LATTICE DYNAMICS OF METALS AND SOLIDIFIED NOBLE GASES

Jitendra Behari

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PREFACE

In the present work we have undertaken mainly the theoretical studies on the lattice dynamics of metals. Solidified noble gases have also been studied and are presented as supplementary to the main work. The investigations have been carried out under the following two heads:

1. Metals:

It is well known that the Cauchy relation ($C_{12} = C_{44}$) does not hold for metals, even approximately, and therefore, any model based on purely central forces will be inadequate. Born[1] considered the presence of ion-ion angular interaction to explain the lattice dynamics of diamond and the concept has been latter extended to the case of metals by Hendricks, Riser and Clark[2], Clark, Gazis and Wallis[3] and Yuen and Varshni[4]. However, these attempts to explain the lattice dynamics of metals met with limited success. This is not surprising because these authors have neglected an important aspect of interaction, namely, the electron ion interaction, which is quite significant for these solids.

In the above studies on metals two distinct trends have emerged to incorporate the presence of angular forces, one due to Clark, Gazis and Wallis[3] (on the lines of Born[1]) and the other that of de Launay[5]. The former is superior in the sense that it is invariant under rigid body rotation while the latter is not. We have used both of them in the present studies. The lattice dynamics of several bcc and fcc metals is studied on a modified angular force mo

where an account is also taken of the presence of conduction electrons (volume forces). The total interaction in metals is supposed to consist of central, angular (both between a pair of ions) and the volume forces. The last of these is alternately called as electron-ion interaction and is accounted through Sharma and Joshi model[6]. The detailed discussions of all these is postponed for the Chapter I.

In the second chapter the form of the modified secular determinant is set up, where the contribution due to all the three interactions is taken care of.

(i) Alkali Metals:

In the studies on alkali metals (lithium, sodium and potassium) we have restricted the central and angular forces to be operative upto second nearest neighbours only. Angular forces are included alternately through both the approaches of Clark, Gazis and Wallis[3] (CGW) and that of de Launay[5]. The scheme of inclusion of all the three types of interactions (as outlined above) is employed to calculate the phonon dispersion relations, phonon spectra, Debye Θ and the Debye-Waller factor of the three metals. A good agreement with the experimental data is obtained on either model. It has been further concluded that the two types of angular forces are equivalent as far as the calculations of their lattice dynamical properties are concerned.

(ii) Fcc Metals:

The cases of three noble metals, namely copper, silver

and gold have also been examined on both the angular forces, in a similar way as has been done for the bcc alkali metals. A good agreement with the experimental data is obtained in all the cases. For gold no neutron scattering results are available so far, therefore, analogy from copper and silver is pushed to assess its behaviour. We find nothing anamolous as far as gold is concerned. A good agreement of phonon dispersion curves for gold is also predicted.

The investigations are conducted by including both types of angular forces in turn and again we are led to conclude their equivalence for the calculated properties in question. No detailed results were available so far for these metals on any angular force model and de Launay[5] has long back sought the quantitative results to establishe their equivalence.

The results for multivalent metals, namely nickel and aluminium are also reported. Looking at the equivalence obtained above only CGW model is employed to study them.

(iii) Bcc Transition Metals:

A similar scheme (except that the central forces are considered to be effective upto third nearest neighbour only) is employed to study the cases of three bcc transition metals (alpha iron, molybdenum and tungsten). In view of the equivalence observed between the two angular force approaches, only one of them (de Launay's[5]) is employed in the studies of these metals. A calculation of various vibrational properties, yields good agreement with the experimental data.

A general conclusion that is drawn from the above studies is that the Cauchy discrepancy is not only because of the electron gas but also due to the ion-ion angular interaction, both the interactions being noncentral in character. It could be read as a revision in Fuchs hypothesis.

2. Solidified Noble Gases:

(i) Use of an Elastic Force Model:

The elastic force model is used in the studies of solidified noble gases too. Central forces of the type as considered by Leighton[7] are assumed to be operative upto second nearest neighbour only. A calculation of various lattice dynamical properties for solid neon[8], argon, krypton[9] and xenon show a very good agreement with the experimental data in almost all the cases.

(ii) Logarithmic Form for the Overlap Repulsion:

Born and Mayer proposed an exponential form $\left(\Phi(r)^{\text{Repulsive}} = a \exp\left(-\frac{r}{\rho}\right)\right.$ of potential for the exchange interaction between a pair of ions. Though it is quantum mechanically well established, it suffers from one disadvantage, for,

$$\Phi(r)^{\text{Repulsive}} = \text{Constant (not infinity) for } r = 0.$$

In order to improve the situation Prakash and Behari[10] suggested a logarithmic form for the said interaction: viz.,

$$\Phi(r)^{\text{Repulsive}} = A \log_e \left[1 + \left(\frac{B}{r}\right)^n\right],$$

where A, B and n are constants. This form of potential was

adopted for the first time to calculate the cohesive energy of the alkali halides. This has also eliminated the ionic radii dependence which are quite uncertain in the Be solids. A similar form of logarithmic function is applied in the studies of solidified noble gases also.

The total interaction is divided into two parts: first is the usual Van der Waals interaction term and the other (of logarithmic form), is adopted for the exchange force (overlap repulsion), The effect of zero point energy is also taken care of on the lines of Gupta and Dayal[11]. A calculation of cohesive energies for krypton and xenon show good agreement with the experimental data.

Detailed calculations of other properties, making use of this potential function are in progress.

The present work has resulted in the following publications:

1. Phonon Dispersion in Copper, J. Behari and B.B. Tripathi, Phys. Letters, 29A (1969) 313.

2. A Modified Angular Force Model in the Studies of Lattice Dynamics of Bcc Metals: An Application to Sodium, J. Behari and B.B. Tripathi, J. Phys. Soc. Japan, 28 (1970) 346.

3. Phonon Dispersion Relations in Noble Metals, J. Behari and B.B. Tripathi, J. Phys. C., 3 (1970) 659.

4. Frequency Spectra and Heat Capacities of Copper, Nickel and Aluminium, J. Behari and B.B. Tripathi, Aust. J. Phys., 23 (1970) 311.

5. Phonon Dispersion in Solidified Argon and Krypton with the Elastic Force Model, J. Behari and B.B.Tripathi, Lett. Nuovo Cim., 3 (1970) 381.

6. Crystal Dynamics of Light Weight Alkali Metals, B.B.Tripathi and J. Behari, J. Phys. C. (To be published).

7. A New Logarithmic Form of Potential in the Studies on Metals, J. Behari, Indian J. Phys. (To be published).

8. Angular Forces and the Lattice Dynamics of Fcc Metals, J. Behari and B.B. Tripathi (Communicated).

9. Lattice Dynamics of Some Bcc Transition Metals, J.Behari and B.B. Tripathi (Communicated).

10. Lattice Dynamics of Solidified Neon, J. Behari and B.B. Tripathi, Nuovo Cim., (To be published).

11. A New Logarithmic Form for the Exchange Interaction in Solidified Noble Gases (Under preparation).

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