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THE ELASTIC CONSTANTS OF MgAg AND $MgCu_2$ SINGLE CRYSTALS

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Abstract—The three independent elastic constants of MgAg and $MgCu_2$ have been determined by the pulse–echo method from 80° to 500°K. The temperature coefficients of all the elastic constants are normal but smaller than the average of their constituent elements. The anisotropy factor is high for MgAg and low for $MgCu_2$, as one would expect from their respective crystallographic configurations. The elastic behavior of $MgCu_2$ was found to be similar to that of the diamond structure.

INTRODUCTION

SINCE many intermetallic compounds of many different crystal structures have been found in alloy systems, the basic reason for their stability has drawn a great deal of attention. However, measurements on elastic constants of these compounds, which may enable one to evaluate the extent of interatomic forces, have been relatively few. It was the intention of the present investigation to determine the elastic constants of two compounds, MgAg and $MgCu_2$, so that a better understanding about the nature of the interaction between neighboring ions in the crystals may be achieved.

MgAg has a CsCl-type structure. The elastic properties of this structure have been the most explored among all intermetallic compounds, both theoretically and experimentally. A metallic compound of this type is characterized by a high degree of anisotropy due to its low resistance to a (110) $[1\bar{1}0]$ shear. $MgCu_2$ is the proto-type cubic Laves phase. It is believed that its stability can be attributed to the fact that it is a close-packed arrangement of unequal spheres. If this interpretation is correct, we may expect that $MgCu_2$ will be fairly isotropic. Both compounds are stable and remain ordered at all temperatures up to the melting point.

EXPERIMENTAL PROCEDURE AND RESULTS

Single crystals of MgAg and $MgCu_2$ of stoichiometric compositions, received from DR. V. B. Kurfman of our laboratory, were grown by the Bridgman method in graphite molds from high purity metals. For each compound, two cylindrical specimens were cut in the [100] and [110] orientations with an electrical discharge machine. The surface finishing was done on metallographic polishing wheels without final etching. The dimensions of each specimen were about 3 cm dia. × 1 cm thick, with misorientation $<2°$ and parrallelism within $\pm 0{\cdot}005$ mm.

Sonic velocities were determined by the pulse–echo technique using a 10 Mc/s rectified pulse of $1{\cdot}5$ μsec duration. The experimental set-up was similar to that of HUNTINGTON.[1] The basic components of the electrical system consisted of an Arenberg PG650C pulsed oscillator, a balancing network, and a WA600C wide-band amplifier, in conjunction with a Tektronix 545A oscilloscope. A 4× magnifying lens mounted in front of the cathode-ray tube screen helped to improve visibility of the echoes. The arrangement of the specimen holder is shown in Fig. 1. The temperatures from 80° to 500°K were measured with a copper–constantan thermocouple embedded in the base of the specimen seat. To bond the X-cut or Y-cut quartz transducer to the specimen, Nonaq was used for low temperatures and Dow Corning 806A silicone resin for high temperatures. For the latter, a thin layer of the resin was first applied to the top surface of the specimen and to the bottom surface of the transducer. These layers were cured separately for an hour at 100°C, then were matched together and baked at 250°C under spring loading for another hour. For $MgCu_2$ specimens, numerous echoes, ~100, were visible, but attenuation in MgAg was high, with only 8 or 9 echoes displayed.

