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ABSTRACT

Beryllium is an ablator material used in inertial-confinement fusion and hypervelocity impact studies. The thermoelastic properties, structural factors, and optical properties of beryllium are important in these studies. In this paper, the static structural factors, ion-ion dynamic structural factors, adiabatic velocity, and optical properties of beryllium along the Hugoniot were calculated by *ab initio* simulations. The static structural factors show that beryllium atoms were randomly distributed. The dynamic structural factors extracted the dispersion relation for collective excitation via the scattering function. By collecting the peak position of the dynamic structural factors, the dispersion relation and adiabatic sound velocity were derived by definition. Using the calculated equation of state, the thermoelastic properties and adiabatic sound velocity have been derived. The two calculated methods for adiabatic sound velocity were verified to be equivalent.

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I. INTRODUCTION

Beryllium is an ablator material in inertial-confinement fusion and hypervelocity impact studies. The physical properties, such as the equations of states (EOS), thermoelastic properties, structural factors, and optical properties are of fundamental importance in understanding the physical process and material composition identification. The EOS are usually determined by shock experiments or *ab initio* calculations. The static structural factors $S(q)$ can

be measured directly by diffraction experiments. The experimental methods for dynamic structural factors are based on scattering experiments using either fast electrons or x rays. On the other hand, the dynamic structure factors are closely connected with the dielectric function via the fluctuation-dissipation theorem, and all other quantities can be derived. The structural factors can be calculated using the trace of the equilibrium structure, by definition. Dynamic ion structural factors of dense plasmas and the warm dense matter are of great importance as they contain the complete information of

the ions in these strongly interacting systems and are also influenced by the electron properties.

Experimentally, the principal Hugoniot, sound velocity, and shear stress of beryllium were measured using magnetically accelerated fly plates on Sandia's Z machine.¹ The dynamic structural factors are the Fourier transform of the space- and time-dependent density-density correlation functions, which furnished a direct measure of the density-fluctuation spectrum of the scattered electrons. The dynamic structural factors of beryllium were determined by inelastic x-ray scattering experiments.² The multi-phase EOS were constructed by functional theory calculation, and thermoelastic data were constructed by experimental and resonant ultrasound spectroscopy measurements.³ Sound velocity can be obtained from inelastic x-ray scattering experiments⁴ or theoretical methods.⁵

The EOS and ion transport properties of warm dense beryllium were calculated by quantum molecular dynamics simulations.⁶ The expanded beryllium evolution from warm dense matter to atomic fluid was calculated by molecular dynamics simulations.⁷ The electrical and optical properties of beryllium along the principal Hugoniot were investigated by using quantum molecular dynamics simulations combined with the Kubo-Greenwood formulation.⁸ The electron heat capacity and electron-phonon coupling factor of beryllium were calculated using *ab initio* theoretical studies.⁹ The premelting hcp to bcc transition of beryllium was calculated by phonon quasiparticles, with anharmonic effects being taken into consideration.¹⁰ Then, the high-pressure phase diagram of beryllium was drawn using first-principles molecular dynamics coupled with the thermodynamic integration method.¹¹ Moreover, the dielectric function by the Kubo-Green formula was used to determine the dynamic structural factors.¹² The x-ray Thomson scattering, ion-ion structural factors, compressibility, phonons, and conductivity of beryllium were calculated by the supposed density functional neutral-pseudoatom hypernetted-chain model, which agrees closely with density-functional-theory molecular-dynamics simulations.¹³ In conclusion, the *ab initio* simulation can collect the structural factors, EOS, thermoelastic properties, sound velocity, and optical properties concurrently.

The comprehensive data about the ion-ion dynamic structural factors allow for the calculation of the dispersion relation for collective excitation. On the one hand, the static and ion-ion dynamic structural factors can be derived by the *ab initio* calculated equilibrium configurations, and the adiabatic sound velocity can be derived using the dispersion relationship derived from the ion-ion dynamic structural factors. On the other hand, the dynamic structural factors are the spectral function of the density-density correlations in the systems and are needed to determine the EOS and transport properties. After a series of *ab initio* simulations, the EOS of beryllium are collected, which can derive the thermoelastic properties, by definition, such as the isothermal bulk modulus and adiabatic sound velocity. From the physical significance, the two methods of adiabatic sound velocity are equivalent. In this paper, the ion-ion dynamic structural factors and optical properties of beryllium along the principal Hugoniot curve were calculated by the *ab initio* molecular dynamics. Then, the adiabatic sound velocities were derived by both the dispersion relationship and the EOS, which check the equivalence of these two methods.

