First-principles equation-of-state table of beryllium based on density-functional theory calculations

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Beryllium has been considered a superior ablator material for inertial confinement fusion (ICF) target designs. An accurate equation-of-state (EOS) of beryllium under extreme conditions is essential for reliable ICF designs. Based on density-functional theory (DFT) calculations, we have established a wide-range beryllium EOS table of density $\rho = 0.001$ to 500 g/cm^3 and temperature $T = 2000$ to 10^8 K . Our first-principle equation-of-state (FPEOS) table is in better agreement with the widely used *SESAME* EOS table (*SESAME* 2023) than the average-atom *INFERNO* and *Purgatorio* models. For the principal Hugoniot, our FPEOS prediction shows $\sim 10\%$ stiffer than the last two models in the maximum compression. Although the existing experimental data (only up to 17 Mbar) cannot distinguish these EOS models, we anticipate that high-pressure experiments at the maximum compression region should differentiate our FPEOS from *INFERNO* and *Purgatorio* models. Comparisons between FPEOS and *SESAME* EOS for off-Hugoniot conditions show that the differences in the pressure and internal energy are within $\sim 20\%$. By implementing the FPEOS table into the 1-D radiation–hydrodynamic code *LILAC*, we studied the EOS effects on beryllium-shell–target implosions. The FPEOS simulation predicts higher neutron yield ($\sim 15\%$) compared to the simulation using the *SESAME* 2023 EOS table. *Published by AIP Publishing.*

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I. INTRODUCTION

Beryllium (Be), which has many applications in nuclear power,¹ electronic,² geophysics,³ and aerospace industries,⁴ is an element of great technological and scientific importance for its simple atomic configurations. In inertial confinement applications (ICF),^{5–7} beryllium has been used as an ablator for indirect-drive fuel capsule designs^{8–11} because of its advantages of high density, low opacity, high thermal conductivity,¹² and low instability growth.^{13,14} Since these target designs are based mainly on the radiation–hydrodynamic simulations where the materials will experience many different pressures (up to 10^5 Mbar) and temperature (up to 10^8 K) conditions,¹⁵ accurate properties of beryllium under such extreme conditions are essential for ICF applications. Experimental data are limited to ≤ 20 Mbar, however, because of the difficulty in generating shocks and measuring them accurately. Hydrodynamic (hydro) simulations require a full equation-of-state (EOS) table to cover all plasma conditions concerned. Therefore, it is of great importance to calculate the EOS of beryllium for a wide range of conditions by using reliable methods. Once the calculated EOS table is benchmarked with experiments, it can be used for reliable ICF and high-energy-density target designs and simulations.

In the 1980s, underground nuclear explosions were used to study the EOS of beryllium. Shock Hugoniot data of beryllium were obtained at pressures up to ~ 17 Mbar (Refs. 16 and 17). In the experiment setup, the impedance-matching technique was used to measure the EOS data relative to a standard

material whose shock Hugoniot data were known beforehand. The standard material chosen was molybdenum whose absolute shock Hugoniot was obtained by simultaneously measuring the particle velocities and shock velocities.¹⁸ Ragan¹⁷ reports that the differences between the experimental data and *SESAME* data in this region are within $\sim 1\%$. In recent years, several groups have continued shock Hugoniot experiments of beryllium. Cauble *et al.*^{19,20} have performed Be-EOS experiments by using a high-intensity laser to generate strong shock waves. Absolute data on the Hugoniot of beryllium between 10 and 15 Mbar were obtained by measuring particle velocity and shock velocity directly using x-ray transmission radiography. The results in this regime agree with the previous experiments. Experimental data for the Hugoniot of beryllium are also available in the pressure ranges of 0.5 to 3.8 Mbar (Ref. 21) and 4 to 11 Mbar.²² Although the superposition of these data gives a single smooth shock Hugoniot curve, the maximum pressure reached by experiments is still far away from the “turnover” regime of peak shock compression in which EOS models tend to differ significantly.

