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Internal particle velocity history measurements are performed on [100] LiF single crystals under plate impact to 2–152 GPa, to investigate the Gruneisen equation of state and shock-induced melting. Hugoniot and sound velocities of LiF are obtained via the Lagrangian analysis. The drop in the longitudinal sound velocity to bulk sound velocity between 134 and 152 GPa, suggests that shock-induced melting initiates at 134–152 GPa. The Gruneisen parameter as a function of shock-state density is determined. Given high-pressure Gruneisen parameters, shock temperature and melting curve of B1 phase LiF are calculated, and consistent with previous molecular dynamics and ab initio calculations, as well as diamond-anvil cell and shock wave measurements. Our calculation suggests that shock-induced melting initiates at 142 GPa, in agreement with our sound velocity measurements. © 2015 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4906558]

I. INTRODUCTION

Phase transitions under high pressure and high temperature conditions have long been a subject of interest for their importance in constructing phase diagrams and multi-phase equations of state. In dynamic compression experiments, precise measurements of sound velocity at high pressures are not only useful for identifying phase transitions with small volume change including melting, which are not discernible on the pressure-density curves, but also for constraining the Gruneisen equations of state.

LiF, an ionic crystal with B1 phase structure (NaCl-type) at the ambient conditions, is chemically stable, and optically transparent with an electronic band gap of 14 eV, and has a high melting temperature. It has important applications to several fields. For example, it is widely used as a substrate in micro-electronics. In diamond anvil cell (DAC) experiments, LiF is used as a pressure-transmitting medium and pressure scale. In dynamic experiments, it is used extensively as a window material for both velocimetric and thermometric measurements for its ability to retain transparency at very high pressures and high temperatures.

In contrast to its extensive applications in dynamic high-pressure experiments, structural stability and melting behavior of LiF under compression are still poorly understood, and controversies exist among both theoretical and experimental results. It was found that LiF B1 phase remains stable up to ~100 GPa and to its high-pressure melting point, and to 300 GPa at 0 K as predicted by first-principles calculation. Ab initio calculations with anharmonic approximation and molecular dynamics (MD) simulations predicted the B1 → B2 structural transition at ~140 GPa, but the calculated melting curves were quite different: the ab initio prediction is much higher than the MD result. It was claimed that the B2 phase melting line is consistent with the shock wave (SW) data obtained by pyrometry. However, the excellent optical transparency of LiF single crystal at very high pressures implies an extremely low emissivity, and the radiation from the impactor-LiF interface also contributes to pyrometric measurements. The low emissivity and the complication incurred by the interfacial radiation render shock temperature determination a challenging task for LiF. Therefore, alternatives to pyrometry are necessary for an accurate determination of melting curves.

In this work, we report results of sound velocity measurements by the Lagrangian wave analysis method on LiF single crystals under plate impact, to investigate solid-solid and solid-liquid phase transitions at high pressures. Based on the measured longitudinal and bulk sound velocities at high pressures and high temperatures, the Gruneisen parameters at various densities are deduced to constraint its Gruneisen equation of state and shock temperature calculations. In addition, shock melting of the B1 phase is identified.

II. EXPERIMENT AND DATA ANALYSIS METHODS

The LiF samples are UV-optics grade single crystals grown via the Czochralski method, with purity better than 99.9%, provided by Anhui Institute of Optics and Fine Mechanics, Chinese Academy of Science. They are disks with optical finish on both [100] surfaces, with a nominal thickness of 3 mm or 5 mm, and a diameter of 30 mm. The average density is 2.638(5) g/cm³, and the longitudinal sound velocity at ambient condition is 6.602(5) km/s determined by an opti-
A 1.433 mm-thick 2024 Al baseplate is used; for other shots, 56-μm-thick stainless steel foils are used.

TABLE I. The shock pressure ranges from 2 GPa to 152 GPa.

