Theoretical Calculations of Temperature Dependence of The Transport properties of Liquid Aluminum

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ABSTRACT

The transport properties i.e. electrical and thermal conductivities of liquid aluminum are calculated over a range of temperatures at and above melting point, 670, 750 and 1050 ^{o}C. The calculations carried out using the solutions of the Boltzmann equation, the structure factors obtained from Monte Carlo simulation, the form factor derived using the Dagen, Rasolt and Taylor (DRT) model potential and the screening function of Geldart and Taylor (GT). The calculated results compared with experimental values.

Key words: Liquid metal, Ziman formula, Boltzmann equation, thermal conductivity, electrical conductivity, Monte Carlo.

حساب خواص النقل الكهربائي والحراري للألمنيوم السائل بتابعية درجة الحرارة

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الملخص

قمنا بحساب الناقلية الكهربائية والحرارية للألمنيوم السائل عند درجة حرارة الانصهار وأعلى من الانصهار –أي عند الدرجات 670 و750 و1050 درجة مئوية. أُجريت الحسابات باستخدام حلول معادلة بولتزمان إذ تم الحصول على عامل البنية للالمنيوم بطريقة مونتي كارلو وحُسب عامل التشكيل باستخدام الكمون المقترح من قبل داجن وراسولت وتايلور وتابع الحجب المقترح من قبل جيلدرت وتايلور. وأُجريت مقارنة النتائج بالقيم التجريبية.

الكلمات المفتاحية: معادن سائلة، علاقة زايمن، معادلة بولتزمان، الناقلية الكهربائية، الناقلية الحرارية، مونتي كارلو.

Introduction

The solutions of the Boltzmann equation using the relaxation time approximation [1] gives the electrical resistivity as:

$$\rho = \frac{3\pi\Omega_0 m_e^{\,2}}{4e^2\hbar^3 k_f^6}\int_0^{2k_F}|W(q)|^2 S(q)q^3 dq \qquad (1)$$

Which is known as the Ziman formula [2]. Where $W(q)$ is the form factor, $S(q)$ is the static structure factor of the liquid and Ω_0 is the ionic volume, e and m_e are the charge and mass of the electron.

The thermal resistivity is given by:

$$\lambda = \frac{3\pi\Omega_0 m_e^{\,2}}{4e^2\hbar^3 k_f^6}\frac{1}{L_0 T}\left[\int_0^{2k_f}|W(q)|^2 q^3 S(q)dq + \frac{3\hbar^2 k_f^2}{2Mk_B T\pi^2}\int_0^{2k_f}|W(q)|^2 q^3 S(q)dq - \frac{\hbar^2 k_f^2}{Mk_B T\pi^2}\int_0^{2k_f}|W(q)|^2 q^5 S(q)dq\right] \qquad (2)$$

Where M is the ionic mass, the second and third terms in thermal resistivity equation give the inelastic part of the electron scattering, equation (2) is used in full in current work but if we neglect the second and the third terms in the last equation (which is justified for high temperatures) we will get the well known Wiedemann-Franz law.

The two components needed to carry out the calculations are the structure factor which can be obtained experimentally from x-ray or neutron diffraction experiments, and theoretically by solving the Integral equation of liquid structure [3], or by Monte Carlo and molecular dynamics simulation [4,5,6], and the form factor, which can be calculated based on a model potential and appropriate screening function. The goal of the current work is to calculate the electrical and thermal properties over a range of temperatures in the liquid state of aluminum and compare the results to the experimental values.

Many results are reported using the Ziman formula but mainly the calculations was carried out at melting point only, in the current work we carry out the calculations over a range of temperature above melting for liquid aluminum using theoretically calculated structure factor from Monte Carlo simulation.

