Reprinted from THE JOURNAL OF CHEMICAL PHYSICS, Vol. 44, No. 12, 4385–4386, 15
Printed in U. S. A.

Effect of High Pressure on the Compressibilities of Five Alloys*

R. L. CLENDENEN AND H. G. DRICKAMER

Department of Chemistry and Chemical Engineering and *Materials Research Laboratory, University of Illinois, Urbana, Illinois*

(Received 18 February 1966)

The effect of high pressure has been measured on a series of alloys, including Fe plus 8 at. % Si, which has a (disordered) bcc structure, Fe_3Al and Fe_3Si, which have an ordered bcc structure, and FeAl and AgMg, which have the CsCl structure. The compressibilities of all the alloys except Fe_3Si decrease with increasing pressure and lie between those of the pure components. For Fe_3Si the compressibility increases slightly with increasing pressure and is less than that either of pure iron or pure silicon.

THE effect of pressure to several hundred kilobars has been measured on the lattice parameters of bcc iron containing 8% silicon, on Fe_3Al and Fe_3Si which have an ordered bcc structure, and on FeAl and AgMg which have the CsCl structure. The iron alloys were obtained from Beck, and were those used in his specific heat work.[1,2] The AgMg was obtained from Busk of the Dow Chemical Company.

TABLE I. V/V_0 vs pressure. Iron alloys and AgMg.

V/V_0	Fe+8.0% Si	Fe_3Si	Fe_2Al	FeAl	AgMg
1.00	0 (kbar)	0	0	0	0
0.99	18	26	16	12	10
0.98	37	52	29	27	19
0.97	56	76	45	43	30
0.96	77	100	62	60	40
0.95	98	125	80	79	52
0.94	120	148	98	99	64
0.93	142	172	118	120	76
0.92	166	195	140	142	88
0.91	191	217	162	165	101
0.90	216	238	185	191	115
0.89	···	260	210	222	130
0.88	···	282	238	260	144
0.87	···	···	268	304	160
0.86	···	···	···	···	175
0.85	···	···	···	···	191
0.84	···	···	···	···	208
0.83	···	···	···	···	226
0.82	···	···	···	···	244
0.81	···	···	···	···	264
0.80	···	···	···	···	285
Markers	Nb	Nb NaF	Nb NaF	Nb CaO	Nb Al NaCl

The high-pressure x-ray techniques have been discussed in detail elsewhere.[3] The smoothed data are listed in Table I; Figs. 1 and 2 show typical results for Fe_3Al and Fe_3Si. As discussed in Ref. 3, the pressures were established by measuring the lattice parameters of markers, substances of known compressibility mixed with the sample. The markers used for each substance are shown in Table I. The metal compressibilities were from shock-wave data[4,5] corrected to 25°C. The salts were the data of Perez-Albuerne and Drickamer[6] and Pagannone and Drickamer.[7]

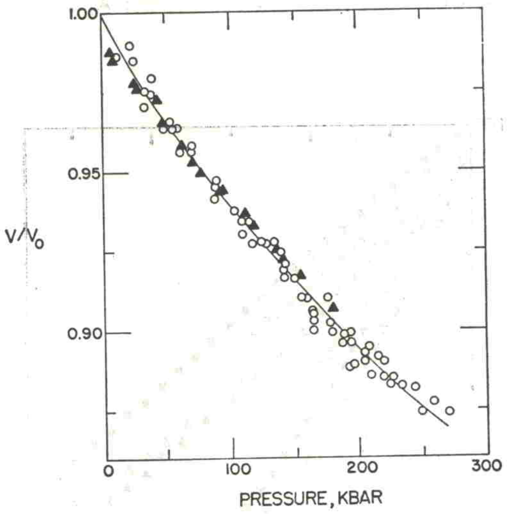

FIG. 1. V/V_0 vs pressure—Fe_3Al. (○, Nb; ▲, NaCl.)

These smoothed results are plotted in Fig. 3 with data on pure iron,[8] silicon,[9] and aluminum.[4] Several points are observable. The bcc iron containing 8% Si has a compressibility very near that of pure iron. By 130 kbar a significant fraction has transformed to the hcp structure, the high-pressure phase of pure iron. (The equilibrium pressure may well be below 130 kbar.) No attempt at detailed study of the hcp phase was made, but at 150 kbar $c/a=1.67$.

Both the ordered Fe_3Al and the FeAl with the CsCl

---

* This work has been supported in part by the U.S. Atomic Energy Commission.

[1] C. H. Cheng, K. P. Gupta, C. T. Wei, and P. A. Beck, J. Phys. Chem. Solids **25**, 759 (1964).

[2] K. P. Gupta, C. H. Cheng, and P. A. Beck, J. Phys. Chem. Solids **25**, 1147 (1964).

[3] E. A. Perez-Albuerne, K. F. Forsgren, and H. G. Drickamer, Rev. Sci. Instr. **35**, 29 (1964).

[4] M. H. Rice, R. G. McQueen, and J. M. Walsh, Solid State Phys. **6**, 1 (1958).

[5] R. G. McQueen and S. P. Marsh, J. Appl. Phys. **31**, 1253 (1960).