Theoretical EOS models are particularly difficult to generate in the so-called warm-dense-matter (WDM) regime, where both strongly coupled ($\Gamma > 1$) and degeneracy effects ($\theta < 1$) are important.²³ In this regime, where traditional classical plasma physics assumptions break down, quantum and many-body effects must be taken into account. Various theoretical models have been developed to predict the EOS of beryllium. *SESAME* EOS²⁴ was constructed using different theoretical models and constrained by the best-available experiment data. The QEOS model²⁵ is a global EOS model based on the simple Thomas–Fermi model developed in the

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1980s. The *INFERNO* model^{26,27} was an atom-in-jellium model that was spherically averaged by taking into account the shell structure of atoms. Self-consistent-field approximation was used in this model, and exchange correlation was introduced to model the many-body and quantum effects. The *Purgatorio* model²⁸ is an upgraded implementation of an *INFERNO* algorithm. Again, both models treat a single average atom in the plasma media. In the past, Benedict *et al.*²⁹ had also constructed an EOS table for Be by using these models. They constructed a multiphase EOS for Be by performing *ab initio* free-energy calculations in both solid and liquid phases. At very high temperatures, the EOS was obtained using the *Purgatorio* model.

Quantum molecular dynamics (QMD),^{30–32} based on the density-functional theory (DFT), has proven to be a reliable method for studying the many-body quantum systems of dense plasmas. QMD simulations have been shown to work well for EOS calculations such as deuterium,^{15,33} CH,^{34,35} silicon,^{36,37} carbon,³⁸ and quartz.³⁹ The most-recent first-principles calculations,^{34,37} which combined the orbital-based-DFT Kohn–Sham molecular dynamics (KSMD) and orbital-free molecular dynamics (OFMD), have established wide-ranged and consistent first-principles EOS (FPEOS) tables for CH and silicon. These studies have also indicated that the observed EOS differences can have significant effects on hydro-simulations. Since beryllium has been considered an efficient ablator for ICF targets, in this work we use first-principle calculations to establish a Be-EOS table in a much wider range of plasma conditions than the limited conditions ($\rho = 4$ to 6 g/cm^3 and $T = 1$ to 10 eV) previously studied.⁴⁰

In this paper, QMD simulations were used to calculate the Be-EOS table for a wide range of densities ($\rho = 0.001 \text{ g/cm}^3 \sim \rho = 500 \text{ g/cm}^3$) and temperatures ($T = 2000 \text{ K}$ to $T = 10^8 \text{ K}$). From the established FPEOS table, we derived the principal Hugoniot curve using the Rankie–Hugoniot equation and compared our calculations with several theoretical models and available experimental data. We also studied the pressure and internal energy differences between FPEOS and *SESAME* 2023 for off-Hugoniot conditions. With the implementation of our FPEOS table of beryllium into our radiation–hydrodynamics code *LILAC*, we investigate the EOS effects on ICF simulations.

The paper is organized as follows: The QMD method is presented in Sec. II. Our FPEOS Hugoniot curve is compared with several theoretical and experimental data in Sec. III. The off-Hugoniot comparisons between FPEOS and *SESAME* 2023 are shown in Sec. IV. In Sec. V, the FPEOS is implemented into *LILAC* to investigate how the different EOS tables will affect ICF implosions using beryllium as the ablator. Our summary is presented in Sec. VI.

II. SIMULATIONS OF QUANTUM MOLECULAR DYNAMICS BASED ON THE DENSITY-FUNCTIONAL THEORY

In recent years, first-principles methods (or *ab initio*), including the DFT-based QMD,^{41–45} path-integral Monte Carlo (PIMC),⁴⁶ and quantum Monte Carlo (QMC),^{47,48}

have made substantial progress in predicting the properties of materials at extreme conditions. QMD, combining the laws of quantum mechanics and classical molecular dynamics, has been proven to be an effective computational approach to treating materials under extreme conditions. Based on the finite-temperature density-functional theory, traditional QMD implementation uses the Kohn–Sham orbitals^{49,50} to represent the many-particle system in terms of single-particle orbitals (denote as “KSMD”). The KSMD method is accurate and computationally efficient at temperatures generally below the electron Fermi temperature T_F . At the high-temperature region ($T > T_F$), however, it becomes impractical because of the increasing number of energy bands needed to represent the thermal-excited electrons according to Fermi–Dirac distribution. In contrast, the other QMD implementation is OFMD,⁵¹ which greatly improves the computational efficiency by eliminating orbitals. In the OFMD treatment, the total free energy of a many-particles system is expressed only in terms of electron density according to an improved Thomas–Fermi–Dirac (TFD) model. The computational efficiency at $T > T_F$ is at the expense of precision resulting from the approximation of the TFD model. Nonetheless, the pressure predicted by OFMD differs from the KSMD prediction by only 1% in the vicinity of Fermi temperature where both methods are applicable.

