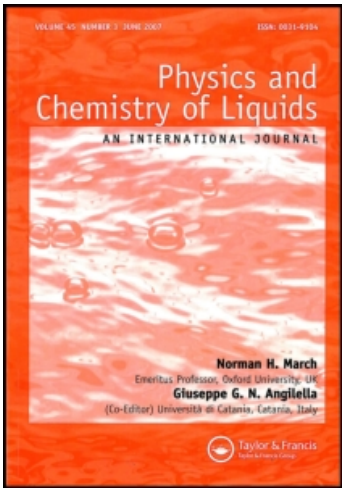

Physics and Chemistry of Liquids
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713646857

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To cite this Article El-daher, M. Sayem and Murphy, R. D.(2000) 'Influence of the Screening Function on Theoretical Calculations of the Structure Factor of Liquid Aluminum', Physics and Chemistry of Liquids, 38: 5, 599 — 606
To link to this Article: DOI: 10.1080/00319100008030306
URL: http://dx.doi.org/10.1080/00319100008030306

Phys. Chem. Liq., 2000, Vol. 38, pp. 599–606
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INFLUENCE OF THE SCREENING FUNCTION ON THEORETICAL CALCULATIONS OF THE STRUCTURE FACTOR OF LIQUID ALUMINUM

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(Received 9 September 1999)

The structure factor $S(k)$ of liquid aluminum is calculated using the Metropolis Monte Carlo method. The effective two-body ion–ion interaction used in the calculations are the Shaw optimized model and the local approximation suggested by Harrison calculated using two screening function in each case, the screening function of Vashishta and Singwi and that of Utsumi and Ichimaru. The calculated structure factors from each case are compared with experiment.

Keywords: Liquid aluminum; structure factor; Monte Carlo; screening function

I. INTRODUCTION

The purpose of this study is to compare the liquid structure factor resulting from Metropolis [1] Monte Carlo calculations using different form of the effective ion–ion interaction potentials. The pair potentials used in the current work are based on pseudopotential theory and given by

$$u(r) = \frac{(Z^*e)^2}{r}\left(1 - \frac{2}{\pi}\int_0^\infty F(q)\frac{\sin qr}{q}dq\right).$$

*Corresponding author.

Here $F(q)$, the energy-wavenumber characteristic, is calculated using the procedures suggested by Shaw [2] and implemented by Bretonnet [3], including effective mass and exchange correlation corrections or directly from the local approximation suggested by Harrison [4] with the screening function added in each of the previous cases. The screening functions studied here are the one suggested by Vashishta and Singwi [5] (VS) and the one suggested by Utsumi and Ichimaru [6] (UI). These two screening functions are used with the above two models in deriving four different pair potentials for liquid aluminum. The resulting pair potentials were used in a Monte Carlo routine in order to obtain the structure factor of liquid aluminum resulting from each case.

II. SCREENING FUNCTIONS

The VS screening function is derived by a self-consistent numerical calculation for the static pair correlation function, correlation energy, compressibility, and the plasmon dispersion relation for the electron liquid in the metallic-density range; it is tabulated [5] for many values of r_s (r_s is the Wigner-Sietz radius). The screening function UI is a fitting formula proposed to reproduce quantum Monte Carlo calculations of the correlation energy done by Ceperly and Alder [7] as well as microscopic theory and to satisfy self-consistency conditions in the compressibility sum rule.

III. COMPUTATION AND RESULTS

The radial distribution function $g(r)$ was calculated for a system of 4394 particle in a cubic box of a side L with the nearest-image periodic boundary convention. The computer calculations were performed at the melting temperature ($T = 667°C$) of liquid aluminum and the results

TABLE I Values of the parameters in the asymptotic fit to $g(r)$

Pair potential	c	$\alpha(A°)^{-1}$	$\gamma(A°)^{-1}$	$r_0(A°)$
Harrison-VS	0.70	0.12	2.6	4.895
Harrison-UI	0.59	0.11	2.6	4.895
Shaw-VS	0.5	0.12	2.6	4.895
Shaw-UI	0.59	0.09	2.6	4.895

