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Volume Compressibility of BeO and Other II–VI Compounds*

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The volume compressibilities of BeO, ZnS, CdS, CdSe, and CdTe have been measured to 45 kbar. Solid–solid transitions were observed in CdS, CdSe, and CdTe at 17.5, 21.3, and 31.8 kbar, respectively, with corresponding volume changes of 16.0%, 16.4%, and 16.4%.

I. INTRODUCTION

THE room-temperature volume compressibilities of BeO, CdS, CdSe, ZnO, CdTe, and ZnS have been measured to 45 kbar as part of a continuing program on the fundamental properties of II–VI compounds. The first four compounds have a wurtzite structure while the latter two have a zinc-blende structure. Table I lists some of the properties of the compounds of interest.

TABLE I. Properties of II–IV compounds.

Compound	Atmospheric crystal structure	Lattice parameters a_0 c_0 (Å)	Bond distance (Å)	Bandgap (eV)	Molecular volume (cc)	Density (g/cc)
BeO	B_9[a]	2.695–4.39	1.64, 1.65	~11.6(R.T.)	8.31	3.010
ZnO	B_9	3.243–5.195	1.95, 1.98	3.14(R.T.)	14.31	5.676
ZnS	B_4[b]	5.412	2.36	3.91(14°K)		4.096
	B_9	3.811–6.234	2.33, 2.33	3.84(14°K)	23.83	4.089
ZnSe	B_4	5.65	2.45	2.820(4°K)	30.35	5.262
ZnTe	B_4	6.07	2.63	2.39(4°K)	34.24	5.636
CdS	B_9	4.14–6.72	2.51, 2.53	2.50(R.T.)	29.94	4.825
CdSe	B_9	4.30–7.01	2.63, 2.64	1.840(1.8°K)	41.00	5.854
CdTe	B_4	6.46	2.78	1.705(2.1°K)	41.00	5.854

[a] B_9 = wurtzite structure.
[b] B_4 = sphalerite structure.

A search of the literature revealed only two studies of isothermal compressibility of II–VI compounds. They are the work of Gutsche[1] on CdS and Weir and Shastis[2] on BeO. The CdS was done using an optical technique. The BeO data were scattered and only extended to 10 kbar.

The results are compared with the adiabatic compressibility calculated from elastic constants. Solid–solid transformations were observed for CdS, CdSe, and CdTe and are compared with previous work.[3–8]

II. EXPERIMENTAL

Method

A die with a tungsten carbide inner core and with steel support rings was used. The method has been described previously[9]; corrections were made for the expansion of the die.[10] Most of the samples were run in a die of 0.500-in. bore; some of the smaller samples, such as ZnO, were run in a 0.312-in. die.

In addition, shock-wave data were obtained for BeO to 1.1 mbar. Techniques for these measurements are described by Rice *et al.*[11]

TABLE II. Source of samples.

Samples	Purity (%)	Sources
CdS	99.99	(1) Harshaw Chemical Company (2) Obtained as a boule from Dr. Norman Tallan WADC
β-ZnS	99.99 99.99 99.98	(1) Harshaw Chemical Company (2) Obtained as a boule from Dr. Norman Tallan WADC (3) Semi Elements, Inc.
α-ZnS	99.99	(1) Harshaw Chemical Company
CdSe	99.98	(1) Semi Elements, Inc. (2) Harshaw Chemical Company
ZnO	99.99	(1) Obtained as pure crystals from Minneapolis Honeywell
BeO	99.95	(1) Obtained as 6-in.-diam block from Dr. S. Carneglia of Atomics International
CdTe	99.99	(1) Obtained from Semi Elements as $\frac{1}{2}$-in. cubes

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Samples

All of the samples with the exception of BeO were single crystals. The polycrystalline BeO had a density of 3.006 g/cm^3, which is 99.88% of theoretical. The sources of the samples are given in Table II.

III. RESULTS AND DISCUSSION

BeO

The BeO samples were right-circular cylinders approximately 0.5 in. in diameter by 1 in. high; they were core drilled out of a 6-in. hot pressed block. The hydrostatic results obtained on the samples are shown in Fig. 1. It is evident that there is considerable scatter in the data, due in part to the low compressibility of BeO. The scatter results in a ±20% error in the data.