II. METHODS AND CALCULATION

A. Structural factor

1. Static structural factor

The radial distribution function $g(r)$ is defined as

$$g(r) = \frac{V}{4\pi r^2 N^2} \left\langle \sum_{i=1}^N \sum_{j=1, j \neq i}^N \delta(r - |\mathbf{r}_i - \mathbf{r}_j|) \right\rangle, \quad (1)$$

where V is the cell volume, N is the number of atoms, r_i and r_j are the atomic coordinates of atoms i and j , respectively, and $\langle \dots \rangle$ means the time or ensemble average.

The definition of static structural factors $S(q)$ is

$$S(q) = \frac{1}{N} \left\langle \sum_{i=1}^N \sum_{j=1}^N e^{i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \right\rangle, \quad (2)$$

where the wave vector q is determined by $2\pi\sqrt{n}/a$, in which a is the lattice parameters of the cell and $n = 0, 1, 2, \dots$. As pointed out, $S(q)$ is computed via the Fourier transform of $g(r)$. $S(q)$ at small q represents the long-ranged structural information of systems. The isothermal compressibility χ ($1/K_T$, where K_T is the isothermal bulk modulus) can be computed from $S(q)$ at $q \rightarrow 0$ with the form¹⁴ of

$$\chi = \frac{\lim_{q \rightarrow 0} S(q)}{n_i k_B T} = \frac{1}{K_T}, \quad (3)$$

where $n_i = N/V$ is the ionic density, k_B is the Boltzmann constant, and T is the temperature. The cubic fitting to yield $S(0)$ is enough.

2. Dynamic structural factor

From the theory of simple liquid,¹⁴ the ion-ion dynamic structure factors $S(q, \omega)$ of warm dense matter in thermodynamic equilibrium¹⁵ characterize the collective dynamics of fluctuations of ionic density over both length and time scales, where ω denotes the frequency. For a system in thermodynamic equilibrium, $S(q, \omega)$ is computed via the Fourier transform of the intermediate scattering function $F(q, t)$,¹⁶

$$S(\mathbf{q}, \omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} F(\mathbf{q}, t) e^{i\omega t} dt. \quad (4)$$

$F(q, t)$ is defined as

$$F(q, t) = \frac{1}{N} \langle \rho(\mathbf{q}, t) \rho(-\mathbf{q}, 0) \rangle, \quad (5)$$

where $\rho(\mathbf{q}, t)$ is the Fourier transform of the real space time-dependent density distribution and contains the ion information at wave number $\mathbf{q}$ and time t ,

$$\rho(\mathbf{k}, t) = \sum_{j=0}^N \exp[i\mathbf{k} \cdot \mathbf{r}_j(t)]. \quad (6)$$

By collecting the peak position of $S(q, \omega)$ at different wave numbers q , the dispersion relation is obtained. The adiabatic speed of sound is estimated by $d\omega/dq|_{q \rightarrow 0}$.¹⁵

B. Thermoelastic properties and adiabatic sound velocity by the equations of state

On the other hand, the adiabatic sound velocity can be calculated from the *ab initio* calculated EOS. From the EOS, the thermoelastic properties can be calculated directly by definition, such as the isothermal bulk modulus, thermal expansion coefficient, heat capacity, and Grüneisen parameter.¹⁷

The isothermal bulk modulus (K_T) is

$$K_T = -V \left(\frac{\partial P}{\partial V} \right)_T. \quad (7)$$

The thermal expansion coefficient (α) is

$$\alpha = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_P. \quad (8)$$

The heat capacity at a constant volume (C_V) is

$$C_V = \left(\frac{\partial E}{\partial T} \right)_V. \quad (9)$$

The Grüneisen parameter (γ) is

$$\gamma = V \left(\frac{\partial P}{\partial E} \right)_V = \frac{\alpha K_T V}{C_V}. \quad (10)$$

The adiabatic bulk modulus (K_S) is

$$K_S = K_T [1 + \alpha \gamma T]. \quad (11)$$

The adiabatic sound velocity (V_P) is

$$V_P = \sqrt{\frac{K_S}{\rho}}. \quad (12)$$

Then, the adiabatic sound velocity at specific temperature and pressure states $V_P(T, P)$ is collected by the calculated isothermal bulk modulus, thermal expansion coefficient, and Grüneisen parameter at the same state.