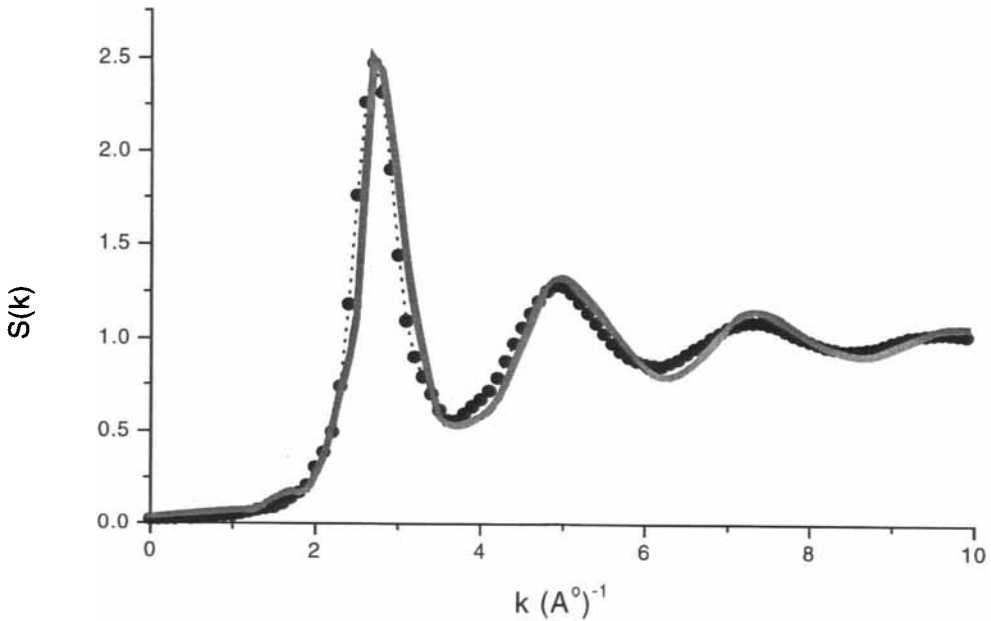

FIGURE 1 Structure factor resulting from Shaw-VS pair potential. Dotted line is the experimental data of Waseda.

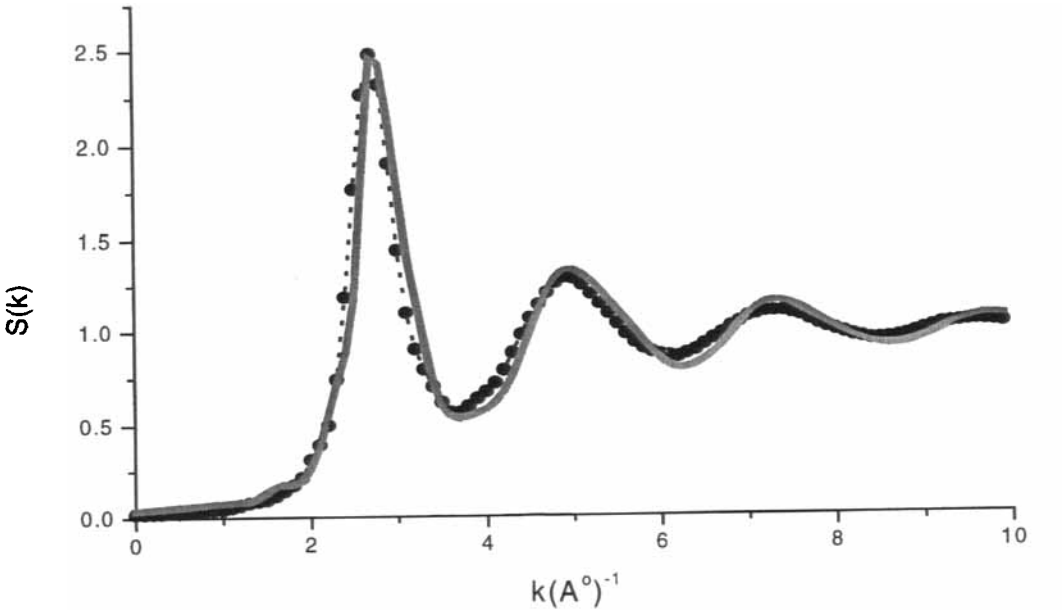

FIGURE 2 Structure factor resulting from Harrison-VS pair potential. Dotted line is the experimental data of Waseda.