A. KSMD

The Vienna *ab initio* simulation package (VASP),^{52–55} one of the implementations of KSMD with finite-temperature DFT utilizing a plane-wave basis, was used to perform our low-temperature ($T < T_F$) calculations. In order to make the wave function near the core regions smoother, a projector-augmented wave (PAW) pseudopotential was generated to replace the pure Coulomb potential. The electron exchange-correlation potential is modeled by the Perdew–Burke–Ernzerhof (PBE) functional in the generalized-gradient approximation (GGA).⁵⁶ The electrons are described by quantum-mechanical wave functions, and the nuclei (ions) are treated as classical particles governed by the Newtonian mechanics.

A cubic reference cell containing 128 Be atoms (64 or 32 at low density) represents the basic work unit in our simulations. The volume of the cubic cell is determined by the mass density. Initially, we set the ions and electrons of the beryllium in the thermodynamic equilibrium with the same temperature. The initial position R and the momentum P are determined by the input parameters (temperature and density). The volume of the reference cell is determined by the number of atoms and the density. The periodic boundary condition was applied to the basic cell to simulate the real plasma environment. The dynamics of the system were calculated in a repeated two-step process: First, we treated the electrons quantum mechanically and found the electronic wave function by solving the Kohn–Sham equations, from which the electronic forces acting on the ions are determined; second, the time evolution of the ions was calculated using Newton’s second law. This two-step QMD cycle was repeated for thousands of time steps, from which the thermodynamic EOS quantities can be determined. In our KSMD simulation, the density varied from $\rho = 0.1 \text{ g/cm}^3$ to $\rho = 50.0 \text{ g/cm}^3$ and the

temperature ranged from $T = 2000$ K to $T = 250\,000$ K. The number of the energy bands changed from 300 to 3800, and the electronic occupation of the highest band was less than 10^{-5} . The time step varied from $\delta t = 2.0$ fs to $\delta t = 0.1$ fs, depending on density and temperature. The PAW potential used all four active electrons with a core radius of $R = 1.3$ bohr. The maximum cutoff energy (ENMAX) was set to $\text{ENMAX} = 2000$ eV. Convergence has been reached for these parameter sets.

B. OFMD

The OFMD⁵¹ method describes the ground-state energy of a many-particle system as a function of electronic density without constructing Kohn–Sham orbitals.⁵⁰ The main feature that distinguishes the OFMD from the KSMD is the expression for the kinetic-energy term. In the OFMD approach, the kinetic energy is derived using the TFD model at a finite temperature plus the von Weizsäcker correction taking into account the gradient correction of electron density. In OFMD simulations, we assume that the beryllium plasmas are in the local thermodynamic equilibrium (LTE); relativistic effects in our simulation region are negligible; and bound states and continuum states are treated in the same way. The cutoff radius was chosen to be less than 10% of the Wigner–Seitz radius to avoid the overlap of regularized ion spheres. The exchange–correlation functional is expressed in the local density approximation of Perdew and Zunger.⁵⁷ The time evolution of the system was also calculated in two steps. The electrons were treated quantum mechanically and ions were classical particles. The difference here is that we minimized the electron-free energy with respect to the electron density directly, rather than minimizing with respect to the orbitals in the KSMD case. In OFMD simulations, we also used 128 atoms in a cubic cell with periodic boundary conditions. The density varied from $\rho = 0.001$ g/cm³ to $\rho = 500$ g/cm³; the temperature ranged from $T = 125\,000$ K to $T = 10^8$ K. The time step varied from $\delta t = 0.116$ fs to $\delta t = 1.9 \times 10^{-4}$ fs. Finally, the EOS quantities of pressure and internal energy were directly evaluated in our OFMD simulations.