<table>
<thead>
<tr>
<th>Shot No.</th>
<th>d (mm)</th>
<th>w (km/s)</th>
<th>(P_{sh}) (GPa)</th>
<th>(u_p) (km/s)</th>
<th>(D) (km/s)</th>
<th>(C_L^0) (km/s)</th>
<th>(C_T^0) (km/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LiF01</td>
<td>4.98(2)</td>
<td>3.150(16) (Cu)</td>
<td>46.65(32)</td>
<td>2.163(42)</td>
<td>8.08(2)</td>
<td>11.09(22)</td>
<td>14.55(16)</td>
</tr>
<tr>
<td>LiF02</td>
<td>5.009(2)</td>
<td>4.090(21) (Cu)</td>
<td>66.61(48)</td>
<td>2.802(45)</td>
<td>8.94(5)</td>
<td>12.77(25)</td>
<td>15.89(18)</td>
</tr>
<tr>
<td>LiF03</td>
<td>5.001(2)</td>
<td>5.160(26) (Cu)</td>
<td>92.68(68)</td>
<td>3.434(66)</td>
<td>9.77(20)</td>
<td>14.46(42)</td>
<td>18.33(40)</td>
</tr>
<tr>
<td>LiF04</td>
<td>5.016(2)</td>
<td>5.190(26) (Cu)</td>
<td>112.74(82)</td>
<td>4.031(85)</td>
<td>10.61(42)</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>LiF05</td>
<td>5.003(2)</td>
<td>4.830(24) (Cu)</td>
<td>102.43(73)</td>
<td>3.782(91)</td>
<td>9.06(42)</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>LiF06</td>
<td>3.055(2)</td>
<td>5.535(28) (Cu)</td>
<td>117.96(88)</td>
<td>4.154(55)</td>
<td>10.61(11)</td>
<td>16.75(33)</td>
<td>20.65(28)</td>
</tr>
<tr>
<td>LiF07</td>
<td>5.021(2)</td>
<td>6.036(30) (Ta)</td>
<td>134.2(10)</td>
<td>4.503(63)</td>
<td>11.09(42)</td>
<td>17.99(32)</td>
<td>21.72(26)</td>
</tr>
<tr>
<td>LiF08</td>
<td>5.010(2)</td>
<td>6.161(31) (Ta)</td>
<td>152.03(12)</td>
<td>4.91(12)</td>
<td>11.73(18)</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>LiF09</td>
<td>5.023(2)</td>
<td>6.087(30) (Pt)</td>
<td>151.51(12)</td>
<td>4.88(10)</td>
<td>11.76(15)</td>
<td>18.75(37)</td>
<td>19.28(26)</td>
</tr>
<tr>
<td>LiF10</td>
<td>1.763(2)</td>
<td>0.198(1) (Cu)</td>
<td>2.00(2)</td>
<td>0.141(2)</td>
<td>5.39(1)</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>LiF11</td>
<td>3.037(2)</td>
<td>0.531(3) (Cu)</td>
<td>5.67(3)</td>
<td>0.375(5)</td>
<td>5.73(2)</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

TABLE I. Data from sound velocity measurements on LiF. d: sample thickness, w: impact velocity, \(P_{sh}\): shock pressure, \(u_p\): particle velocity of sample, \(D\): shock velocity, \(C_L^0\) and \(C_T^0\): the Lagrangian bulk and longitudinal sound velocities, respectively. Numbers in parentheses are uncertainties in the last one or two significant digits.

FIG. 1. Schematics of experimental setup (a), and x-t diagram and interface velocity profiles (b) for sound velocity measurements based on the Lagrangian analysis method. \(\Delta t_1\) and \(\Delta t_2\) are the thickness of sample (LiF1), and the transit time for shock wave and release waves to traverse the sample, respectively. ss: stainless steel; DPS: Doppler pin system for particle velocity measurement.

The experimental results of 11 shots are summarized in Table I. The shock pressure ranges from 2 GPa to 152 GPa.

Here, \(d\) is the original sample thickness, \(\Delta t_1 = t_3 - t_1\), and \(\Delta t_2 = t_4 - t_2\). \(t_1\) and \(t_3\) denote the arrival time of the shock wave at the driver-sample and sample-window interfaces, respectively, and \(t_2\) and \(t_4\) denote the instants of the rarefaction wave arriving at the front and rear interfaces, respectively. A particular advantage of using LiF as window material is the exact match of shock-impedance between the sample and the window, and sound velocity along the releasing path in LiF can be determined precisely. This assembly eliminates the wave reflections at the sample/window interface with impedance mismatch.

III. RESULTS AND DISCUSSION

The experimental results of 11 shots are summarized in Table I. The shock pressure ranges from 2 GPa to 152 GPa.
Interfacial velocity profiles at the front and rear surfaces of the LiF samples are obtained, and corrected for the index of refraction of LiF. For clarity, only six shots are displayed in Fig. 2 with the time zero shifted to the instant when the shock wave reaches the front surface of the LiF sample. As the shock wave arrives at the two interfaces in sequence, there is a velocity jump to the steady shock state at $t_1$ and $t_3$, and release begins upon the arrival of the rarefaction wave reflected from the rear surface of the flyer plate at $t_2$ and $t_4$ (indicated by arrows, Fig. 2), respectively. The releasing portions on all measured wave profiles exhibit a typical elastic-plastic transition. The plateau value is the true particle velocity $u_p$. Shock velocity $D$ is determined from the time difference between the shock rises of the two profiles, and the sample thickness. The $D - u_p$ data obtained for LiF in this study is plotted in Fig. 3, and are in excellent agreement with literature results. Linear fitting of all the data points yields $D = 5.201(25) + 1.323(9) u_p$.