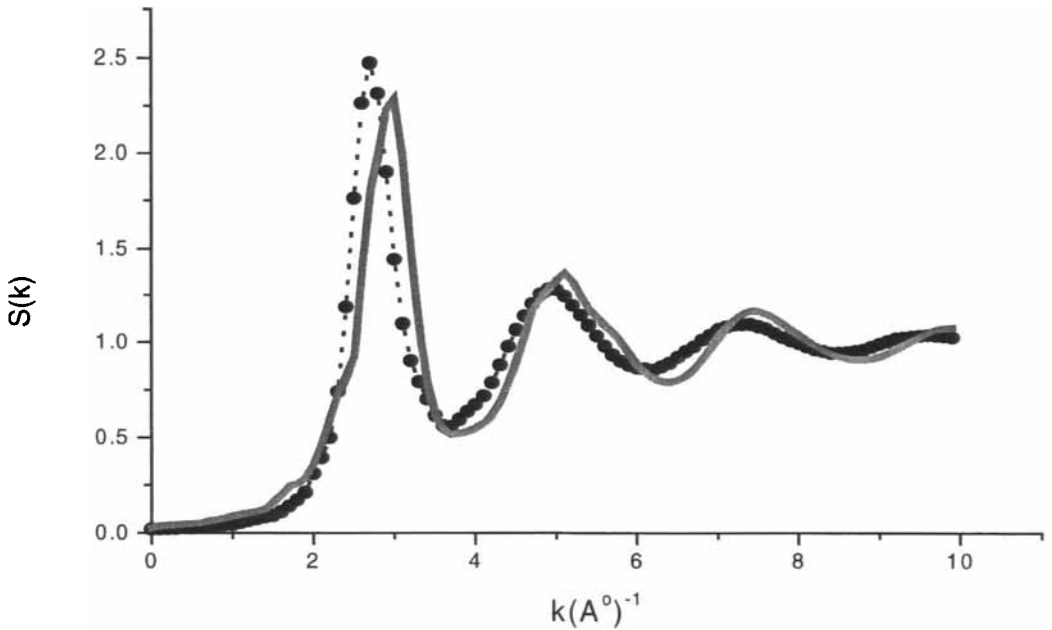

FIGURE 3 Structure factor resulting from Shaw-UI pair potential. Dotted line is the experimental data of Waseda.

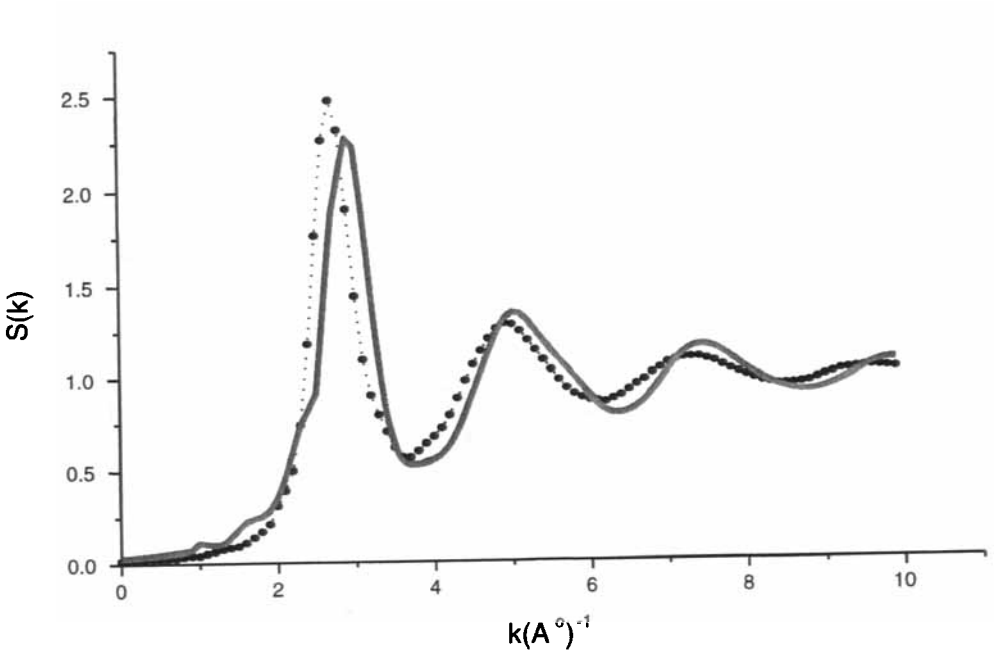

FIGURE 4 Structure factor resulting from Harrison-UI pair potential. Dotted line is the experimental data of Waseda.

compared with X-ray diffraction [8] results at the same temperature. After initial (equilibrating) calculations which eliminated any trace of the initial distribution of the particles, the radial distribution function was obtained for the region $0 < r < L/2$. In order to obtain the structure factor accurately we need to account for the asymptotic behavior of $g(r)$ for $r > L/2$. One way of doing so, used in previous work [9, 10], is to assume that $g(r)$ followed the asymptotic form

$$g(r) - 1 \rightarrow (c/r)\exp(-\alpha r)\cos[\gamma(r - r_0)]$$

The quantities c, α, γ and r_0 are chosen to fit the region $10\,\text{A}^\circ < r < 21\text{A}^\circ$ are listed in Table I. The calculated structure factors $S(k)$ for each case are given in Figures 1, 2, 3 and 4.

IV. CONCLUSION

The theoretical results of $S(k)$ were generally in good agreement with the experimental X-ray diffraction results. The results near $k = 0$ are satisfactory; oscillations noted in previous work [9, 10] were not present here because a larger system was used. The structure factor resulting from the pair potentials with the VS screening function gave significantly better agreement, especially at the main peak, which was tilted slightly forward in the case of the pair potential with the UI screening function. Overall the theoretical calculation of $S(k)$ is sensitive to the choice of the screening function especially at the main peak.

Acknowledgments

The authors would like to thank J. L. Bretonnet for kindly providing the ionic pair potential used in this work. MSE wishes to thank J. William Fulbright Foreign Scholarship for their support throughout the current work. Some of the computations were performed using computer hardware provided by a grant to RDM from the Air Force Office of Scientific Research.

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