Combining the calculations of KSMD and OFMD, we examined the widely ranged beryllium conditions in the pressure–temperature (P – T) space. The pressure and internal energy were obtained for all the sampled density and temperature points ($\rho = 0.001$ to 500 g/cm³ and $T = 2000$ to 10^8 K). We make the transition from KSMD to OFMD at the temperature point $T = 250\,000$ K, where their differences are within $\sim 1\%$. The total pressures as a function of the beryllium temperature are shown in Fig. 1 for different densities. We plot the temperature ranging from $T = 10^2$ K to $T = 10^8$ K and the pressure ranging from $P = 10^{-5}$ Mbar to $P = 10^7$ Mbar. It is noted that we have done extrapolations to extend the temperatures down to zero Kelvin. Overall, we ascertain that the FPEOS table of Be presented here is accurate within an error bar of $\sim 1\%$ in both pressure and internal energy. The Be-FPEOS table established here is available as an open source data set for the community (upon request).

FIG. 1. The pressure as a function of beryllium plasma temperature for all densities ($\rho = 0.001$ to 500 g/cm³) by our first-principle Kohn–Sham and orbital-free molecular dynamics calculations.

III. COMPARISONS BETWEEN FPEOS AND SESAME EOS FOR THE PRINCIPAL HUGONIOT

The shock Hugoniot curve can be derived from the resulted FPEOS table according to the Rankine–Hugoniot equation

$$\text{Hug} = E_f - E_0 + \frac{1}{2}(P_f + P_0)\left(\frac{1}{\rho_f} - \frac{1}{\rho_0}\right) = 0,$$

where the initial pressure, internal energy, and density of the beryllium before the shock are represented by (P_0, E_0, ρ_0) and the quantities after shock are given by (P_f, E_f, ρ_f) .

To reach low- T conditions outside our calculation range (2000 K to 10^8 K), we have extrapolated our EOS table from the lowest-temperature points in our KSMD calculations, guided by direct KSMD calculations. To compute the principal Hugoniot, we chose the initial state to be the solid beryllium, ($\rho = 1.84$ g/cm³) at ambient temperature ($T = 300$ K). Substituting the EOS data into the Hugoniot equation, we can derive the principal Hugoniot of Be. We compare the beryllium FPEOS Hugoniot curve with the *SESAME* model,²⁴ the *Purgatorio* model,²⁸ the QEOS model,²⁵ *INFERNO*,^{26,27} and experimental data^{17–22} in Fig. 2, in which the Hugoniot pressure is plotted as a function of shock density. These EOS models, even built decades ago, are still used for ICF and HED plasma simulations. For example, the average-atom based *INFERNO* and its improved version *Purgatorio* models were used as the building-blocks for constructing the Livermore Equation-of-State (LEOS) tables; While the QEOS is still being used, in spite of its inaccuracy in warm-dense matter regime, for electron-ion temperature relaxation modeling in a recent paper,⁵⁸ due to its analytical simplicity, *SESAME* EOS²⁴ was constructed using various combinations of different theoretical models and constrained by the best-available experimental data in different regions. The standard approach of *SESAME* assumes that three parts contribute to the Helmholtz

FIG. 2. The Rankine-Hugoniot curve of beryllium predicted by the first-principles equation of state (FPEOS) (solid blue line) is compared with the *SESAME* 2023 model²⁴ (dashed red line), the *Purgatorio* model²⁸ (dotted-dashed green line), the *QEOS* model²⁵ (dashed orange line), the *INFERNO* model^{26,27} (dotted-dashed blue line), and available experiments (various symbols) by Regan,¹⁷ Cauble *et al.*,^{19,20} Isbell *et al.*,²¹ and Nellis *et al.*²²

free energy: the zero-temperature isothermal (cold curve), the thermal ionic part, and the thermal electronic part. The thermal electronic part is based on the TFD theory at finite temperature; the ionic part is modeled with the Debye theory; and the zero-temperature isothermal is constructed from the shock-wave data and calculations based on the Mie-Grüneisen theory. The quotidian equation-of-state (*QEOS*) model²⁵ also decomposed the Helmholtz free energy into three parts: ion-free energy, electron-free energy, and a semi-empirical correction for chemical bonding effects and quantum effects. The ion thermodynamic properties were constructed by a multiphase EOS, combining the Debye model for the solid Lindemann melting law⁵⁹ and a fluid scaling law. The electron-free energy was calculated using the modified TFD theory without exchange; the correlation is not complete since it considers only plasma ion correlation through the ion-sphere model assuming weak coupling. In general, the *QEOS* model predicts more ionization due to its underestimation of the negative electron-ion interactions, especially in the intermediate density range. This results in less compressible behavior for most materials including Be.