C. Optical property

In the current *ab initio* simulations, the optical properties are calculated by the dielectric function. From the Kubo–Greenwood formula, the frequency dependent dielectric function¹⁸ $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$ is collected. Here, $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$ are the real and imaginary parts of the dynamical dielectric response function $\epsilon(\omega)$, respectively. Then, the main optical spectra, such as the reflectivity $R(\omega)$, adsorption coefficient $I(\omega)$, energy-loss spectrum $L(\omega)$, and refractive index $n(\omega)$, can be obtained from the dynamical dielectric response function $\epsilon(\omega)$.

Then the absorption coefficient $I(\omega)$ is

$$I(\omega) = \sqrt{2}\omega \left[\sqrt{\epsilon_1(\omega)^2 + \epsilon_2(\omega)^2} - \epsilon_1(\omega) \right]^{1/2}. \quad (13)$$

The energy-loss spectrum $L(\omega)$ is

$$L(\omega) = \epsilon_2(\omega) / [\epsilon_1(\omega)^2 + \epsilon_2(\omega)^2]. \quad (14)$$

The absorption coefficient and emission coefficient are either continuous or linear. The simulating optical spectra of atomic and molecular gases at different thermodynamic conditions are calculated based on the NIST databases and semi-classical quantum theory, which correspond to the line-by-line spectrum. For the continuous spectrum, the black body radiation theory is usually adopted for the solid or liquid. The difference between the black body radiation theory, the semi-classical quantum theory, and our calculated optical properties is discussed in this study.

D. Calculation details

The *ab initio* molecular dynamics calculations are implemented in the plane wave density functional Vienna *Ab initio* Simulation Package (VASP) code.^{19,20} The projector augmented waves (PAWs)^{21,22} and generalized gradient approximation (GGA) in the parameterization of Perdew, Burke, and Ernzerhof²³ were adopted. The plane wave cut-off was 800 eV, which was sufficient to ensure that the pressure converges with 1% accuracy. The selected time step was 1 fs in all the calculations. An accurate calculation of the dynamic structural factors requires an ensemble averaged over a large number of particles and a long time scale. We selected 256 atoms as a cell, and beryllium atoms were randomly distributed in the cell. The density and temperature at the Hugoniot state were referred to from Refs. 6 and 8. The density ranged from 3.8 to 5.8 g/cm³, and the temperatures ranged from 0.95 to 10.65 eV. The long-term correlation function was collected by the NVT ensemble with the equilibrium volume and when the total time exceeded 20 ps. For the calculation of ion–ion dynamic structural factors, the ion movement was extracted from the trajectories of the equilibrium configurations. Then, the optical property was calculated using the Kubo–Greenwood formula and the Chester–Thellung–Kubo–Greenwood formula, as implemented in the VASP. The optical property was obtained by averaging ten snapshots extracted from the last 6000 time steps in each MD trajectory with an interval of 600 time steps.

III. RESULTS

A. Static structural factor

The static structural factors of beryllium were calculated using Eq. (2) and are shown in Fig. 1. An *ab initio* simulation for these conditions has already been carried out.^{6,8} Our simulation uses a larger energy cut-off, a larger number of ions, and a larger number of time steps, which likely leads to more accurate results. The calculated shape of the static structural factors near 3 eV was consistent with the reported experimental results¹³ and *ab initio* calculated results.²⁴ The *ab initio* calculated peaks of the static structural factors of beryllium at low temperatures were notable, while the peaks approached disappearance as the temperature increased. The static structural factors showed that beryllium was randomly distributed in the cell, which was consistent with the analysis of the radial distribution function. As temperature increased, the main peak position of $S(q)$ increased and the peak strength decreased, as shown in the inset of Fig. 1. At higher temperature along the principal Hugoniot state, the mean atom distance decreased as the temperature increased, and the system was distributed homogeneously. In the long-wavelength limit, $\lim_{q \rightarrow 0} S(q)$ was correlated with the

