi(r) \cdot 10^2$ eV.

r [Å]	0.0	0.1	0.2	0.3	0.4
2					
3	-3.19	-0.10	0.97	2.01	2.97
4	3.44	3.13	2.68	2.11	1.54
5	-1.29	-1.51	-1.70	-1.85	-1.83
6	1.21	1.36	1.33	1.23	1.18
7	0.00	-0.11	-0.27	-0.46	-0.63
8	-0.41	-0.13	0.14	0.36	0.54
9	0.32	0.24	0.14	0.02	-0.09
10	-0.37	-0.31	-0.26	-0.19	-0.10
11	0.34	0.34	0.30	0.21	0.11
12	-0.20	-0.22	-0.21	-0.19	-0.16
13	0.13	0.17	0.16	0.15	0.12
14	-0.05	-0.07	-0.08	-0.08	-0.09

TABLE 1 (cont).

r [Å]	0.5	0.6	0.7	0.8	0.9
2	13.40	-3.82	-5.48	-5.66	-5.03
3	3.61	3.89	4.14	3.96	3.78
4	1.10	0.70	0.16	-0.46	-0.92
5	-1.54	-1.00	-0.32	0.33	0.85
6	1.17	1.06	0.78	0.43	0.16
7	-0.72	-0.77	-0.79	-0.76	-0.64
8	0.68	0.74	0.69	0.57	0.43
9	-0.18	-0.27	-0.35	-0.40	-0.40
10	0.02	0.14	0.21	0.26	0.29
11	0.04	0.00	-0.04	-0.10	-0.15
12	-0.13	-0.10	-0.06	-0.00	0.06
13	0.12	0.11	0.10	0.05	0.00
14	-0.10	-0.10	-0.09	-0.06	-0.05

TABLE 2
PAIR INTERACTION POTENTIAL IN LIQUID Sn $\Phi(r) \cdot 10^2$ eV.

r [Å]	0.0	0.1	0.2	0.3	0.4
2					
3	-2.91	-3.03	-2.69	-1.83	-0.77
4	0.55	0.85	0.99	1.04	1.16
5	0.92	0.71	0.55	0.37	0.14
6	-0.66	-0.68	-0.69	-0.66	-0.58
7	0.25	0.27	0.39	0.51	0.57
8	0.29	0.20	0.10	-0.02	-0.14
9	-0.36	-0.34	-0.28	-2.22	-0.15
10	0.24	0.26	0.26	0.25	0.24
11	-0.02	-0.06	-0.08	-0.10	-0.15
12	-0.15	-0.15	-0.09	-0.00	0.05
r [Å]	0.5	0.6	0.7	0.8	0.9
2				7.41	-1.89
3	-0.32	-0.02	-0.02	0.17	0.31
4	1.29	1.28	1.22	1.20	1.13
5	-0.07	-0.22	-0.36	-0.50	-0.61
6	-0.49	-0.38	-0.19	-0.05	0.21
7	0.58	0.61	0.62	0.53	0.40
8	-0.27	-0.36	-0.39	-0.38	-0.36
9	-0.07	0.05	0.14	0.17	0.20
10	0.22	0.19	0.16	0.12	0.06
11	-0.19	-0.20	-0.17	-0.14	-0.13
12	0.06	0.07			

Fig. 3 also shows the potential calculated on Al with a hard core $1/r^{12}$ used by Schiff¹⁶⁾ to fit the potential calculated by Pick¹⁷⁾ from the pseudopotential theory

$$V(r) = \varepsilon [(\cos 2 K_F r) / r^3] [A + B/r^2 + C/r^4] + [(\sin 2 K_F r) / r^4] (D + E/r^2) + F/r^{12}. \quad (5)$$

We have used $\varepsilon = 0.05$ eV and $\sigma = 2.5$ Å while the other parameters are given in¹⁵⁾. As it can be seen the agreement is good for the well depth of the potential, but the wavelength and the phase are not in agreement.

The comparison and the agreement with the results from the other methods are rather good and this approximation seems to be useful for the liquid metals.

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POTENCIJAL INTERAKCIJE U TEČNOM Al I Sn

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Sadržaj

Dobijen je potencijal interakcije između parova atoma u tečnom aluminijumu i kalaju merenjem statičkog strukturnog faktora metodom neutronske difrakcije. Izračunavanje potencijala se zasniva na aproksimaciji totalne korelacione funkcije.

Rezultati ukazuju da u tečnim metalima potencijal interakcije u velikoj meri zavisi od oblika parne korelacione funkcije.