Monte Carlo Simulation

We derived an effective potential based on the ab-initio model potential suggested by Dagens, Rasolt and Taylor [7] and the screening function of Geldart and Taylor [8] and used this potential in Metropolis Monte Carlo algorithm starting with an initial cubic cell with a side of 43 A° and a sample of 4394 atoms distributed on (BCC) positions, the MC code used generates new configuration few hundred times to eliminate any trace of the initial (BCC) distribution before starting to accumulate statistical data in 2000 loops -this was checked in an earlier published work (by the Author) and found satisfactory. The radial distribution function $g_{MC}(r)$ is obtained for ($r \leq 21.5\ A^{\circ}$). And the asymptotic behavior of g(r) was taken into account by adding its contribution analytically to the calculation of the structure factor S(k) which is calculated from the equation:

$$S(q) = 1 + n\int [g(r) - 1] e^{i\vec{q}\vec{r}}\, dr \qquad (3)$$

The integration in the equation (3) is a three dimensional Fourier transform and n is the number density, we carried this integration out using the Filon method [9] for integration, the results of Monte Carlo simulation is given in Fig. (1), (2) and (3) compared to the experimental data of Waseda[10].

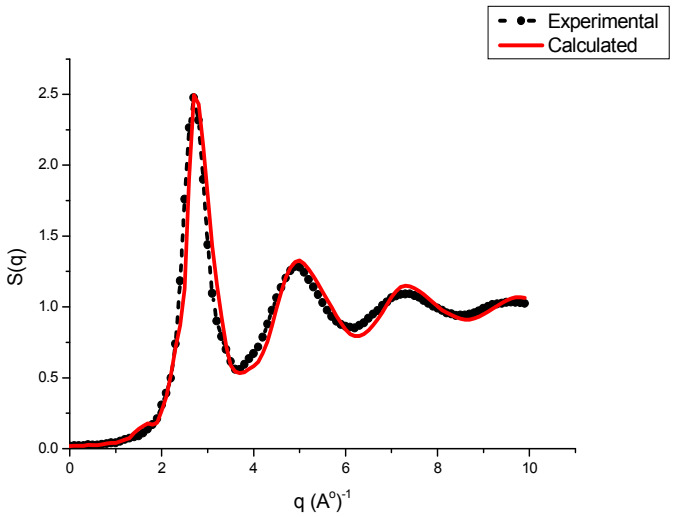

Fig (1) The calculated structure factor S(q) of aluminum at melting point Compared to experiment.

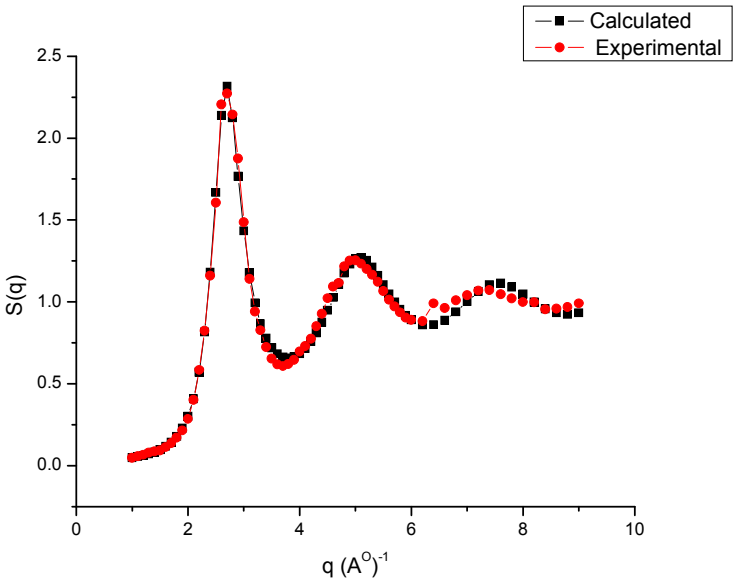

Fig (2) The calculated structure factor S(q) of aluminum at T=750°C Compared to experiment.