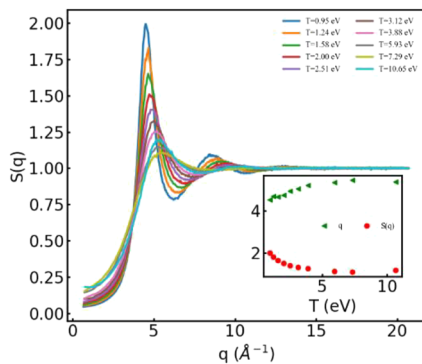


FIG. 1. Static structural factors of Be along the Hugoniot labeled by density. The inset shows the maximum peak of $S(q)$ with different values of q and $S(q)$.

isothermal compressibility using Eq. (3), and the isothermal compressibility was determined from the EOS using Eq. (7). $\lim_{q \rightarrow 0} S(q)$ increased as pressure increased, which affected the adiabatic sound velocity. The calculated long-wavelength limit $\lim_{q \rightarrow 0} S(q) = 0.046$ for $T = 0.95$ eV and $\rho = 3.8$ g/cm³ was consistent with $\lim_{q \rightarrow 0} S(q) = 0.046$ by isothermal compressibility from the EOS reported earlier⁶ at the same state.

B. Dynamic structural factors

The dynamic structural factors $S(q, \omega)$ via the intermediate scattering function were determined using Eq. (4) and are shown in Fig. 2(a). It exhibited the well-known sharp plasmon peak below a so-called plasmon critical wavevector q_c ,²⁵ which is of the order of the Fermi wavevector. The undesired peaks were attributed to

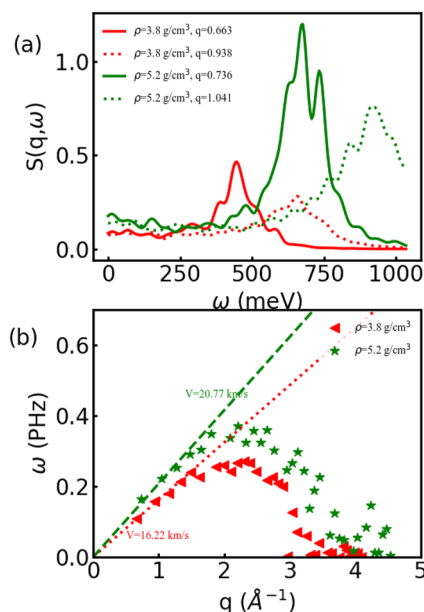


FIG. 2. *Ab initio* calculated (a) dynamic structural factors and (b) dispersion curve.

the limited number of atoms in the cell with only 256 atoms. The dispersion relation of the collective excitation has been determined by analyzing the position of the side peaks. The position of the peak of the resonance against the wave number yielded the dispersion relation for a different state, shown in Fig. 2(b). The slope of the dispersion relation for the small wave vector was the adiabatic sound velocity, and the corresponding sound velocities were determined via linear fits to the dispersion relation at small wave vectors $d\omega/dq|_{q \rightarrow 0}$. By fitting the dispersion relation, the adiabatic sound velocity was 16.22 km/s at $\rho = 3.8$ g/cm³ and 20.77 km/s at $\rho = 5.2$ g/cm³.

C. Adiabatic sound velocity by dynamic structural factors and EOS

From the EOS of beryllium reported earlier,⁶ the thermoelastic properties along the Hugoniot state were collected. The isothermal compressibility (bulk modulus) calculated by the EOS was directly used in the calculation of the adiabatic sound velocity. The adiabatic sound velocities of beryllium along the Hugoniot state calculated by EOS and dynamic structural factors are shown in Fig. 3. We determined $V = 15.92$ km/s at $T = 0.95$ eV and $P = 397.39$ GPa, and these values agreed with the adiabatic sound velocity $V = 16.22$ km/s extracted from the fitting dispersion relation, shown in Fig. 3. The adiabatic sound velocity increased at elevated temperature and density. The adiabatic sound velocity ranged from 15.92 to 25.22 km/s by the EOS and ranged from 16.22 to 23.43 km/s by the fitting dispersion relation. The adiabatic sound velocity difference between the two methods was within 8%. The adiabatic sound velocity difference between the experimental data¹ and our calculated results originated from the difference in Hugoniot states. Our calculated pressures were slightly higher than those in Ref. 1. The adiabatic sound velocity by ion–ion dynamic structural factors may be limited by the size of the supercell (which limited the number of small q) and time steps, as well as data post-processing.

