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LETTER TO THE EDITOR

Extrapolated values of lattice constants of some cubic metals at absolute zero

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Abstract. The equation $a_T = a_0 \exp(CE_T)$ where a_T is the lattice constant of a cubic metal at T K, C is a constant and $E_T = \int_0^T C_V(T)\mathrm{d}T$ where $C_V(T)$ is the atomic heat of the metal at T K and constant volume was observed by Mitra and Mitra to yield the value of a_0, the lattice constant at absolute zero, for copper, and has since been confirmed by Kroeger. In the present work, the same formula has been used to extrapolate the value of a_0 for some cubic elements. These values of a_0 have been compared with experimental measurements of a_0 for these metals at temperatures very close to 0 K and the agreement between these two sets of observations is found to be excellent. This gives us a method for predicting a_0 from measurements at relatively high temperature.

Mitra and Mitra (1963), using their own x-ray diffraction data for spectroscopically pure copper in the temperature range 300–800 K and the macroscopic interferometric data for the same metal in the temperature range 80 to 800 K due to Nix and Macnair (1941), showed that for this entire temperature range, the relation

$$a_T = a_0 \exp[CE_T] \tag{1}$$

remains valid. Here

a_T is the lattice constant at T K

a_0 and C are constants for the sample under study,

and

$$E_T = \int_0^T C_V(T)\,\mathrm{d}T \tag{2}$$

where C_V is the atomic heat of the metal at constant volume and at T K. a_0 and C are obtained from intercept and slope respectively of the plot of ln a_T against E_T for the metal under study. From equation (2), at $T = 0$ K, $E_T = 0$ and if equation (1) is valid up to 0 K, $a_0 = a_T$ at 0 K has the significance of being the lattice constant of the metal at absolute zero. The value of lattice constant at absolute zero for copper is 3.6024 Å as predicted by Mitra and Mitra (1963). From the data of Kroeger (1977) we get a_0 for copper to be 3.6029 Å. Both these data are shown in table 1. This agreement is excellent.

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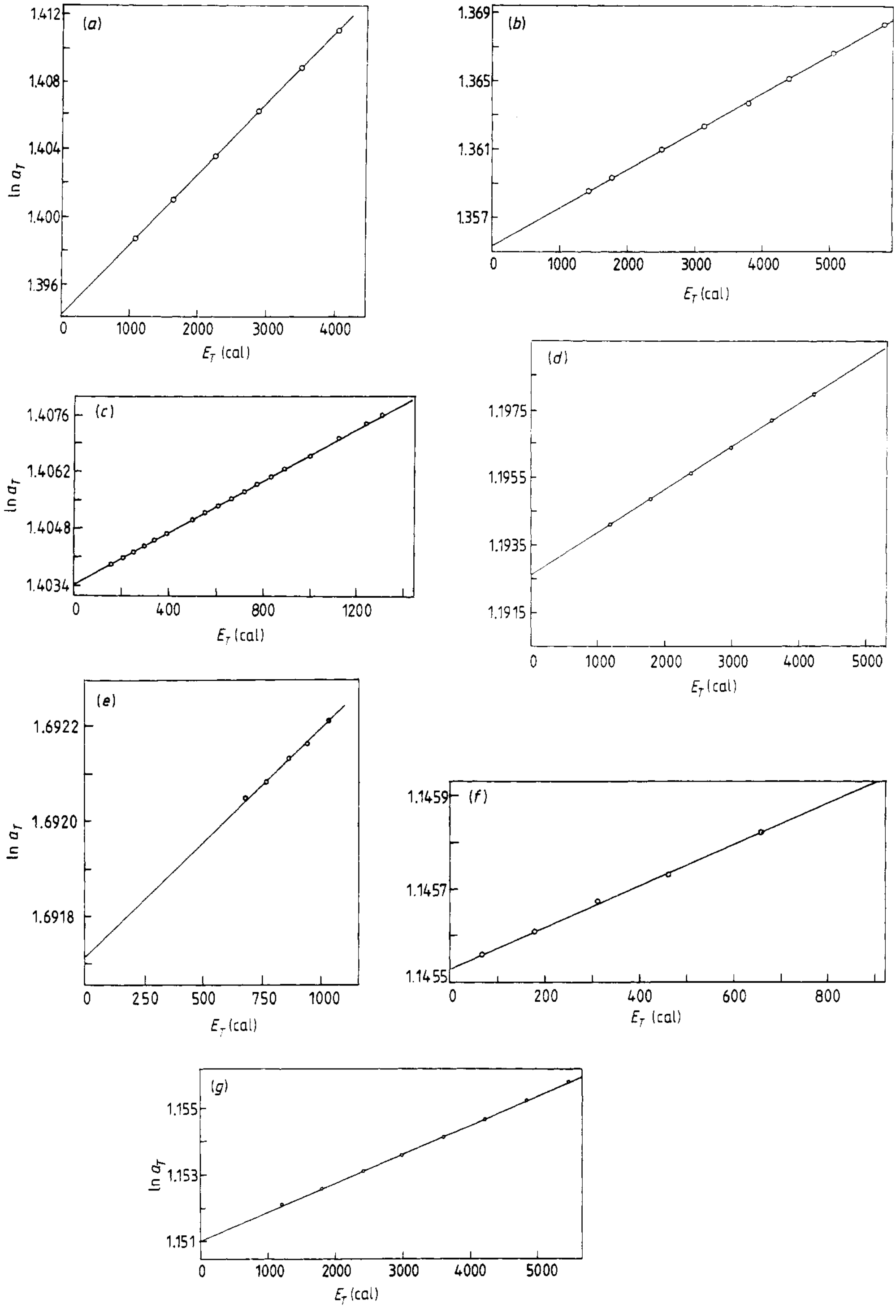