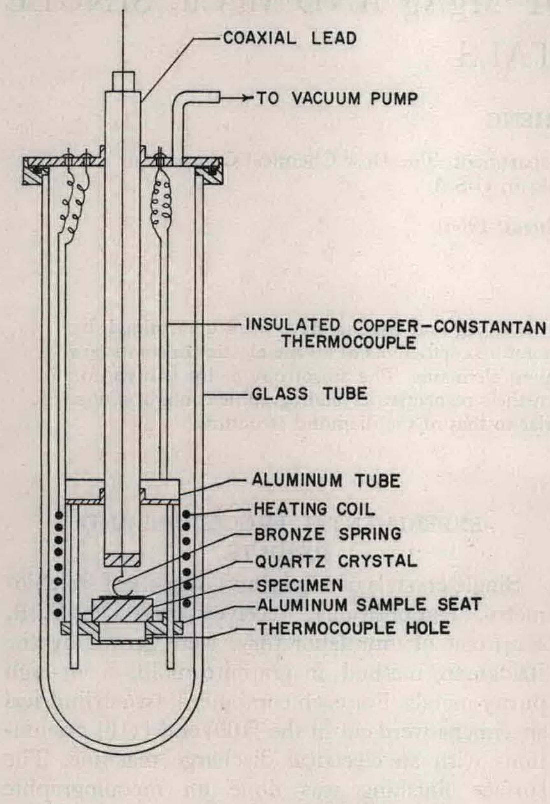

FIG. 1. The sample holder.

The room temperature densities were taken as 6·042 g/cm³ for MgAg and 5·76 g/cm³ for $MgCu_2$.[(2)] The linear coefficients of thermal expansion were determined experimentally. The average values between 0° and 250°C were found to be $22{\cdot}8\times10^{-6}$ (MgAg) and $18{\cdot}7\times10^{-6}$ cm/cm/°C ($MgCu_2$). The latter value is significantly smaller than the previously reported one.[(3)] For each compound, five velocities were measured and the elastic constants were computed with two internal checks. Transit-time corrections of 0·025 μsec and 0·04 μsec were subtracted from the observed delay times in calculating the longitudinal and transverse velocities respectively.

The adiabatic elastic constants of MgAg and $MgCu_2$ from 80° to 500°K are shown in Figs. 2 and 3, and listed in Tables 1 and 2. The estimated over-all accuracy is ±1 percent for C_{11} or C_{44}, and ±2 percent for C_{12}. They follow the normal features of temperature dependence with an approach to zero slope towards 0°K, and a negative slope at higher temperatures. The temperature coefficients are smaller than the average of the constituent elements. The low temperature data extrapolated to 0°K give the Debye temperatures at 315°±3°K (MgAg) and 380°±4°K ($MgCu_2$) by using BLACKMAN's formula.[(4)]

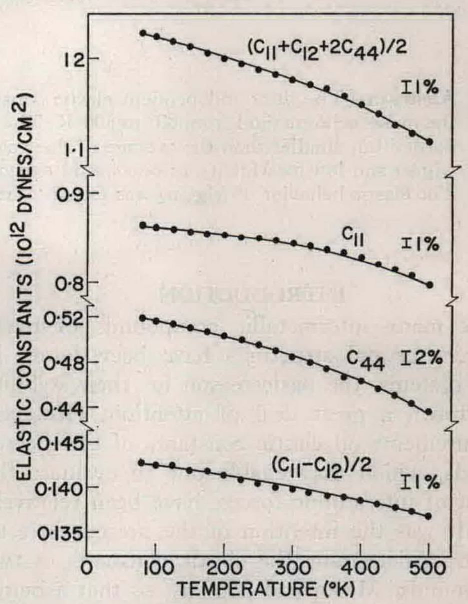

FIG. 2. The temperature dependence of elastic constants of MgAg.

DISCUSSION

As one can see from Fig. 2, with decreasing temperature MgAg exhibits a strong tendency to increase its anisotropy factor, C/C'. [Here $C = C_{44}$ and $C' = (C_{11}-C_{12})/2$.] This trend is even

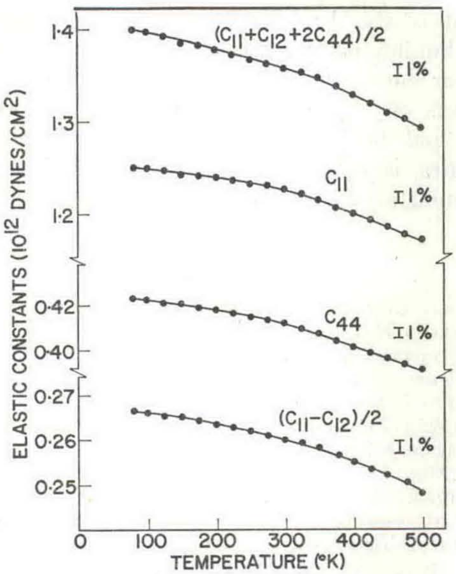

FIG. 3. The temperature dependence of elastic constants of $MgCu_2$.

