

## INTERACTION POTENTIAL IN LIQUID METALS

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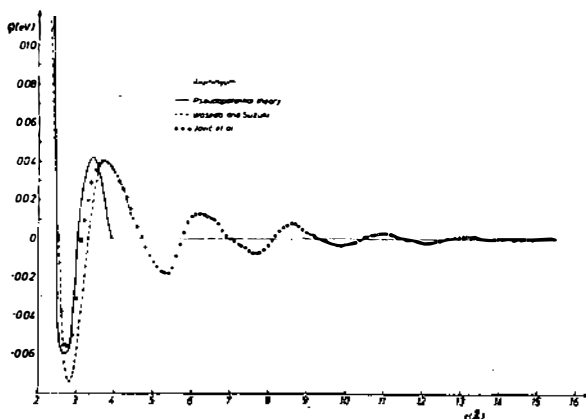
In the last decade, the numerous experimental and theoretical investigations have been devoted to the study of simple liquids, particularly to the liquid metals. The knowledge of a structure factor  $S(Q)$  over a wide momentum transfer range and a large interval of temperature provides the possibility to calculate the correlation functions.

The information about the structure and correlation functions could be useful for a better understanding of the nature and interatomic forces in liquid metals. One of the most important quantities which gives the information about the microscopic properties and the structure of a liquid metal is the atomic radial distribution function  $g(r)$ . If  $g(r)$  is known as a function of temperature, and the pair interaction potential can be calculated from the other sources, then all the equilibrium properties of the liquid metals can be obtained. On the other hand, the accurate knowledge of  $g(r)$ , especially of small distances, is important for the evaluation of the transport properties. The atomic radial distribution function can be obtained from the experimental structure factor data using the Fourier transform over the momentum transfer space<sup>1,2</sup>.

The another correlation function, which plays a very important role in the study of liquid metals, is a direct correlation function  $c(r)$  introduced by Ornstein-Zernike. This function includes the fact that the total correlation function between two atoms is a sum of a direct effect due to a pair of atoms and an indirect one from all the other atoms. The direct correlation function

$c(r)$  can be calculated from the experimental structure factor<sup>3)</sup>.

If we can define  $g(r)$  and  $c(r)$  from the experimental data, then we can try to obtain the interatomic potential directly using the approximate relations between the correlation functions and the potential by the existing Born-Green's and Percus-Yevick's theories of the liquid state. In order to obtain the interaction potential on liquid aluminium we used an approximation for  $v(r) = -k_B T c(r)$ . This offers a method of finding an asymptotic pair potential from the measured structure factor through the direct correlation function. The obtained potential is shown in Figure and



compared with the interaction potential for the liquid aluminium obtained from the pseudopotential theory<sup>4)</sup> and the Born-Green equation<sup>5)</sup>.

#### References

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