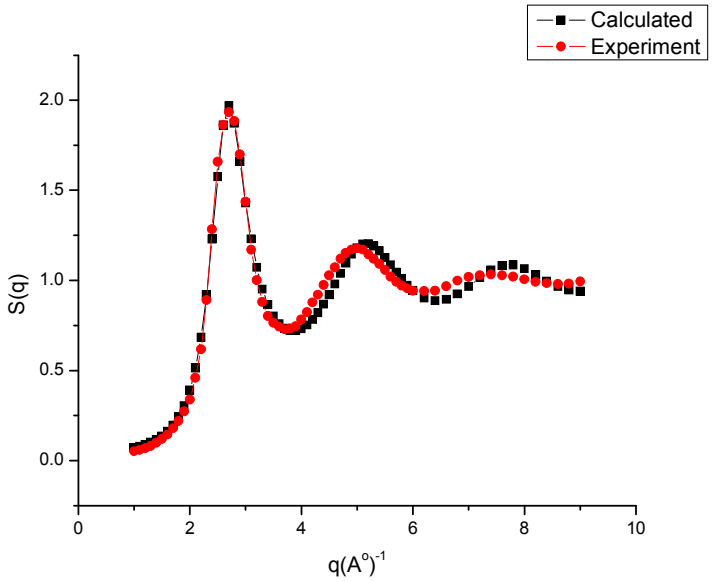

Fig (3) The calculated structure factor S(q) of aluminum at T=1050 °C Compared to experiment

The calculated structure factor agrees well with the experimental results obtained by X-ray diffraction in all three cases but there is a small shift in the third peak in the case of 750 ^{o}C and 1050 ^{o}C, which does not affect the transport properties calculations because only the first peak is included in the calculation as it is clear from the limits of the integration in the previous equations.

Application to Aluminum

The calculation of transport properties using equations (1) and (2) is carried out at the temperatures 670, 750 and 1050 ^{o}C, the corresponding ionic volumes and other temperature dependent parameters used in the calculations are given in Table I. where the density values used are those of Waseda [10].

Table I. Volume dependent parameters for Al

T C^{o}	**670**	**750**	**1050**
Density g/cm^{3}	2.37	2.35	2.27
Ω_0 au^{3}	127.78	128.78	133.10
lattice constant a $\overset{o}{A}$	4.231	4.242	4.289
Wave number k_f au^{-1}	0.8858	0.8833	0.8739
Fermi Energy E_f Ryd.	0.785	0.780	0.764

The structure factor used in the current work obtained from Monte Carlo simulation and the form factor derived using the DRT [7] model potential parameters and the screening function suggested by Geldart and Taylor [8]. These calculation require only the ionic volume given in table I., and the model potential parameters. We calculated the form factor and used it in equations (1) and (2) to obtain the electrical and thermal resistivities. The results are given in Table II. and compared with the electrical resistivity experimental results of [11].

Table II. Theoretical and experimental electrical resistivity and thermal conductivity for Al.

T C^o	670	750	1050
ρ_e 10^{-8} Ω m	23.72	24.69	28.13
$\rho_{exp.}$ 10^{-8} Ω m	24.2	25.5	29.8
Error %	1	3	5
κ $Wm^{-1}K^{-1}$	97.1	101.32	114.9
$\kappa_{exp.}$ $Wm^{-1}K^{-1}$	93.5	97.0	107.0
Error %	4	4.5	7

Theoretical calculations using Quantum Molecular dynamics code and the Kubo greenwood formula done by Knider and coworkers [12] at temperature 730 C^o gave electrical resistivity value (27.72) and after additional theoretical correction a value of (25.45), the methods used in reference [12] are far more demanding -from computational point of view- than the method adopted in the current work.

Discussion and Conclusion

The calculated results agree very well with the experimental values and close to other theoretical results [12] over the range of temperature studied. This is attributed in our opinion to the inclusion of the inelastic part of the electron scattering, the use of adequate screening function in the derivation of the form factor and the accuracy of the structure factor obtained from Monte Carlo simulation.

In conclusion we can say that the calculations of the transport properties of liquid aluminum obtained by using the form factor derived and using the DRT model potential and the screening function of Geldart and Taylor gives results in good agreement with experiment. However further studies needed to check the validity of the method used near critical point and the liquid vapor coexistence line.

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