

Crystal dynamics of solidified argon

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(Received 13 April 1973)

Usual van der Waal's forces and a logarithmic form for the repulsive interaction is assumed between a pair of atoms in the studies on solidified noble gases. Interactions are confined to the nearest neighbours only, where the effect of zero-point energy is also taken into account. Our earlier work on solidified krypton and xenon is extended to include argon also. A calculation is made for cohesive energy, phonon dispersion relations in the three symmetry directions and the Debye temperature. These results are found to be in fairly good agreement with the experimental data.

1. INTRODUCTION

Inert gas solids form an ideal subject of investigation from a theoretical point of view. It has become customary to assume a form of interatomic potential containing a number of parameters, provided it is consistent with the physics of the situation. Recently Behari (1972) adopted a simple logarithmic form for the overlap repulsion along with the usual van der Waal's interaction between a pair of atoms in the case of inert gas solids. The interaction was supposed to be effective upto the nearest neighbour only, when the effect of zero-point energy was also taken into account on the lines of Gupta & Dayal (1966). A number of lattice dynamical properties were studied relating to solidified krypton and xenon. A satisfactory agreement with the experimental data was found in most of the cases. In view of its earlier success it seems interesting to extend this work to include solidified argon, which also on many accounts approximates to an ideal situation in a solid.

2. INTERATOMIC POTENTIAL AND THE METHOD OF CALCULATION

The potential function can be written as

$$\Phi(r) = -\frac{C}{r^6} + A \log_e \left[1 + \left(\frac{B}{r} \right)^m \right], \quad \dots \quad (1)$$

where the symbols have their usual meaning as mentioned earlier (Behari 1972). The value of m is chosen to be equal to 14 on the basis of the conclusions derived

by Mason & Rice (1954). B is chosen to be equal to the ionic radii of the substance in question and the remaining two parameters (C and A) are determined by applying the conditions of crystal stability and the compressibility as discussed before (Behari 1972).

3. COMPARISON WITH THE EXPERIMENTAL RESULTS

The expression for cohesive energy is the same as mentioned before. Its value comes out to be -1.65 K cal/mole, in close agreement with the experimental data (-1.84 K cal/mole) (Pollack 1964).

The form of the secular determinant remains the same as mentioned earlier. It is solved for selected values of wave vectors in the first Brillouin zone to obtain phonon dispersion relations and the complete vibration spectra. The method of subdivision of the Brillouin zone and the consequent mode of calculation of specific heat is as discussed before (Behari 1972). Phonon dispersion curves are plotted in figure 1 along with the experimental results. The experimental plots are due to Batchelder *et al* (1970) and Egger *et al* (1968). It can be seen that our results are in fairly good agreement with these data.

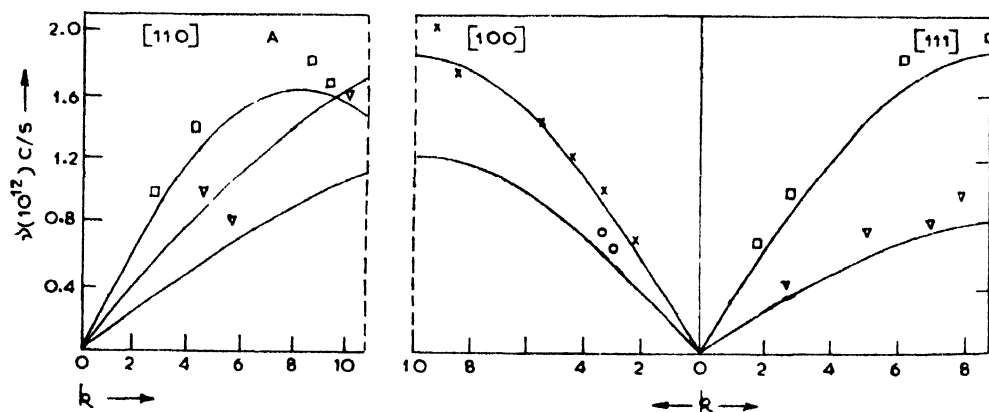


Fig. 1. Phonon dispersion in solidified argon. k is in units of $(1/10a)$.

[□, ○, ▽] Experimental points are as indicated on the graph.

$(\theta - T)$ curves are plotted in figure 2 along with the experimental results due to Peterson *et al* (1966). It can be assessed from this graph that within the limits of approximations involved in our theoretical analysis, our results compare favourably with the experimental findings.

It is thus inferred that the logarithmic form for the overlap repulsion in conjunction with the Van der Waal's forces is able to interpret well the lattice dynamical properties of solidified noble gases. Some disagreement between the theoretical and experimental results may be attributed to the neglect of distant neighbour interactions and the anharmonicity.

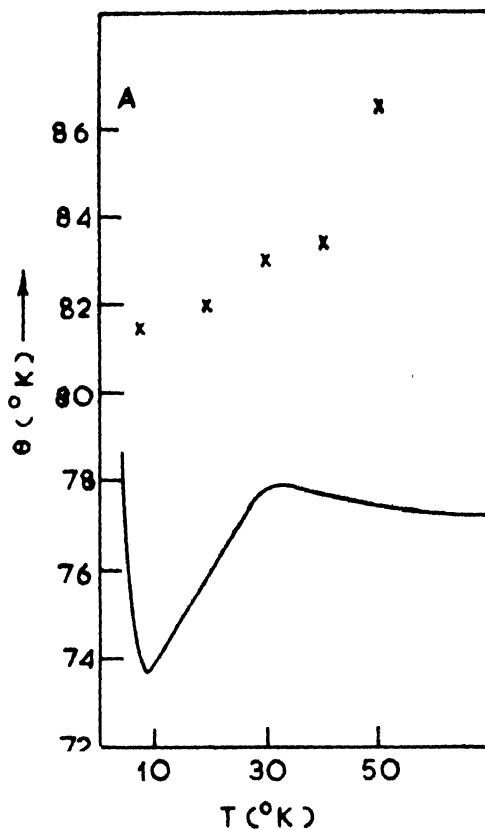


Fig. 2. ($\theta-T$) curve for solidified argon.
 x represent the experimental points.

ACKNOWLEDGMENT

The author is thankful to Dr. B. B. Tripathi for his valuable suggestions during the course of investigation. Financial assistance from CSIR is also thankfully acknowledged.

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