JOURNAL OF SOLID STATE CHEMISTRY 60, 128–130 (1985)

BRIEF COMMUNICATIONS

Pressure Dependence of the Grüneisen Parameter of Silver Bromide

P. C. SHARMA*

Department of Physics, Tuskegee University, Tuskegee, Alabama 36088

P. MOHAZZABI

Department of Mechanical Engineering, Tuskegee University, Tuskegee, Alabama 36088

AND K. P. ROY

Department of Physics, Banaras Hindu University, Varanasi-221005, India

Received October 19, 1984

For the first time, the Grüneisen parameter of silver bromide is calculated as a function of pressure by using the Callaway integral technique and pressure dependence of the thermal conductivity. The values are reported up to 2.0 GPa at 130 and 292 K. Good agreement between theory and experiment is obtained in the low-pressure region where the latter data exist. © 1985 Academic Press, Inc.

I. Introduction

Even though the Grüneisen parameter is known for many materials, its pressure dependence has not been extensively studied. Recently, the pressure dependence of the longitudinal and transverse phonon velocities in cesium, silver, and sodium chlorides have been measured (*1*). From these data, the pressure dependence of the Grüneisen parameters can be obtained using (*2*)

$$\gamma_i = \frac{1}{3} + B_T \left(\frac{\partial \ln v_i}{\partial P}\right)_T, \qquad (1)$$

where v_i and γ_i are the phonon velocities and the Grüneisen parameters, respectively, and the subscript i stands for the longitudinal and transverse phonon modes. P and T are the pressure and the absolute temperature, respectively. B_T is the isothermal bulk modulus.

In a previous work (*3*) we have used the pressure dependence of the Grüneisen parameter of silver chloride and the Callaway integral technique (*4*) to explain the pressure dependence of the thermal conductivity of this material which could not be explained otherwise. Recently, pressure dependence of thermal conductivity of silver bromide has been measured (*5*). Siliver

* To whom correspondence is to be addressed.

0022-4596/85 $3.00

TABLE I

EXPERIMENTAL THERMAL CONDUCTIVITIES AND THE ELASTIC CONSTANTS OF SILVER BROMIDE AS A FUNCTION OF PRESSURE AT 130 AND 292 K

Pressure (GPa)	κ_{expt} (W/m · K)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)
		T = 130 K		
0.0	1.500	66.220	33.770	7.904
0.5	1.736	71.523	35.447	7.720
1.0	1.971	76.825	37.123	7.535
1.5	2.207	82.128	38.800	7.351
2.0	2.443	87.430	40.476	7.166
		T = 292 K		
0.0	0.685	53.908	30.082	7.271
0.5	0.779	59.828	32.353	7.138
1.0	0.872	65.747	34.623	7.005
1.5	0.966	71.667	36.894	6.872
2.0	1.059	77.586	39.165	6.739

bromide, being the same type of material as silver chloride, is expected to be explained by the Callaway integral technique. However, due to lack of experimental and theoretical data on the pressure dependence of the Grüneisen parameter of silver bromide, we decided to use the thermal conductivity data and predict the pressure dependence of the Grüneisen parameter.

II. Theory

Thermal conductivity of a nonmetallic solid is given by (*4*)

$$\kappa = \frac{k}{2\pi^2 v}\left(\frac{kT}{\hbar}\right)^3 \int_0^{\theta/T} \frac{x^4 e^x}{(e^x - 1)^2 \tau_c^{-1}}\, dx, \quad (2)$$

where x is a dimensionless parameter given by $x = \hbar\omega/kT$, with ω the phonon frequency, k the Boltzmann constant, T absolute temperature, and $\hbar = h/2\pi$, where h is the Planck constant. θ is the Debye temperature and v is the average phonon velocity in the solid. τ_c^{-1} is the combined relaxation rate of the different phonon scattering processes. At the temperatures of our interest, only the phonon–phonon interaction mode is dominant, and therefore

$$\tau_c^{-1} = \tau_{ph\text{-}ph}^{-1} = A\omega^2 T = A\left(\frac{k}{\hbar}\right)^2 x^2 T^3. \quad (3)$$

In this expression A is given by (*6*)

$$A = \frac{4\pi k a \gamma^2}{\sqrt{2}\, M v^3}, \quad (4)$$

where M is mass per unit cell, a is the lattice parameter, and γ is the average Grüneisen parameter. Combining Eqs. (2), (3), and (4) we obtain

$$\kappa = \frac{M}{4\sqrt{2}\,\pi^3 a}\left(\frac{k}{\hbar}\right)\left(\frac{v}{\gamma}\right)^2 \int_0^{\theta/T} \frac{x^2 e^x}{(e^x - 1)^2}\, dx. \quad (5)$$

