



FIG. 3. The temperature dependence of elastic constants of MgCu<sub>2</sub>.

Table 1. The adiabatic elastic constants of MgAg (in units of 10<sup>12</sup> dyn/cm<sup>2</sup>)

T(°K)	C <sub>11</sub>	C <sub>12</sub>	C <sub>44</sub>
80	0.865	0.579	0.520
100	0.863	0.578	0.517
150	0.859	0.575	0.511
200	0.855	0.572	0.504
250	0.851	0.570	0.496
300	0.846	0.567	0.485
350	0.839	0.560	0.474
400	0.831	0.553	0.464
450	0.816	0.540	0.452
500	0.798	0.524	0.438

stronger in the isostructural phases, ordered CuZn<sup>(5)</sup> and cubic AuCd<sup>(6)</sup>. The anisotropy factor also increases from MgAg (~3.5) to CuZn (~8) to AuCd (~12). This is understandable from the viewpoint that the ion-ion distance in MgAg is quite large compared to that in CuZn or AuCd. Therefore, we expect that the contribution arising from a short-range repulsion term is less in the case of MgAg, and its anisotropy should be also less pronounced. The absence of phase transformation in MgAg may well be attributed to its relatively low anisotropy. The recently reported

Table 2. The adiabatic elastic constants of MgCu<sub>2</sub> (in units of 10<sup>12</sup> dyn/cm<sup>2</sup>)

T(°K)	C <sub>11</sub>	C <sub>12</sub>	C <sub>44</sub>
80	1.250	0.717	0.423
100	1.249	0.717	0.422
150	1.243	0.714	0.420
200	1.239	0.712	0.418
250	1.232	0.709	0.415
300	1.228	0.706	0.412
350	1.214	0.697	0.407
400	1.200	0.690	0.402
450	1.185	0.681	0.396
500	1.171	0.675	0.391

elastic data on NiAl,<sup>(7)</sup> given its  $C/C' = 3.28$  at room temperature, also support the above postulation.

Theoretical calculations of elastic constants of b.c.c. metals are due to FUCHS, ZENER, JONES and ISENBERG<sup>(8-11)</sup>. Following FUCHS and ISENBERG<sup>(8,11)</sup> we may divide the crystal energy into a number of terms as:

$$W = W_0 + W_F + (W_E - W_S) + W_I.$$

Here,  $W_0$  is the energy of the lowest  $S$  state,  $W_F$  is the Fermi energy,  $W_E$  is the electrostatic energy,  $W_S$  is the self-energy of a Wigner-Seitz sphere, and  $W_I$  is the overlap energy between neighboring ions. From the values of measured elastic constants, the lattice spacing and an assumed effective charge of  $\sqrt{2}$ , we may estimate at least semi-quantitatively, the separate contributions to the three physically meaningful shear and bulk moduli,  $C$ ,  $C'$ , and  $B$ . According to ISENBERG's scheme,<sup>(11)</sup>  $W_0$ ,  $W_F$  and  $W_S$  are nearly functions of volume only, and therefore have no contribution to  $C$  and  $C'$ . While under condition of hydrostatic compression,  $(W_E - W_S) \approx 0$ , the contribution of this term to  $B$  is negligible. The results of the calculation are presented in Table 3. To  $C'$ , the contribution of the nearest neighbors turns out to be slightly negative. Therefore, the stability of the MgAg crystal is apparently dominated by the next nearest neighbor interaction, a condition already known to exist in the CuZn crystal.

The results for MgCu<sub>2</sub>, with twenty-four atoms per unit cell and supposed to be a space-filling compound, indicate that it is fairly isotropic. In

Table 3. contributions to the elastic constants of MgAg in units of  $10^{12}$  dyn/cm<sup>2</sup>

Contributions from	C	C'	B
$W_E - W_S$	0.29	0.04	—
$W_0 + W_F$	—	—	0.32
$W_1$ Nearest neighbors	0.23	-0.046	0.26
Next nearest neighbors	<0.01	0.145	0.10
Total	0.52	0.14	0.68

fact, another Laves phase compound of hexagonal structure, CaMg<sub>2</sub>, whose elastic constants have been reported,<sup>(12)</sup> is also isotropic. The mechanical behaviors<sup>(13)</sup> and elastic properties of MgCu<sub>2</sub> are very similar to those of the diamond-structure elements. This may be due to the fact that they belong to the same space group  $O_h^7 - Fd\bar{3}m$ . A comparison between the elastic properties of MgCu<sub>2</sub> and those of the three IVa elements<sup>(14)</sup> is shown in Table 4. All the numbers in this table are supposed to be unity if any of the idealized conditions are obeyed. BORN's relation<sup>(14)</sup> is based on a two-force-constant model for crystals with a diamond lattice, taking into account only the forces between nearest neighbors. Harrison's

relation is also based on a two-force-constant model but implicitly introduces the second nearest neighbor interaction.<sup>(14)</sup> The fact that the elastic constants of MgCu<sub>2</sub> fit Harrison's relation perfectly, and better than those of the diamond structures, is very interesting, if an extension of his formulation to the cubic Laves phase is justified.

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Table 4. A comparison of MgCu<sub>2</sub> with the diamond structure elements

Crystal	Anisotropy	Born's relation	Harrison's relation
	$\frac{2C_{44}}{C_{11} - C_{12}}$	$\frac{4C_{11}(C_{11} - C_{44})}{(C_{11} + C_{12})^2}$	$\frac{(7C_{11} + 2C_{12})C_{44}}{3(C_{11} + 2C_{12})(C_{11} - C_{12})}$
Diamond	1.54	1.49	1.18
Si	1.56	1.08	1.14
Ge	1.67	1.01	1.20
MgCu <sub>2</sub>	1.59	1.07	1.00