Figure 1. Plots of ln a_T against E_T for (*a*) aluminium ($a_0 = 4.0317$ Å), (*b*) palladium ($a_0 = 3.8779$ Å), (*c*) silver ($a_0 = 4.0690$ Å), (*d*) niobium ($a_0 = 3.3027$ Å) (*e*) silicon ($a_0 = 5.4289$ Å), (*f*) molybdenum ($a_0 = 3.1441$ Å), (*g*) tungsten ($a_0 = 3.1613$ Å).

Table 1. Values of lattice constants of cubic metals at absolute zero.

	Values of lattice constant in Å.			
Metals	Extrapolated	Reference to date for drawing $\ln a_T - E_T$ curve†	Reported	Reference
Al	4.0317	a	4.0318	b
			4.0315	c
Pd	3.8779	d	3.8782	e
Ag	4.0690	f	4.0695	b
Nb	3.3022	g	3.3027	h
Si	5.4289	i	5.4293	j
Mo	3.1441	f	3.1441	b
W	3.1613	d	3.1618	f
Cu	3.6024	k	3.6029	l

† Values of C_v for above metals at different temperatures have been taken from Hultgren *et al* (1963). From these values E_T at different T have been calculated.

[a] Our data
[b] Straumanis and Woodward (1971)
[c] Bandopadhyay and Gupta (1978)
[d] Dutt and Dayal (1963)
[e] King and Manchester (1978)
[f] Nix and Macnair (1942)
[g] Vasyutinskii *et al* (1966)
[h] Roberge (1975)
[i] Straumanis and Aka (1952)
[j] Batchelder and Simmons (1964)
[k] Mitra and Mitra (1963)
[l] Kroeger (1977)

This led us to investigate whether for other cubic metals, for which the lattice constants at temperatures very near to absolute zero has been determined experimentally, equation (1) can predict accurately the value of a_0. Figure 1 shows the plots of $\ln a_T$ against E_T for eight metals and table 1 shows the value of a_0 obtained from these plots and of lattice constants for the respective metals at temperatures very near to absolute zero as measured by various workers. The observations confirm that equation (1) is valid at all temperatures between absolute zero and relatively high temperatures and the linear plot of $\ln a_T$ againat E_T yields values of a_0 which are the lattice constants of the metals at absolute zero. The importance of this work is that it enables one to predict a_0 from experimental observation of a_T at relatively high value of T. Details of this work is to be published soon.

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