ANOMALIES OF THE SHOCK COMPRESSIBILITY OF WATER

G. E. Bogdanov and A. P. Rybakov

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We analyzed the available experimental data on the shock-wave compressibility of water. The results were approximated by three rectilinear segments in wave–mass velocity coordinates. The calculated temperatures of shock-compressed water were compared with the melting curve of ice VII. We found that breaks in the D–u curve correspond to intersection points of the Hugoniot curve with the water–ice VII phase equilibrium curve. A correlation of these results with the findings of other authors suggests that the Hugoniot curve of water crosses into the solid-phase region of ice VII.

The shock-wave compressibilities of different substances display a common feature: the Hugoniot functions, e.g, the pressure–volume curves, are not smooth. The discontinuities denote phase transitions, i.e., structural changes in the crystal lattice or changes in the atomic electron structure (see [1, 2]). The Hugoniot curve is usually plotted from measurements of the shock-wave kinematic parameters, viz., the wavefront velocity (wave velocity) and the material particle velocity behind the wavefront (mass velocity). The Hugoniot curve is thus representative of the relationship between the wave and mass velocities.

As a most abundant substance on earth, after has been extensively studied, specifically to investigate the fundamental high-pressure behavior of substances, as well as with a view to solving a range of practical problems. Many studies have been devoted to the relative position of the shock compressibility curves and the liquid–solid equilibrium curve of water. It has not been conclusively determined whether the Hugoniot curve "crosses over" into the solid-state region or not. This is illustrated in Fig. 1, where T–p coordinates are used to plot the melting curve of ice VII from the data in [3] (dashed line) and the Hugoniot curves from the data of different authors (solid lines) – 1 is taken from [4], 2 from [5], 3 from [6], 4 from [7], 5 from [8], 6 from [9], 7 from [10], and 8 from [11], The cross indicates the intersection point [10] of the Hugoniot curve of water with the melting curve of ice VII, while line 8 marks the pressure [11] at which shock-compressed water underoges a phase transition. The discrepancy stems from an inaccurate experimental wave–mass velocity formula, i.e., an inaccurate pressure–volume relationship for shock-wave compression, as well as from differences in the equations of state assumed for temperature calculations. In this study we review the existing data in order to determine whether the Hugoniot curve of water crosses the region of ice VII. The results below confirm that such is the case.

1. The phase transition indicated by a break in the Hugoniot curve at p = 11.5 GPa [11].

2. The phase transitions indicated by viscosity changes under shock compression [12-14], Mineev and Zaidel' [13] conclude from their experimental viscosity data that water is in the solid phase in the 8.0 to 15.0 GPa pressure range. This range may vary, considering that the measurements in [13] include the pressure and viscosity, while the temperatures are derived by calculation [6].

TABLE 1

c_0, km/sec	β	σ_D, km/sec	Range of u, km/sec
1,45	2,166	0,094	$0 < u < 0{,}7$
1,879	1,680	0,19	$0{,}75 < u < 2$
2,963	1,185	0,19	$2{,}2 < u < 9$

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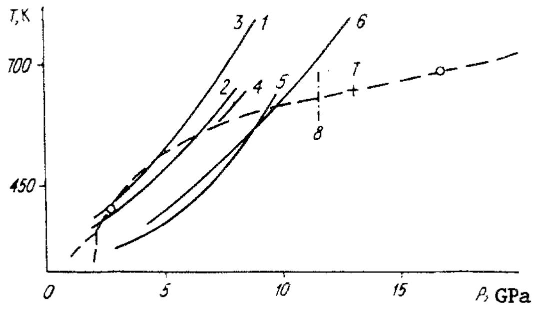

Fig. 1

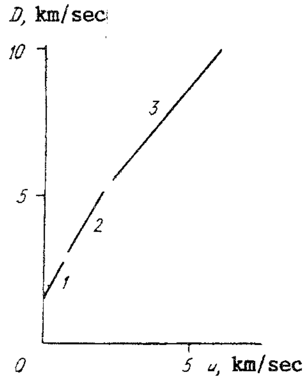

Fig. 2

3. The shock-compressed water temperature measured at p ~30 to 40 GPa [7, 15]. The experimental data are ~10% lower than the calculated values [6]. The calculated temperature–pressure Hugoniot curve [6] intercepts the ice VII region in the 3.0 to 4.5 GPa pressure range. Since the actual temperatures are lower than those calculated in [6], the pressure range within the Hugoniot curve of water and the melting curve of ice VII intersect may well be larger than that.

4. The data of [10], which give the intersection point of the Hugoniot curve of water with the melting curve of ice VII at T = 645 K and p = 13 GPa.