The *INFERNO* model^{26,27} is a spherically averaged atom-in-jellium model,⁶⁰ which improves the *ion-spherical model* by introducing the self-consistent-field (SCF) approximation.⁶¹ The electron density is written as the sum of normalized one-electron orbital functions. The free energy of the system is expressed in terms of the electron density. Exchange and correlation terms are modeled using local density approximations. Minimizing the free energy with respect to density yields one-electron Dirac equations, which can be solved self-consistently. A finite number of bound states and a continuum state are treated equally to ensure the continuity thermodynamic quantities by numerical differentiation. However, the single-particle orbitals can spread out over the boundary of the cell. There is no effective way to separate the cell from outside media. The *Purgatorio* model²⁸ is an upgraded implementation of the *INFERNO* model, which

treats continuum-state resonances by improving the automated quadrature method. Phase-amplitude algorithms were used for continuum orbitals. Again, both models treat a single average atom in the plasma media.

Figure 2 shows that the FPEOS Hugoniot pressure of beryllium is in good agreement (within 10%) with the widely used *SESAME* model (*SESAME* 2023) in the low-compression-ratio region ($\rho/\rho_0 < 3$); however, the pressure differences can be up to 30% in the high-compression region. For example, at a constant pressure of 26 Mbar, the FPEOS table predicted a shock density of $\rho \approx 5.8 \text{ g/cm}^3$, while the *SESAME* table gives a shock density of $\rho \approx 6.0 \text{ g/cm}^3$ —a difference of $\sim 3\%$. At constant density $\rho = 4.7 \text{ g/cm}^3$, the FPEOS table predicts that the Hugoniot pressure should be 8.5 Mbar, which is $\sim 8\%$ higher than the pressure predicted by *SESAME* (~ 7.8 Mbar). For a high density of $\rho = 7.8 \text{ g/cm}^3$, however, the *SESAME*-predicted shock pressure ($P \sim 357.6$ Mbar) is $\sim 20\%$ higher than FPEOS calculations ($P \sim 285.7$ Mbar). Figure 2 also shows that the peak compression ratio decreases slightly from 4.33 (FPEOS calculation) to 4.26 (*SESAME* prediction), which indicates that under shock compression, beryllium is slightly softer than the *SESAME* model near the maximum compression. As the shock pressure continues to increase, the density predicted by both the FPEOS and *SESAME* reaches an ideal gas limit ($\rho/\rho_0 = 4$).

Figure 2 also indicates that under shock compression, beryllium is slightly softer in FPEOS than predicted by *QEOS*. This is mainly because the *QEOS* model overestimates the ionization of electrons, leading to too-large a pressure along the Hugoniot curve for the same shock density. It also shows that the shock Hugoniot curve of beryllium is much stiffer in FPEOS than *INFERNO* and *Purgatorio* predictions. The peak compression ratio predicted by the *INFERNO* and *Purgatorio* models is $\sim 10\%$ higher than FPEOS. This level of discrepancy could lead to a significant difference in hydro simulations. Experimental data for beryllium have also been plotted in Fig. 2 for comparison. Several experimental methods have been used to generate shock waves, from explosion driven to laser driven. In the pressure region under 10 Mbar, our FPEOS's are in good agreement with these experiments (see the inset in Fig. 2). Most of models seemed to agree well with the available experimental data except the *QEOS* model, which generally overestimates the Hugoniot pressures. To the best of our knowledge, no published experiments data have been found above 20 Mbar. Future experimental data are needed to benchmark the theoretical models in the pressure region ranging from 50 Mbar to 500 Mbar.