Table 1. The adiabatic elastic constants of MgAg (*in units of* 10^{12} dyn/cm^2)

T(°K)	C_{11}	C_{12}	C_{44}
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

Table 2. The adiabatic elastic constants of $MgCu_2$ (*in units of* 10^{12} dyn/cm^2)

T(°K)	C_{11}	C_{12}	C_{44}
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

stronger in the isostructural phases, ordered CuZn[(5)] and cubic AuCd[(6)]. The anisotropy factor also increases from MgAg ($\sim$3·5) to CuZn ($\sim$8) to AuCd ($\sim$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 elastic data on NiAl,[(7)] given its $C/C' = 3{\cdot}28$ 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[(8–11)]. Following FUCHS and ISENBERG[(8,11)] 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,[(11)] 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, $(W_E - W_S) \simeq 0$, 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 $MgCu_2$, 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^2

Contributions from	C	C'	B
$W_E - W_S$	0·29	0·04	—
$W_0 + W_F$	—	—	0·32
W_I 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, $CaMg_2$, whose elastic constants have been reported,[12] is also isotropic. The mechanical behaviors[13] and elastic properties of $MgCu_2$ 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 $O_h{}^7 - Fd3m$. A comparison between the elastic properties of $MgCu_2$ and those of the three IVa elements[14] 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[14] 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.[14] The fact that the elastic constants of $MgCu_2$ 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.

Table 4. *A comparison of* $MgCu_2$ *with the diamond structure elements*

Crystal	Anisotropy $\frac{2C_{44}}{C_{11}-C_{12}}$	Born's relation $\frac{4C_{11}(C_{11}-C_{44})}{(C_{11}+C_{12})^2}$	Harrison's relation $\frac{(7C_{11}+2C_{12})C_{44}}{3(C_{11}+2C_{12})(C_{11}-C_{12})}$
Diamond	1·54	1·49	1·18
Si	1·56	1·08	1·14
Ge	1·67	1·01	1·20
$MgCu_2$	1·59	1·07	1·00

REFERENCES

1. HUNTINGTON H. B., *Phys. Rev.* **72,** 321 (1947).
2. PEARSON W. P., *A Handbook of Lattice Spacings and Structures of Metals and Alloys* pp. 293, 584. Pergamon Press, London (1958).
3. SMITH J. F. and OGREN J. R., *J. appl. Phys.* **29,** 1523 (1958).
4. BLACKMAN M., *Phil. Mag.* **42,** 1441 (1951).
5. MCMANUS G. M., *Phys. Rev.* **129,** 2004 (1963).
6. ZIRINSKY S., *Acta Met.* **4,** 164 (1956).
7. WASILEWSKI R. J., *Trans. Am. Inst. Min. Met., Petrol. Engrs* **236,** 455 (1966).
8. FUCHS K., *Proc. R. Soc.* **A153,** 622 (1936).
9. ZENER C., *Phys. Rev.* **71,** 846 (1947).
10. JONES H., *Proc. Phys. Soc. Lond.* **49,** 250 (1937); *Phil. Mag.* **43,** 105 (1952).
11. ISENBERG I., *Phys. Rev.* **83,** 637 (1951).
12. SUMER A. and SMITH J. F., *J. appl. Phys.* **33,** 2283 (1962).
13. MORAN J. B., *Trans. Am. Inst. Min., Met., Petrol., Engrs* **233,** 1473 (1965).
14. HUNTINGTON H. B., *Solid. St. Phys.* **7,** 300 (1958).