Table 4

Average values of K_T' for b.c.c. transition metals as derived from equation (1) using the shock wave data [14-15]

Metals	Molar volume, cm^3	K_T'
Ta	10.8	4.10
Nb	10.8	3.90
W	9.6	4.18
Mo	9.4	4.32
V	8.4	4.00

general trend is for K_T' to increase with decreasing Ω_o. The data points of most of the f.c.c. and h.c.p. metals fall within $\pm$ 10 per cent of the straight line shown in Figure 1. Exceptions are Ag and Au, which are discussed later, and Ru. Recent work at the University of Hawaii indicates that the ultrasonic value of K_T' is subject to reexamination. Our analysis of the Ru high pressure x-ray data [9] gives $K_T' = 4.7 \pm 2.2$, which is more consistent with the other data, but is still poorly determined.

The general relation between K_T' and Ω_o shown in Figure 1 can be understood from a relatively simple model originally proposed by Mott and Jones [20] for the bulk modulus of metals. This model considers two contributions to K_T:

$$K_T = K_F + K_{SR} \tag{4}$$

where K_F is due to the volume dependence of the Fermi energy of the free electrons, and K_{SR} represents a short-range repulsive interaction between ion cores.

We assume a free electron gas model for the Fermi contribution. The bulk modulus of the electron gas is

$$K_F = \frac{2}{3}\frac{E_F}{\Omega_o} Z^* \tag{5}$$

where Z^* is the effective number of free electrons per atom, and E_F is the Fermi energy which is proportional to $\Omega_o^{-2/3}$. Differentiating (5) with respect to pressure we get

$$K_F' = \frac{dK_F}{dP} = \frac{5K_F}{3K_T} \quad . \tag{6}$$

The short-range repulsive energy is assumed to be given by a Born-Mayer potential of the form

$$W(r) = A \exp[-B(r/r_0 - 1)] \tag{7}$$

where A and B are material parameters and r is the interatomic separation. Fuchs [21] considered a central force model for the f.c.c. structure and found the short-range contribution to K to be

$$K_{SR} = \frac{2r^2}{3\Omega_o}\frac{d^2W(r)}{dr^2} \tag{8}$$

when only nearest neighbor interactions are taken into account. Since an atom has twelve nearest neighbors in both h.c.p. and f.c.c. structures, (8) should be a reasonable approximation for the h.c.p. metals also. Now (7) and (8) can be combined to give

$$K_{SR} = \frac{2B^2A}{3\Omega_o} \tag{9}$$

and further differentiation with respect to pressure yields

$$K_{SR}' = \frac{dK_{SR}}{dP} = \frac{K_{SR}}{3K_T}(B+1) \tag{10}$$

Using (4), (6), (10), and the pressure derivative of (4) we find

$$K_T' = \frac{5}{3} + \frac{K_{SR}}{K_T}\left(\frac{B-4}{3}\right) \quad . \tag{11}$$

Equation (11) predicts that for very large Ω_o (when $K_{SR} \sim 0$), $K_T' \to 5/3$. The straight line in Figure 1 was in fact obtained by fixing the intercept at 5/3 and using the well defined cluster of rare earths (Gd, Dy, and Er) to determine the slope. The good agreement over the large range of Ω_o values indicates that K_T' is linear in Ω_o^{-1} and hence, from (11), and assuming B is roughly constant (a reasonable assumption), K_{SR}/K_T is approximately proportional to Ω_o^{-1}. At higher Ω_o^{-1}, $K_{SR} \sim K_T$, and we might expect K_T' to level off and become less dependent on Ω_o. It may be noted here that a linear $K_T' - \Omega_o^{-1}$ relationship is probably the simplest that is consistent with the data for close-packed metals, and it does not seem that a more sophisticated formula would be justified.

In case of Au and Ag, the anisotropy in the Fermi surface may affect the K_F term and thus produce a deviation from the first term (5/3) in equation (11). Such a conclusion is consistent with the calculation of Hsieh and Bolsaitis [22].

Referring again to Figure 1, we find that the b.c.c. transition metals Ta, Nb, W, Mo, and V fall in a cluster of points below the straight line. The relatively small variation among the K_T' values (3.90-4.32) is in contrast to the large range in the K_T' values (3.23-6.66) for the close-packed structures. This is not unexpected in view of the relatively greater influence of the electronic band structure on the elastic moduli for the b.c.c. metals [23]. Note also that the short range contribution must be