III. Results and Discussion

The values of the quantities used in our calculations are presented in Tables I and II. The experimental thermal conductivities, κ_{expt}, are obtained from the results of Ross and Andersson (*5*). The elastic constants C_{11}, C_{12}, and C_{44} are calculated using the extrapolated data on the elastic constants and their pressure derivatives (*7*). Values of a, ρ (density), and θ at different pressures are obtained using the compressibilities (*8*) and the low-pressure thermodynamic Grüneisen parameter (*9*). The temperature variations of a, ρ, and θ in the temperature range of this work are very small and, therefore, neglected. The average phonon velocities of Table III are cal-

TABLE II

LATTICE PARAMETER (a), DENSITY (ρ), AND THE DEBYE TEMPERATURE (θ) OF SILVER BROMIDE AS A FUNCTION OF PRESSURE

Pressure (GPa)	a (Å)	ρ (g/cm³)	θ (K)
0.0	5.7745	6.4772	144.0
0.5	5.7533	6.5484	147.6
1.0	5.7495	6.5614	148.2
1.5	5.7129	6.6845	154.5
2.0	5.6956	6.7428	157.4

TABLE III

CALCULATED PHONON VELOCITY AND THE GRÜNEISEN PARAMETER OF SILVER BROMIDE AT DIFFERENT PRESSURES

Pressure (GPa)	v/γ (m/sec)	v (m/sec)	γ
	$T = 130$ K		
0.0	932	1884	2.021
0.5	1001	1924	1.941
1.0	1071	1971	1.870
1.5	1130	2000	1.828
2.0	1189	2036	1.784
	$T = 292$ K		
0.0	931	1718	1.845
0.5	994	1773	1.807
1.0	1050	1833	1.769
1.5	1106	1874	1.754
2.0	1159	1921	1.733

culated in the following way. The longitudinal and transverse phonon velocities, $v^{(l)}$, $v_1^{(t)}$, and $v_2^{(t)}$, are first calculated for each of the main crystal directions [100], [110], and [111] (*8*). In each direction, the average phonon velocity is then obtained using

$$v_{[hkl]} = \frac{v^{(l)} + v_1^{(t)} + v_2^{(t)}}{3}. \quad (6)$$

Finally, the weighted average of the phonon velocities are obtained from

$$v = \tfrac{1}{13}\,(3v_{[100]} + 6v_{[110]} + 4v_{[111]}). \quad (7)$$

The numbers 3, 6, and 4 account for the multiplicities of the corresponding crystal directions.

Values of the Grüneisen parameter at different pressures are calculated from Eq. (5) and listed in Table III. Our calculated low-pressure Grüneisen parameter values of 2.02 and 1.85 compare reasonably well with the low-pressure thermodynamic value of 2.27 (*9*), i.e., a difference of 11 and 18.5%, respectively. The Grüneisen parameter with values of 1.13 and 3.00 obtained from Bridgman's data using the Murnaghan equation and the modified Murnaghan equation (*10*) differ from the thermodynamic value by 50 and 32%, respectively. Clearly, our low-pressure values are in better agreement with the thermodynamic Grüneisen parameter than those obtained from the Bridgman data. The high-pressure Grüneisen parameters could not be compared with the experimental results due to lack of the data.

Acknowledgments

We thank Professor G. Backstrom and Dr. P. Andersson of the University of Umea, Sweden, for the excellent hospitality provided to one of us (P. C. S.) at their laboratory and for providing the experimental data. We also thank Dr. O. C. Williamson, Dean, College of Arts and Sciences, and Dr. V. G. Harris, Dean, School of Engineering and Architecture of the Tuskegee Institute, for their interest and encouragement.

References

1. F. F. VORONOV AND S. B. GRIGOR'EV, *Sov. Phys. Solid State* **18,** 325 (1976).
2. F. W. SHEARD, *Philos. Mag.* **3,** 1381 (1958).
3. K. P. ROY, P. MOHAZZABI, AND P. C. SHARMA, *Canad. J. Phys.* **62,** 89 (1984).
4. J. CALLAWAY, *Phys. Rev.* **113,** 1046 (1959).
5. R. G. ROSS AND P. ANDERSSON, *High Pressure Sci. Technol. AIRAPT Conf., 8th, and EHPRG Conf., 19th* (1981).
6. M. ROUFOSSE AND P. G. KLEMENS, *Phys. Rev. B: Condens. Matter* **7,** 5379 (1973).
7. K. F. LOJE AND D. E. SCHUELE, *J. Phys. Chem. Solids* **31,** 2051 (1970).
8. D. E. GRAY (Coord. Ed.), "American Institute of Physics Handbook," 3rd ed., pp. (3)99–(3)100 and (4)46, McGraw–Hill, New York (1972).
9. J. AKELLA, S. N. VAIDYA, AND G. C. KENNEDY, *J. Appl. Phys.* **40,** 2800 (1969).
10. S. N. VAIDYA AND G. C. KENNEDY, *J. Phys. Chem. Solids* **32,** 951 (1971).