D. Optical properties

The absorption coefficients of beryllium at the Hugoniot state were calculated (shown in Fig. 4), which was consistent with

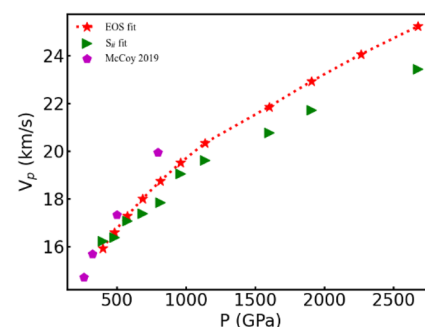


FIG. 3. Sound velocity of beryllium along the Hugoniot. The “EOS” and “ S_u ” labels correspond to the adiabatic sound velocity calculated by the EOS and ion–ion dynamics structural factor, respectively. The “McCoy 2019” label is the experimental data from Ref. 1.

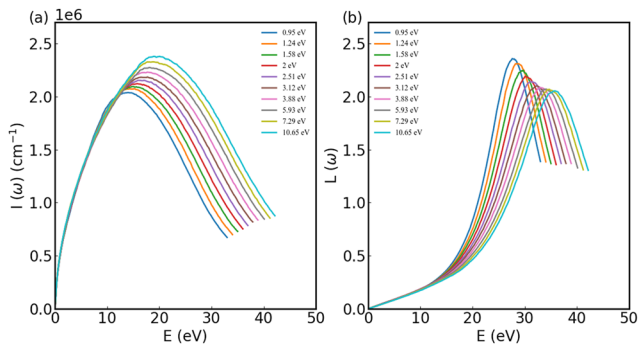


FIG. 4. *Ab initio* calculated (a) absorption coefficient and (b) energy loss spectrum of beryllium along the Hugoniot state.

Ref. 8. The Hugoniot state corresponded to the first stage of hypervelocity impact, which corresponds to a warm dense plasma and was constructed for continuous optical spectra. The *ab initio* calculated absorption spectra of beryllium along the Hugoniot were continuous without any line characteristic, which has been reported.⁸ The beryllium atoms in these shocked warm dense states were as closely condensed as the properties of black body radiation, which show a continuous characteristic. At the later stage of the hypervelocity impact, the plasmas were quickly expanded at high temperature and low density, and the plasmas show an atomic or ionic characteristic, which corresponded to a line characteristic spectrum. The line spectrum of the hypervelocity impact was constructed at the later stage of the impact, which corresponds to a low density gas and can be calculated using SpectraPlot.²⁶ Atomic optical spectroscopy results calculated using SpectraPlot²⁶ were different from our results about beryllium along the Hugoniot state. The energy-loss spectra were also collected, which also show a notable peak around 30 eV, and high temperature/pressure states always shifted to the high energy.

IV. CONCLUSIONS

In conclusion, we have determined the static structural factors, ion-ion dynamic structural factors, adiabatic sound velocity, and optical properties of beryllium along a shock Hugoniot by *ab initio* molecular simulations. The static structural factors showed that beryllium atoms are randomly distributed in the cell. The calculation results of the structural factors can be used for a direct comparison of inelastic x-ray scattering spectral experiments. The adiabatic sound velocity calculated from the dispersion relation for the ion-ion dynamic structural factors and EOS was equivalent. From the equivalence of the calculation method of the adiabatic sound velocity, it can be seen that the dynamic structural factor method is appropriate when the adiabatic sound velocity at a specified state is needed and that the EOS method is appropriate when the adiabatic sound velocity at a certain range is needed. The optical spectra were continuous along the Hugoniot without any line characteristics, which can provide data for the first stage of hypervelocity impact. However, when the line atomic optical spectrum was needed, more calculations should be performed.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Wei-Jie Li: Conceptualization (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **Jie Zhou:** Formal analysis (equal). **Zi Li:** Formal analysis (equal); Methodology (equal); Software (equal); Writing – review & editing (equal). **Yunliang Zhu:** Formal analysis (equal). **Han-Dong Hu:** Resources (equal). **Hao Ma:** Resources (equal). **Zhe Ma:** Supervision (equal). **Cong Wang:** Funding acquisition (equal); Methodology (equal); Supervision (equal); Writing – review & editing (equal). **Ping Zhang:** Project administration (equal); Supervision (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding authors upon reasonable request.

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