Our isothermal compressibilities (at 1 atm) are shown in Table III. Adiabatic compressibilities as calculated from elastic constant data[12–18] are also listed. The agreement between the isothermal and adiabatic compressibilities for BeO is considered reasonable due to the scatter in the hydrostatic data. The isothermal compressibility should be larger than the adiabatic by a term $(1+\alpha\gamma T)$, where α is the volume coefficient of thermal expansion, γ the Gruneisen constant, and T the absolute temperature (°K). In the case of BeO this term is very small, so the two compressibilities should be about the same.

TABLE III. Isothermal and adiabatic compressibilities.

Compound	K_s (adiabatic) ($\times 10^3$ kbar^{-1})	K_T (isothermal) ($\times 10^3$ kbar^{-1})
BeO	0.397	0.411
ZnO	0.697	2.22
ZnS[a]	1.275	1.30
CdS	1.626	2.62
CdSe	1.879	3.56
CdTe[a]	2.360	3.96
ZnSe	1.680	2.469
ZnTe	1.962	2.427

[a] Sphalerite form, $K_s=3(s_{11}+s_{12})$ (cubic), $K_s=2(s_{11}+s_{12}+2s_{13})+s_{33}$ (hexagonal).

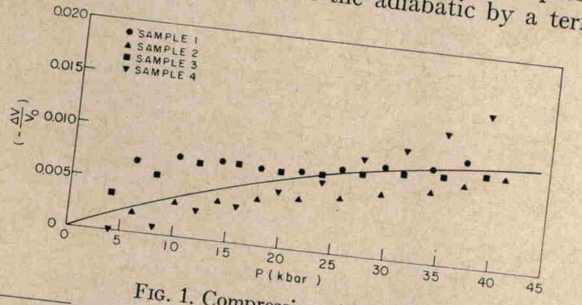

FIG. 1. Compression of BeO.

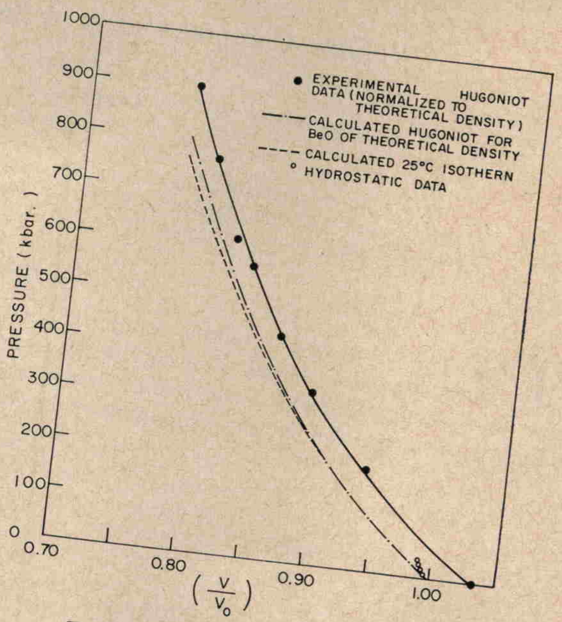

FIG. 2. Pressure vs V/V_0 for BeO.

TABLE IV. Evaluated constants.

Compound	$10^3 a$ (kbar)$^{-1}$	$-10^5 b$ (kbar)$^{-2}$	$10^6 c$ (kbar)$^{-3}$
BeO	0.413	0.43	⋯
CdS[a]	2.63	8.0	1.43
CdSe[a]	3.58	1.39	2.98
CdTe[a]	3.98	8.8	1.09
ZnO	2.22	0.37	⋯
ZnS	1.31	0.410	⋯

[a] Low-pressure fit only.

Table IV tabulates the calculated coefficients a, b, and c which were obtained by a least-squares fit to an equation of state of the form $-\Delta V/V_0=ap+bp^2+cp^3$. The compressibility at $P=0$ is the a in the preceding equation. Table V is a comparison of the experimental data with values calculated from the equation of state.

In addition to the hydrostatic experiments, dynamic data were also obtained for BeO. The methods have been described in the literature.[11,19] These data are presented in Table VI. Unfortunately the samples were not at theoretical density ($\rho_0=3.0096$ cm^3).

The data were corrected for density and temperature effects as follows: First, the Mie–Gruneisen and Dugdale–McDonald equations were used to obtain a fit of the Gruneisen γ with volume. The method is described in Ref. 11. The constants used are shown in Table VII. Then the Mie–Gruneisen and Hugoniot equations were

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