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LINDEMANN LAW FOR IDEAL SOLIDS

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Abstract—The applicability of the Lindemann law of melting is investigated for the simple solids like neon, argon, krypton, and xenon by lattice dynamics, and is found to hold good for the class. It is observed that the law is structure as well as interaction dependent, and holds separately for each class of solids having similar structure and interparticle interactions.

1. INTRODUCTION

ACCORDING to the Lindemann law [1], the melting temperature of a solid is attained when the root-mean square amplitude of its atomic vibration becomes a certain fraction of the nearest neighbour distance. It was also suggested that the fraction, the so called Lindemann parameter, might be the same for all solids. But Shapiro [2], on the basis of his lattice dynamical studies of a number of f.c.c. and b.c.c. metals, has concluded that the Lindemann parameter is structure dependent and has different values for different classes of solids.

Recently, Crawford and Daniels [3], van Witzenberg and Stryland [4], and Peterson *et al.* [5] have provided some such experimental data for solidified Argon. This substance belongs to that class of solids (rare-gas solids) which are known to be almost ideal [6]. It will therefore be interesting to test the validity of the law and to find the Lindemann parameter for the class of ideal solids.

2. LINDEMANN PARAMETER

The mean-square-amplitude of oscillation of a monatomic lattice in quasi-harmonic approximation at T °K is given as

$$\langle U^2 \rangle_T = \frac{1}{mN} \sum_{\mathbf{q},j} \frac{\varepsilon(\mathbf{q},j)}{\omega_j^2(\mathbf{q})}, \tag{1}$$

where m and N are respectively the mass and the number of atoms constituting the lattice, $\omega_j(\mathbf{q})$ is the angular phonon frequency corresponding to the wave vector $\mathbf{q}$ and the polarization j, and

$$\varepsilon(\mathbf{q},j) = [\langle n[\omega_j(\mathbf{q})] \rangle + \tfrac{1}{2}]\hbar\omega_j(\mathbf{q}), \tag{2}$$

is the average energy of the $(\mathbf{q},j)$ phonon mode. Here $\langle n[\omega_j(\mathbf{q})] \rangle$ stands for the Bose occupation number. Thus

$$\langle U^2 \rangle_T = \frac{\hbar}{2mN} \int_0^{\omega_{\max}} \operatorname{Coth}\left(\frac{\hbar\omega}{2kT}\right) \frac{g(\omega)}{\omega} \, d\omega, \tag{3}$$

and the Lindemann parameter

$$\delta = (\langle U^2 \rangle / r^2)^{\frac{1}{2}}_{T_m}, \tag{4}$$

where $r(=a\sqrt{2})$ is the nearest neighbour distance, and T_m is the melting temperature of the solid.

The phonon spectra $g(\omega)$ for the face-centred cubic solids Ne, Ar, Kr, and Xe have been computed by a quasi-harmonic central-force rigid atom model [7]. The model assumes weak long-range attractive and strong short-range repulsive interatomic forces derivable from two-body (exp, 6) potential function, and takes care of interactions up to fourth neighbours. It estimates zero-point energy and its volumes derivatives by Debye theory of specific heats, and includes them in the calculation by iteration. The Lindemann parameters "δ", so calculated, are presented in Table 1.

TABLE 1. LINDEMANN PARAMETERS FOR IDEAL SOLIDS

Solids	T_m (°K)	$a_{T_m} \times 10^8$ (cm)	$U_T^2 \times 10^{16}$ (cm^2)	δ
Neon	24·6	4·537	0·1844	0·1338
Argon	83·8	5·468	0·1928	0·1136
Krypton	115·8	5·817	0·2041	0·1097
Xenon	161·4	6·353	0·1891	0·0968

All experimental data including the melting temperature (T_m), and the lattice parameters (a_{T_m}) have been taken from [12].

3. DISCUSSION

The values of the parameters "δ" show a small scatter, and cluster about 0·1134. The δ's for Argon, Krypton, and Xenon are almost the same as the cluster value of the group. However, δ (Ne) "0·1334" is a little larger than any of these including the cluster value, but it cannot be taken as the refutation of the Lindemann theory, since Neon lies very close to Helium in the periodic table and its properties are intermediate between solid helium and other heavier rare gas solids of this group. It is well known [8] that the interaction in the case of helium is of different type and quantum effects are predominant. It is, therefore, expected [9] that δ (Ne) calculated taking all quantum effects into account will be close enough to the cluster value (0·1134) of the group. As far as this value of the average Lindemann parameter is concerned no standard is claimed keeping in regard the accuracy of the experimental data used and the simplicity of the Lattice dynamical model employed for its computation. However, it is not very much different from the ones already determined by earlier workers [3, 5, 10, 11].

It is interesting to compare this cluster value (0·1134) of the Lindemann parameter of f.c.c. rare-gas solids with that (0·0710) of another group of f.c.c. metals (Al, Cu, Ag, Au, Pb, and Ni) determined by Shapiro [2] using a force-constant model. The difference in the two values is sufficiently large, and is quite inconsistent with the conclusion of Shapiro [2], according to whom all f.c.c. solids must have the same Lindemann parameter. The author is of the view that the large difference in the values of the δ's of the two groups of f.c.c. solids is due to the difference in the nature of interactions present in them.

It may, therefore, be concluded that the Lindemann law is not only structure dependent, as inferred by Shapiro [2], but is also interaction dependent; and holds separately for each class of solids having similar structure as well as interparticle interactions.

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Абстракт—На основе динамики решеток, исследуется применимость закона плавления Линдеманна для простых твердых тел, как неон, аргон, криптон и ксенон. Определяется что этот закон надлежашми образом имеет силу для этого класса. Наблюдается что закон зависит как от структуры так и от взаимодействия. Он является применимым отдельно для кажого класса твердых тел, имеющих подобную структуру и междучастичные взаимодействия.