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The Phonon Theory of Liquid Thermodynamics

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ABSTRACT: The phonon dispersion curves of some liquid metals, viz. Na (Z = 1), Mg (Z = 2), Al (Z = 3) and Pb (Z = 4), have been computed using our model potential. The charged hard sphere (CHS) reference system is applied to describe the structural information. Our model potential along with CHS reference system is capable of explaining the phonon dispersion relation for monovalent, divalent, trivalent and tetravalent liquid metals.

KEYWORDS. Pseudopotential; phonon dispersion curves.

I. INTRODUCTION

The attempts to study the phonon dispersion curves of liquid metals using the pseudopotential theory are very rare and not exhaustive [1–3]. Srivastava [1] and Gajjar *et al* [3] have reported the phonon dispersion of some simple liquid metals. It was found that the maximum deviation takes place in the vicinity of the first spherical Brillouin zone. This region lies nearly at half the distance of the first peak in the structure factor. Thus the choice of the structure factor also plays a vital role in the study of phonon dispersion curves of liquid metals. It was also observed that generally people have used the hard sphere reference system to describe the structural information, which is independent of the model potential. To describe the structural information we adopt here the charged hard sphere (CHS) reference system [4–7].

The present paper deals with the computation of the phonon dispersion curves of some liquid metals, viz. Na (Z = 1), Mg (Z = 2), Al (Z = 3) and Pb (Z = 4), with the aim to explore the application of our newly constructed form of the pseudopotential [4,5].

The choice of the pseudopotential form factor is certainly an important factor in the study of metallic properties and its actual form is much more sensitive to the choice of dielectric function of the electron gas. Hence, the purpose of the present paper is not only to generate the phonon dispersion curve, but also to see the influence of various local-field correction functions in the screening. So we incorporated three different forms of the exchange and correlation functions, viz. Hartree (H) [8], Taylor (T) [9] and Sarkar *et al* (SS) [10].

II. THEORY

To compute the phonon dispersion relations of liquid metals, the most frequently used approach of Hubbard and Beeby [11] is adopted. With the physical argument that the product of the static pair correlation function $g(r)$ and the second deriv-ative of the interatomic potential $\Phi(r)$ is peaked near the hard sphere diameter σ, Hubbard and Beeby [11] have derived the expression for the longitudinal phonon frequencies $\omega_L(q)$ and the transverse phonon frequencies $\omega_T(q)$ as [11,12],

Table 1. Parameters and constants used in present computation.

Metal	T (K)	$q_0/2k_F$	ρ (g/cm^3)	Z	η	k_F (Å^{-1})	r_c (Å)
Na	378	0.98	0.928	1	0.46	0.2509	0.7650
Mg	953	0.83	1.545	2	0.46	0.3675	0.6167
Al	943	0.76	2.370	3	0.45	0.4690	0.5278
Pb	613	0.84	10.66	4	0.46	0.4318	0.5186

his model potential is continuous in r-space and it is the modified version of the Ashcroft's empty core model. In comparison with Ashcroft's empty core model potential, we have introduced $(Ze^2/r)\exp(-r/r_c)$ as a repulsive part outside the core which vanishes faster than only Coulomb potential $(-Ze^2/r)$ as $r \to \infty$. Here, *Z, e, q* and r_c are the valency, electronic charge, wave vector and the parameter of the potential, respectively. In the present investigations, the parameter of the potential is determined by employing values of the wave vector, q_0, where the form factor takes first zero value, i.e. $W(q) = 0$ for $q = q_0$. For the present model potential, the condition is $q_0 r_c = 1.3439$ [5]. Therefore, the potential parameter r_c becomes $r_c = 1.3439/(q_0/2k_F)2k_F$. From these relations, one can easily evaluate the value of r_c by substituting the observed value of $(q_0/2k_F)$ [13].

III. RESULTS AND DISCUSSION

The constants and parameters used in the computations are tabulated in table 1. The computed phonon dispersions and structure factors are shown in figure 1 for liquid metals, viz. Na ($Z = 1$), Mg ($Z = 2$), Al ($Z = 3$) and Pb ($Z = 4$).

