Short Communications

Aust. J. Phys., 1974, **27**, 129–30

Melting Criterion for Cubic Metals Based on a Modified Angular Force Model

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Abstract

A modified angular force model for the lattice dynamics of metals is used to test Lindemann's melting criterion by computing the ratio γ_m of the mean square amplitude of thermal vibrations to the square of the interatomic spacing at the melting point for a number of cubic metals belonging to different groups in the periodic table.

Lindemann (1910) suggested that the melting temperature of a material is attained when the mean square amplitude of thermal vibrations reaches a certain fraction of the square of the interatomic spacing. This fraction γ_m, the so-called Lindemann's parameter, is presumed to be the same for all monatomic solids, but in fact it is found to vary considerably when a simple Debye model is applied to solids. In this note, we report the results of using the modified noncentral force model described by Behari and Tripathi (1969).

The ratio γ of the mean square amplitude of thermal vibration $\langle \delta R_i^2 \rangle$ and the square of the interatomic spacing R_0 can be written (Pines 1963) in terms of the average energy of the phonon in the mode $(\boldsymbol{q},j)$. The summation over $\boldsymbol{q}$ may be replaced by an integration over allowed values of $\boldsymbol{q}$ within the first Brillouin zone. In the present work the integration was performed numerically using a modified Houston spherical six-term integration procedure, as elaborated by Betts *et al.* (1956). This method gives proper weight to each reciprocal lattice point and is inherently preferable to the sampling technique which relies merely on taking a very large number of points in the reciprocal space. The six directions used in the calculations were [100], [110], [111], [210], [211] and [221].

The calculated values of γ_m for a number of metals crystallizing in a cubic system are presented in Table 1, together with the numerical values of the elastic constants and other relevant parameters used in the computations. It is seen that although γ_m has roughly the same value for elements belonging to one particular group in the periodic table there is a wide variation in γ_m from one group to another. Alkali metals exhibit the maximum r.m.s. amplitude while the smallest value is for the transition metal chromium of group VIB. This variation is consistent with the nature of binding in metals.

The results of this study suggest that the Lindemann hypothesis of a constant γ_m for all solids is not adequate. Too much reliance should not be placed therefore on values of the Debye temperature Θ_D derived from the Lindemann melting criterion.

Table 1. Values of γ_m for cubic metals

Cubic metal	Table group	T_m (K)	Lattice param. (Å)	Elastic constants* c_{11}	c_{12}	c_{44}	Reference†	Ratio γ_m
Li	IA	452·0	3·500	1·481	1·248	1·077	1	0·0282
Na	IA	370·0	4·240	0·808	0·664	0·586	2	0·0234
K	IA	337·0	5·344	0·457	0·374	0·263	3	0·0217
Cu	IB	1356·0	3·616	16·840	12·140	7·540	4	0·0140
Ag	IB	1233·0	4·080	12·400	9·340	4·610	4	0·0124
Au	IB	1336·0	4·070	18·600	15·700	4·200	4	0·0151
Al	IIIA	932·0	4·050	10·732	6·094	2·832	5	0·0124
Pb	IVA	600·0	4·940	4·950	4·230	1·490	6	0·0097
V	VB	1983·0	3·028	22·795	11·870	4·255	7	0·0184
Nb	VB	2773·0	3·301	23·500	12·100	2·820	8	0·0218
Ta	VB	3269·0	3·303	26·100	15·740	8·180	9	0·0176
Cr	VIB	1890·0	2·880	35·00	6·780	10·080	10	0·0080
Mo	VIB	2900·0	3·141	44·080	17·240	12·160	9	0·0082
W	VIB	3660·0	3·160	50·100	19·800	15·140	11	0·0084
Fe	VIII	1808·0	2·866	23·350	13·550	11·800	12	0·0108
Ni	VIII	1723·0	3·524	24·600	15·000	12·200	13	0·0114

* In units of 10^{11} dyn cm^{-2} (10^{10} Pa).

† References to crystal data: 1, Nash and Smith (1959); 2, Sharma and Joshi (1963); 3, Bender (1939); 4, Huntington (1958); 5, Schmunk and Smith (1959); 6, Waldorf and Alers (1962); 7, Alers (1960); 8, Wasilewski (1965); 9, Featherston and Neighbours (1963); 10, Bolef and De Klerk (1963); 11, Wright (1930); 12, Rayne and Chandrasekhar (1961); 13, De Klerk (1959).

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Manuscript received 26 April 1973, revised 13 September 1973