Studies of the optical properties of shock-compressed water report no variations in the 3.0 to 10.0 GPa range [16] or 4.0 to 30.0 range [17]. This has led Kormer et al. [7], and Kormer [15] to conclude that water remains in the liquid phase throughout the Hugoniot curve. The data of [11] show, however, that the transparency of shock-compressed water changes at p = 11.5 GPa, confirming the presence of a phase transition as indicated by a break in the Hugoniot curve at that pressure.

The object of our study is to plot the wave–mass velocity Hugoniot function of water and use it with the equation of state to obtain the shock-compression T–p curve (compared to the phase equilibrium curve).

The D–u function is derived from the experimental data. The shock compressibility of water has been well investigated [1, 4, 8, 11, 18-31]). The results are plotted in the wave–mass velocity (D–u) plane in the form of three segments, each of which can be approximated by a linear function. This piecewise linear approximation is done by the method of least squares applied to each segment. The D–u function is plotted over the experimental range in Fig. 2. Listed in Table 1 are the coefficients c_0 and β of the D–u function, i.e.,

$$D = c_0 + \beta u, \qquad (1)$$

and the shock-wave velocity root-mean-square errors σ_D.

Analysis of the diagrams in Fig. 1 and the experimental curve in Fig. 2 suggests that segments 1 and 3 of the D–u plot correspond to the shock compression of liquid water, while segment 2 may be the Hugoniot curve either of the solid phase, i.e., ice VII, or of a mixture of liquid and solid phase. This makes it very difficult to derive an equation of state for segment 2. Calculation of the temperature for states over this segment would thus yield indeterminate results. We will therefore consider the liquid-phase temperature over segments 1 and 3. The temperature is calculated from the equation of state given in [9]. The relationship between the shock-compressed pressure p and density ρ is obtained from the law of conservation of momentum on the wavefront, by means of Eq. (1) with the coefficients c_0 and β from Table 1. The cold compression curve for the low-temperature segment 1 is taken from [32]. The test point is the initial state under normal conditions. The parameters of the intersection point of this Hugoniot segment with the melting curve of ice VII are T = 400 K and p = 2.7 GPa. The equation of state used for the high-temperature segment is taken from [9]. We performed preliminary calculations to test the resultant values against available data [15, 27]; we assume that thermal electron excitation has a negligible effect on the pressure and internal energy within the given range of state parameters. Using the equation of state from [9] with the values of c_0 and β given in Table 1 for segment 3, we can then calculate the temperatures over the Hugoniot curve in the neighborhood of the melting curve. The intersection point of the high-temperature Hugoniot segment 3 with the ice VII curve has the coordinates T = 695 K and p = 16.7 GPa.

The intersection points of the Hugoniot curve with the melting curve of ice VII are denoted by circles in Fig. 1. Each intersection of the Hugoniot curve with the melting curve actually covers a temperature and pressure range. These values, together with the data of [10, 11], indicate that the Hugoniot curve intersects the ice VII—water boundary in the range of ~12 to 16 GPa. According to Table 1 the coefficient of variation in this pressure range is 3.5%. This corresponds to an interval of $\pm\sigma_p$. In order to determine more accurately the pressure and temperature ranges of intersection of the Hugoniot and melting curves in segment 2 of the D—u plot, we need to include in the internal-energy equation a term for the heat of fusion of ice VII over the intersection of the ice VII-water phase equilibrium curve. The problem in this case is that the solid and liquid-phase fractions present in the shock-compressed state cannot be precisely defined.