Here also it may be seen from figure 1 that the dispersion of the longitudinal phonon exhibits oscillatory behaviour extending to the large wave vector transfer region. But in the case of transverse phonon, the oscillatory behaviour seems quite insignificant for high *q* value. This indicates that the transverse phonon undergoes larger thermal modulation than the longitudinal phonon, which may be connected with the instability of transverse phonons in liquids. The $\omega \to q$ curves for trans-verse phonons attain maxima at a high *q* value than the longitudinal phonon curve. The influence of the exchange and correlated motion of electron through various local-field correction functions raises the phonon modes more than those due to sta-tic Hartree effect. The inclusion of local-field correction does not affect the position of the maxima, minima and the crossing of ω_L and ω_T modes, very significantly. The position of the first minimum roughly coincides with the first peak in the structure

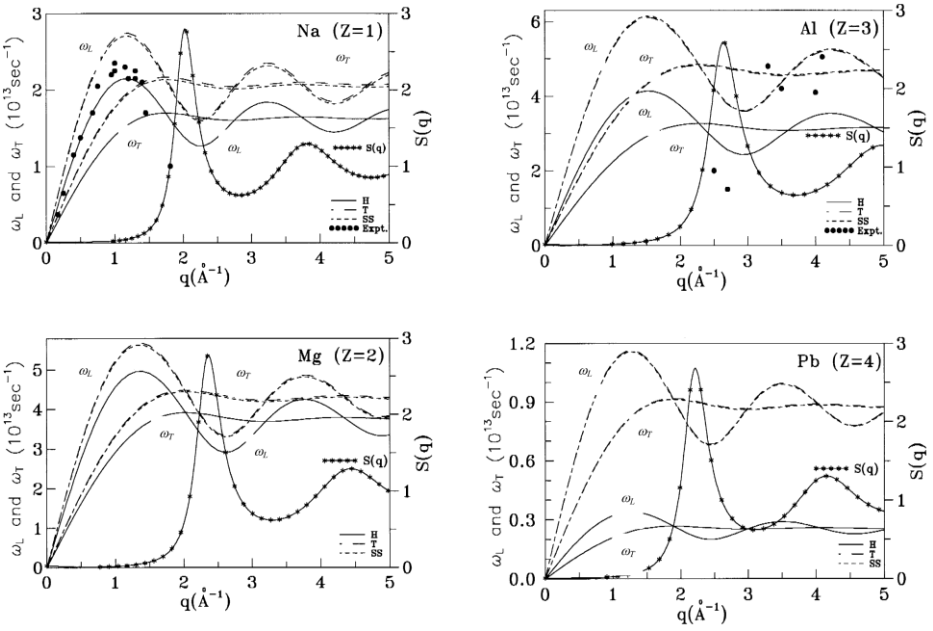

Figure 1. Phonon dispersion curves for liquid Na, Mg, Al and Pb.

factor of the respective systems. The computer simulations and analytical calcula-tions have demostrated that this minimum arises from a process analogous to the Umklapp scattering in the crystalline solids. This sharp first maximum in the static structure factor acts like a smeared-out reciprocal lattice vector. In our literature survey we have found experimental phonon frequencies only for liquid Na [14] and Al [15]. The comparison of the presently computed result for liquid Na with the experimental results [14] is highly encouraging. As the experimental results [15] for Al are only few in numbers, a conclusive comparison with the presently calculated results is not made. For Mg and Pb, the experimental results are not available but the behaviour of the present results does not show any abnormality. Thus, in the absence of experimental results such calculations may be considered as one of the guidelines for further theoretical or experimental investigations. This is very much essential for obtaining concrete conclusions. Finally, we conclude that our model potential [4,5] along with CHS reference system [4–7] is capable of explaining the phonon dispersion relation for liquid metals.

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REFERENCES

[1] S K Srivastava, *J. Phys. Chem. Solids* **36**, 993 (1975)
[2] S K Srivastava and Ram Dawar, *Ind. J. Pure Appl. Phys*. **31**, 520 (1993)
[3] P N Gajjar, B Y Thakore and A R Jani, *Acta Phys. Pol*. **A94**, 520 (1993)
[4] P B Thakor, P N Gajjar and A R Jani, *Indian J. Pure Appl. Phys.* **45**, 509 (2007)
[5] P B Thakor, P N Gajjar and A R Jani, *Commun. Phys.* **14**, 15 (2004)
[6] H B Singh and A Holz, *Phys. Rev.* **A28**, 1108 (1983)
[7] R V Gopal Rao and U Bandyopadhya, *Indian J. Phys.* **A65**, 286 (1991)
[8] W A Harrison, *Pseudopotential in the theory of metals* (W A Benjamine Pub. Co., New York, 1967)
[9] R Taylor, *J. Phys.* **F8**, 1699 (1978)
[10] A Sarkar, D Sen, S Haldar and D Roy, *Mod. Phys. Lett. (USA)* **B12**, 639 (1998)
[11] J Hubbard and L Beeby, *J. Phys.* **C2**, 556 (1969)
[12] B Y Thakore, P N Gajjar and A R Jani, *Bull. Mater. Sci.* **23**, 101 (2000)
[13] V Heine, M L Cohen and D Weaire, *Solid State Physics* (Academic Press, New York, 1970) Vol. 24
[14] W C Pilgrim, S Hosokawa, H Saggau, H Sinn and E Burkel, *J. Non-Cryst. Solids* **96**, 250 (1999)
[15] S J Cocking, *Adv. Phys.* **16**, 189 (1967)

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