[6] E. A. Perez-Albuerne and H. G. Drickamer, J. Chem. Phys. **43**, 1381 (1965).

[7] M. Pagannone and H. G. Drickamer, J. Chem. Phys. **43**, 2266 (1965).

[8] A. S. Balchan and H. G. Drickamer, Rev. Sci. Instr. **32**, 308 (1961).

[9] P. W. Bridgman, Proc. Am. Acad. Arts Sci. **77**, 189 (1949).

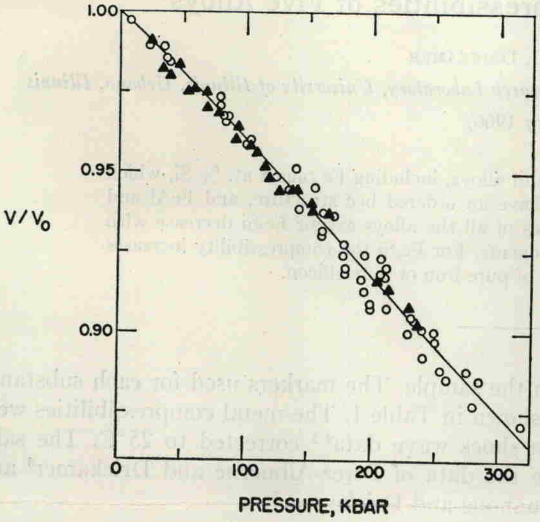

Fig. 2. V/V_0 vs pressure—Fe_3Si. (○, Nb; ▲, NaF.)

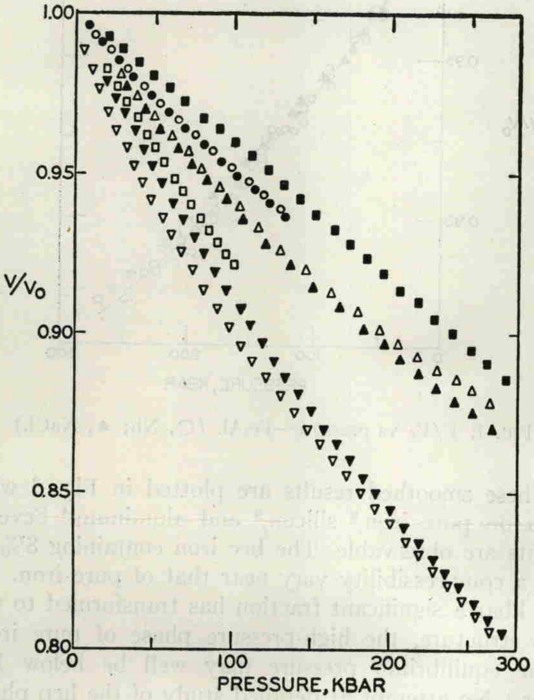

FIG. 3. V/V_0 vs pressure for iron and alloys. ○, Fe; ●, Fe+8.0% Si; ■, Fe_3Si; □, Si(Bridgman); △, FeAl; ▲, Fe_3Al; ▼, AgMg; ▽, Al (shock data).

structure have very nearly the same compressibility, intermediate between pure iron and pure aluminum. The compressibility decreases with increasing pressure as is usual for metals. On the other hand, Fe_3Si is less compressible than either pure iron or pure silicon and has a compressibility which actually increases slightly with increasing pressure. The binding is evidently very different in this alloy. Quite possibly the closer packing accounts for the compressibility less than silicon and the covalent forces account for the compressibility less than iron. There is no simple way of discussing the increase in compressibility with pressure. The AgMg exhibits typical metallic behavior like its analog FeAl.

TABLE II. Initial lattice parameters and Murnaghan constants.

Material	a_0	B_0 (kbar)	B_0'	B_0/B_0' (kbar)
Fe (pure)	2.866	5.0	1780	360
Fe+8% Si	2.860	4.6	1740	370
Fe_3Al	5.792	4.6	1360	300
FeAl	2.909	5.6	1380	240
AgMg	3.311	3.6	860	240
Fe_3Si	5.655	···	···	···

The data have been fit to the Murnaghan[10] equation

$$P=(B_0/B_0')[(V_0/V)^{B_0'}-1]. \qquad (1)$$

The results are listed in Table II along with the atmospheric lattice parameters. In Murnaghan's derivation B_0 is the zero-pressure bulk modulus and B_0' its pressure derivative evaluated at zero pressure. Here they have been treated as empirical constants giving the best least-squares fit to the data over the entire range of pressure and volume. They may therefore not correspond exactly to the coefficients evaluated at 1 atm. Further, the calculated pressures are somewhat insensitive to small variations in B_0 and B_0' if appropriately balanced, so that one should not interpret differences of the order of 10% or so from one material to the next. The results do illustrate the close similarity among Fe, Fe plus 8% Si, Fe_3Al, and FeAl in considerable contrast to the Fe_3Si.

ACKNOWLEDGMENTS

The authors wish to thank Professor Paul Beck of the University of Illinois and Dr. R. S. Busk of Dow Chemical Company for the samples.

---

[10] F. D. Murnaghan, *Finite Deformation of an Elastic Solid* (John Wiley & Sons, Inc., New York, 1951).