Finally, we plotted the shock temperature as a function of shock pressure in Fig. 3(a) along the principal Hugoniot. The ion-ion pair correlation functions $g(r)$ are shown in Fig. 3(b) to study the structure change along the principal Hugoniot. Figure 3(a) indicates that the shock temperature predicted by FPEOS is $\sim 5\%$ to 8% lower than the *SESAME* prediction. Figure 3(b) shows that the ion-ion pair correlation changes for four different densities and temperatures. Note that the peaks in the pair correlation function gradually disappear as the density and temperature increase from $T = 31\,250 \text{ K}$ and $P = 7.99 \text{ Mbar}$ to $P = 27.4 \text{ Mbar}$,

FIG. 3. (a) The shock-temperature comparison between FPEOS and SESAME; (b) the quantum molecular dynamics (QMD)-predicted pair correlation functions of Be shock approximately along the principal Hugoniot at temperature $T = 2000$ K, $T = 15\,625$ K, $T = 31\,250$ K, and $T = 125\,000$ K.

respectively, which indicates a change in the material structure from solid state to liquid state.

IV. COMPARISONS BETWEEN FPEOS AND SESAME EOS FOR OFF-HUGONIOT CONDITIONS

Next, we compare the pressure and internal energy of beryllium plasma for off-Hugoniot plasma conditions between FPEOS and SESAME 2023 in Figs. 4–11. Figure 4(a) shows the pressure as a function of density for beryllium at $T = 31\,250$ K, $T = 125\,000$ K, and $T = 250\,000$ K, while the internal energy comparisons are plotted in Fig. 4(b). Figure 4(b) indicates that the internal energy per atom reaches minimum at density ~ 2.5 g/cm³ for $T = 31\,250$ K; this internal energy minimum, manifesting the maximum electronic-ion interaction, increases with temperature, and the corresponding density having minimum internal energy also increases with temperature.

In order to compare the differences between the two EOS models, we plot the pressure differences in percentage between FPEOS and SESAME versus the density at $T = 31\,250$ K in Fig. 5(a), while the internal energy differences are plotted in Fig. 5(b). Figure 5(a) indicates that FPEOS pressure is lower than SESAME pressure within 20% for low density ($\rho < 2$ g/cm³). The trend is reversed, however, for the high-density region ($\rho > 2$ g/cm³). In other words, FPEOS pressure is higher than SESAME pressure for $\sim 7\%$ at $\rho = 3$ to 5 g/cm³. The difference in internal energy shows a similar trend with a difference on the level of $\sim 5\%$. Similar to Fig. 5, Fig. 6 compares FPEOS and SESAME for $T = 125\,000$ K. In this

higher-temperature situation, we notice that the zero-crossing density point approaches ~ 5 g/cm³. The maximum pressure and internal energy differences are $\sim 20\%$ and $\sim 10\%$, respectively. At $T = 250\,000$ K, we plot the comparisons in Fig. 7 in the same way. We can no longer see the cross point in the pressure difference diagram. The differences between FPEOS and SESAME are still within 20% and $\sim 5\%$ for pressure and internal energy, respectively.

In addition to the isothermal condition, we also compare the pressure and internal energy differences between FPEOS and SESAME at constant density, plotted in Figs. 8–11 as functions of temperature. Figure 8(a) shows the pressure as a function of temperature for beryllium at $\rho = 5$ g/cm³, while the internal energies are compared in Fig. 8(b). From the figures, we see that both pressure and internal energy differences are quite small between FPEOS and SESAME in log-scale plots. To better analyze the data, we plot the percentage differences between FPEOS and SESAME versus the temperature for densities of $\rho = 5$ g/cm³, $\rho = 10$ g/cm³, and $\rho = 50$ g/cm³, respectively, in Figs. 9–11. Figure 9(a) indicates that SESAME-predicted pressure is $\sim 6\%$ lower than FPEOS for $T = 10^5$ K. The trend reverses, however, in the high-temperature region $10^5 < T < 10^7$ K also with a cross zero point. The pressure differences between FPEOS and SESAME reach maximum in the warm dense region $T \sim 10^5$ to 10^6 K, where interparticle interactions strongly affect the property of the plasma. For temperatures higher than 10^7 K, FPEOS and SESAME are in good agreement as the two EOS models both reach the ideal gas limit correctly. Similar to

FIG. 4. The off-Hugoniot equation-of-state (EOS) isothermal comparisons between FPEOS and SESAME 2023. The (a) pressure and (b) internal energy are plotted as functions of the beryllium density for $T = 31,250$ K, $T = 125,000$ K, and $T = 250\,000$ K.