The Lagrangian longitudinal sound velocity $C^L$ at the Hugoniot state can be calculated with Eq. (2). $C^L$ at a given particle velocity along the release path is obtained in a similar way, and a typical curve of $C^L$ as a function of particle velocity is shown in Fig. 4 for shot LiF07. For most of the velocity profiles obtained, the elastic-plastic transition point during unloading is smeared by the Bauschinger effect, so the Lagrangian bulk sound velocity $C^B$ cannot be directly measured from the velocity profiles. Asay et al. proposed a method to deduce $C^B$ at the Hugoniot state by linearly extrapolating the plastic unloading portion to the Hugoniot state in the plot of $C^L$ against engineering strain ($e$). For the plastic segment, $C^L(u)$ relation shows better linearity than $C^L(e)$. Bezruchko et al. have also concluded that the plastic release wave velocity is approximately a linear function of particle velocity. Therefore, the plastic unloading part of the $C^L(u)$ curve is used for linear extrapolation to obtain $C^B$ at the Hugoniot state. The uncertainty in sound velocity measurements is $\sim 3\%$ in our work, smaller than those in previous works since impedance match at the sample-window interface is achieved in our experiments. The Lagrangian sound velocity can be converted to Eulerian sound velocity via $C^E = \left(\frac{\rho_0}{\rho}\right)C^L$.

The Lagrangian (longitudinal and bulk) sound velocities at different shock pressures are plotted in Fig. 5 along with the literature results. The approach of constant Poisson’s ratio and linear dependences of the Lagrangian sound speed on the particle velocity were discussed earlier by Vorob’ev and Kanel et al. Dashed curves are calculations assuming a constant Poisson’s ratio of $\nu = 0.333$. Our measurements are in excellent agreement with previous measurements at low pressures. Both longitudinal and bulk sound velocities increase monotonically as the shock pressure increases, and the longitudinal sound velocity drops to the bulk sound velocity in the pressure range of 134–152 GPa. This drop is a result of shock-induced melting.

The measured bulk sound velocity data can be used to calculate the Gruneisen parameter $\gamma$. Brown deduced an
expression for calculating $\gamma$ from the Rankine-Hugoniot relations, the linear Hugoniot $D-u_p$ relation ($D=C_0+su_p$), and the thermodynamic equation, as follows:

$$\gamma = \frac{\rho_0}{\rho_0 \eta^2} \left[ (1 + \eta) + R^2 (1 - \eta) \right],$$

(3)

where $\eta = u_p/D$, $R^2 = C_b^L/D$, and $\rho_0$ and $\rho$ are densities at the initial and compressed states, respectively. Given the bulk sound velocities and the Hugoniot data measured in this study, the Gruneisen parameter $\gamma$ is calculated with Eq. (3) at six shock pressures, and plotted in Fig. 6 along with the ambient value. All data points can be fitted with a power law, $\gamma/\gamma_0 = (\rho_0/\rho)^{0.842}$.

The Lindemann melting curve of LiF at high pressures can be calculated by the following expression:\(^\text{27}\)

$$T_m = T_{m0} \left( \frac{V_m}{V_{m0}} \right)^{2/3} \exp \left[ -2 \int_{V_{m0}}^{V_m} \frac{\gamma}{V} dV \right],$$

(4)

where $T_{m0}$ is the melting temperature at the ambient pressure, and $V_m(=1/\rho_m)$ and $V_{m0}(=1/\rho_{m0})$ are the specific volumes of melting state at the ambient and high pressures, respectively. Applying the Gruneisen equation of state to the melting state relative to the isentropic state, we can calculate the corresponding pressure with

$$p_m = p_S + \left( \frac{\gamma}{V} \right)_m C_V (T_m - T_S).$$

(5)

Here, the temperature ($T_s$) on the isentrope is\(^\text{28}\)

$$T_S = T_0 \exp \left( -\int_{V_0}^{V_m} \frac{\gamma}{V} dV \right).$$

(6)

The shock temperature $T_H$ can be calculated by the following expression:\(^\text{28}\)

$$T_H = T_S + \frac{V p_S - p_S}{C_V}.$$

(7)

The expressions for the pressure ($p_{\text{H}}$) on the Hugoniot and ($p_s$) on the isentrope are given in the Appendix. $C_V$ is calculated with the Debye model. Note that the electronic contribution to the heat capacity\(^\text{27}\) is ignored, and this may lead to overestimation of the calculated shock temperature. $T_0 = 298$ K is the ambient temperature. The calculated shock temperature along the Hugoniot of the B1 phase is shown as bold blue curve in the lower panel of Fig. 7.