LITERATURE CITED

1. L. V. Al'tshuler, "The use of shock waves in high-pressure physics," Usp. Fiz. Nauk, No. 2 (1965).
2. Ya. B. Zel'dovich and Yu. P. Raizer, Physics of Shock Waves and High-temperature Hydrodynamic Processes [in Russian], Nauka, Moscow (1966).
3. W. F. T. Pistorius, Martha C. Pistorius, J. P. Blakey, L. J. Admiraal, "Melting curve of ice VII to 200 kbars," Chem. Phys., No. 3 (1963).
4. G. A. Gurtman, J. W. Kirschand, and C. R. Hastings, "Analytical equation of state for water compressed to 300 kbars," J. Appl. Phys., No. 2 (1971).
5. M. Comperthwaite and R. Shaw, "Equation of state for liquids. Calculation of shock temperature of carbon tetrachloride, nitromethane, and water in the 100-kbar region," J. Chem. Phys., No. 2 (1970).
6. M. H. Rice and J. M. Walsh, "Equation of state of water to 250 kbars," J. Chem. Phys., No. 4 (1957).
7. S. B. Kormer, K. B. Yushko, and G. B. Krishkevich, "Phase transitions of water to ice VII under shock compression," Zh. Éksp. Teor. Fiz., 54, No. 6 (1968).
8. A. A. Bakanova, V. N. Zubarev, Yu. N. Sutulov, and R. F. Trunin, "Thermodynamic properties of water at high pressures and temperatures," Zh. Eksp. Teor. Fiz., 68, No. 3 (1975).
9. B. V. Zamyshlyaev and M. G. Menzhulin, "Interpolation equation of state for water and water vapor," Prikl. Mekh. Tekh. Fiz., No. 3 (1971).
10. Ronald C. Schroeder and William H. McMaster, "Compression freezing and melting of water and ice," J. Appl. Phys., No. 6 (1973).
11. L. V. Al'tshuler, A. A. Bakanova, and R. F. Trunin, "Phase transitions in water compressed by strong shock waves," Dokl. Akad. Nauk SSSR, 121, No. 1 (1958).
12. A. D. Sakharov, R. M. Zaidel', V. N. Mineev, and A. G. Oleinik, "Experimental study of shock-wave stability and mechanical strength at high pressures and temperatures," Dokl. Akad. Nauk SSSR, 159, No. 5 (1964).
13. V. N. Mineev and R. M. Zaidel', "Viscosity of water and mercury under impact load," Zh. Éksp. Teor. Fiz., 54, No. 6 (1968).
14. V. N. Mineev and E. V. Savinov, "Viscosity and fusion temperature of aluminum, lead, and sodium chloride," Zh. Éksp. Teor. Fiz., 52, No. 3 (1967).
15. S. B. Kormer, "Optical studies of the properties of shock-compressed condensed dielectrics," Usp. Fiz. Nauk, No. 4 (1968).
16. J. M. Walsh and M. H. Rice, "Dynamic compression of liquids from measurements on strong shock waves," J. Chem. Phys., No. 4 (1957).
17. Ya. B. Zel'dovich, S. B. Kormer, M. V. Sinitsyn, and K. B. Yushko, "Study of the optical properties of transparent materials at ultrahigh pressures," Dokl. Akad. Nauk SSSR, 138, No. 6 (1961).
18. I. I. Shirindzhanov, L. V. Al'tshuler, and S. B. Brusnikin, "Anomalies of the shock and isentropic compressibility of water," Fiz. Goreniya Vzryva, No. 5 (1983).
19. M. A. Cook, R. T. Keyes, and W. O. Ursenbach, "Measurements of detonation pressures," J. Appl. Phys., 33, No. 12 (1962).
20. I. C. Skidmore and E. Morris, "Experimental equation of state data for uranium and its interpretation in the critical region," Symposium on Thermodynamic Nuclear Materials, Vienna (1962).

21. L. V. Al'tshuler, S. B. Kormer, M. I. Brazhnik, et al., "Isentropic compressibility of aluminum, copper, lead, and iron at high pressures," Zh. Éksp. Teor. Fiz., 38, No. 4 (1960).
22. J. Berger and C. Faquignon, "Shock wave data on water," in: Compendium of Shock Wave Data, Vol. 1, Sec. A-2, University of California Press, Livermore (1966).
23. M. A. Podurets, G. V. Simakov, R. F. Trunin, et al., "Compression of water by strong shock waves," Zh. Éksp. Teor. Fiz., 62, No. 2 (1972).
24. N. M. Kuznetsov, "Equation of state and specific heat of water in a wide range of dynamic parameters," Prikl. Mekh. Tekh. Fiz., No. 1 (1961).
25. L. V. Al'tshuler, G. I. Kanel', and B. S. Chekin, "New measurements of the viscosity of water behind shock wave fronts," Zh. Éksp. Teor. Fiz., 72, No. 2 (1977).
26. A. P. Rybakov, Shock Waves in Condensed Media [in Russian], Part 2, Daugavpils (1986), Department of the Latvian Research Institute of Scientific Information, No. 98-La, November 27, 1987.
27. G. A. Lyzenga, T. J. Ahrens, W. G. Wellis, and A. C. Mitchell, "The temperature of shock-compressed water," J. Chem. Phys., 77, No. 12 (1982).
28. LASL Shock Wave Hugoniot Data. Univ. of California Press, Berkeley (1980).
29. A. C. Mitchell and M. J. Nellis, "Equation of state and electrical conductivity of water and ammonia shoked to the 100 GPa (1 Mbar) pressure range," J. Chem. Phys., 77, No. 12 (1982).
30. L. P. Volkov, N. P. Voloshin, R. A. Mangasarov, et al., "Shock compressibility of water at a 1-Mbar pressure," Pis'ma Zh. Éksp. Teor. Fiz., No. 9 (1981).
31. Francis H. Ree, "Molecular interaction of dense water at high temperature," J. Chem. Phys., 77, No. 12 (1982).
32. A. P. Rybakov, "Corresponding states in shock-compressed condensed substances," Zh. Khim. Fiz., No. 4 (1972).