FIG. 5. Lagrangian longitudinal and bulk sound velocities versus shock pressure for LiF in comparison with literature data. Dashed curves are calculations assuming Poisson’s ratio $\nu = 0.333$. The parameters used in the calculation are: $\rho_0 = 2.638$ g/cm$^3$, $C_0 = 5.201$ km/s, $s = 1.323$, and $\gamma = \gamma_0 (\rho_0/\rho)^{0.842}$. Inset is a magnified plot of the area within the rectangle.

FIG. 6. Gruneisen parameter versus $\rho_0/\rho$ for LiF. $\gamma_0 = 1.63$ at the ambient condition is taken from Ref. 26.

FIG. 7. (Top) Eulerian longitudinal and bulk sound velocities versus shock pressure for LiF. Dash lines are ab initio calculations from Ref. 4. Solid lines are our calculation. (Bottom) Phase diagram of LiF. Red and blue lines are calculated melting and shock temperature for B1 phase LiF, respectively. Open triangles and filled squares are MD simulations from Ref. 8 and DAC measurement from Ref. 2, respectively. SW temperature data from Ref. 9 is shown as solid diamond. Black solid lines are ab initio calculations for B1 and B2 phases of LiF from Ref. 4.
APPENDIX: DERIVATION FOR THE ISENTORE

Following Ahrens et al., the pressure \( p_H \) on the isentrope can be derived with from following equation:

\[
p_H - p_S = \frac{\gamma}{V} (E_H - E_S)\tag{A1}
\]

Using a commonly used form

\[
\frac{\gamma}{V} = \left( \frac{\rho}{\rho_0} \right)^{\gamma_0} (V/V_0)^{\gamma_0 - 1}
\]

we have

\[
\frac{\gamma}{V} (E_H - E_S) = \gamma_0 (V/V_0)^{\gamma_0 - 1}
\]

Differentiating the above equation with respect to \( V \) yields

\[
\frac{dp_H}{dV} - \frac{dp_S}{dV} = \frac{\rho_0 C_0^2}{V_0^2} \left(\frac{V}{V_0}\right)^{\gamma_0 - 2} - \frac{(\rho_H - \rho_S)(q - 1)}{V_0^2} \left(\frac{V}{V_0}\right)^{\gamma_0 - 2}
\]

\[
= \frac{\gamma_0}{V_0} \left( \frac{dE_H}{dV} + p_S \right)
\]

Here, \( p_H = \rho_0 C_0^2 \frac{\gamma_0}{1 - \eta_0} \), \( E_H = \frac{\gamma_0}{2(1 - \eta_0)} \), and \( \eta = u_0/D = 1 - V/V_0 \).

Substituting these relations and their derivatives into Eq. (A4), one obtains

\[
\frac{dp_S}{d\eta} = \left( \gamma_0 (1 - \eta)^{\gamma_0 - 1} - (q - 1)(1 - \eta)^{-1} \right) p_S
\]

\[
= \rho_0 C_0^2 \left[ (1 + s\eta) - \gamma_0(1 - \eta)^{\gamma_0 - 1} \right] \frac{(1 - \eta) \eta}{(1 - s\eta)^3} + \frac{(q - 1) \eta}{(1 - \eta)(1 - s\eta)^2}
\]

(A5)

Integration of this equation yields

\[
p_S = \rho_0 C_0^2 (1 - \eta)^{\gamma_0 - 1} \exp \left[ -\frac{\gamma_0}{q} (1 - \eta)^{\gamma_0} \right]
\]

\[
\times \int_0^\eta G(x) \exp \left[ \frac{\gamma_0}{q} (1 - x)^{\gamma_0} \right] dx.
\]

(A6)

Here,

\[
G(x) = (1 - x)^{\gamma_0 - 1} \times \left[ \frac{(1 + sx) - \gamma_0(1 - x)^{\gamma_0 - 1}}{(1 - sx)^3} + \frac{(q - 1)x}{(1 - x)(1 - s x)^2} \right]
\]

\[
V_0(= 1/\rho_0) \text{ and } V(= 1/\rho) \text{ are specific volumes at the ambient condition and shock states, respectively.}
\]

IV. CONCLUSION

Internal velocity profiles in plate impact experiments are obtained for [100] LiF single crystals in the pressure range of 2–152 GPa, and the shock-velocity–particle-velocity relation and sound velocities of LiF, deduced. The drop in the longitudinal sound velocity to bulk sound velocity between 134 and 152 GPa indicates that shock-induced melting begins at 134–152 GPa. Gruneisen parameters are determined as a function of density using the measured bulk sound velocities. Given Gruneisen parameters, shock temperature and melting curve of the B1 phase LiF are calculated. Our calculation suggests that shock-induced melting occurs at pressure of 142 GPa, consistent with sound velocity measurements.

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