FIG. 5. The (a) pressure and (b) internal energy differences in percentage are shown as functions of density at $T = 31\,250\text{ K}$.

FIG. 6. The (a) pressure and (b) internal energy differences in percentage are shown as functions of density at $T = 125\,000\text{ K}$.

FIG. 7. The (a) pressure and (b) internal energy differences in percentage are shown as functions of density at $T = 250\,000\text{ K}$.

FIG. 8. The off-Hugoniot EOS isochoric comparisons between FPEOS and SESAME 2023. The (a) pressure and (b) internal energy are plotted as functions of the plasma temperature for beryllium at $\rho = 5\text{ g/cm}^3$.

FIG. 9. The (a) pressure and (b) internal energy differences in percentage are shown as functions of temperature at $\rho = 5 \text{ g/cm}^3$.

FIG. 10. The (a) pressure and (b) internal energy differences in percentage are shown as functions of temperature at $\rho = 10 \text{ g/cm}^3$.

FIG. 11. The (a) pressure and (b) internal energy differences in percentage are shown as functions of temperature at $\rho = 50 \text{ g/cm}^3$.

Fig. 9, Figs. 10 and 11 show the EOS comparisons for the cases of $\rho = 10 \text{ g/cm}^3$ and $\rho = 50 \text{ g/cm}^3$. At these two higher-density conditions, the maximum discrepancy also appears at a temperature around $T \sim 10^6 \text{ K}$. In general, the differences between *SESAME* and *FPEOS* are within 10% to 20%. In some special cases, for example at $\rho = 7.8 \text{ g/cm}^3$ along the Hugoniot curve, the difference can be up to 30%. Next, we will explore how the EOS differences will affect the ICF/HED high-energy-density plasma situation.

V. THE EFFECTS OF BERYLLIUM FPEOS ON HED-PLASMA SIMULATIONS

Implementing the *FPEOS* table of beryllium into our radiation-hydrodynamics code *LILAC*, we can examine the EOS effects on HED plasma simulations. As mentioned previously, we have extrapolated our EOS table to a

low-temperature point outside our calculation range (2000 K to 10^8 K), guided with direct KSMD calculations at low temperatures. The range of the extrapolated EOS table is wide enough for *LILAC* simulations. Since plasmas generally undergo several regimes including both strongly coupled and degenerate regions during the ICF implosion, an integrated ICF implosion can be used to study the EOS effects. In this section, we simulate a National Ignition Facility (NIF)-type direct-drive implosion. Figure 12 shows the step laser pulse and dimensions of the target. The duration of the laser pulse is 10 ns with a total energy of 1.5 MJ. The capsule of the simulation had a 80- μm Be layer filled with deuterium-tritium (DT) gas. The initial pressure of the gas was 3 atm. We launched two simulations: one used beryllium *FPEOS* and the other used the *SESAME-2023*. For DT gas the two simulations used the same *FPEOS* table¹⁵ and the first-principles opacity table.⁶² Both simulations used the same nonlocal

FIG. 12. The dimensions of the target (inset) and the laser pulse shape for implosion simulations to study how EOS differences will affect hydro simulations. The capsule was made of a 80- μm Be layer filled with 1420 μm of deuterium–tritium (DT) gas. The duration of the step laser pulse was 10 ns with a total energy of 1.5 MJ.

thermal-transport model⁶³ and cross-beam energy transfer modeling⁶⁴ in the laser-absorption package. The results of 1-D *LILAC* radiation–hydrodynamic simulations are shown in Figs. 13 and 14, which compare both density and electron temperature profiles predicted by FPEOS (solid blue line) and *SESAME* 2023 (dashed red line) simulations. Once the lasers were launched, the Be layer was ablated, which resulted in a shock propagating into the shell.

Figure 13 shows a snapshot of the density and temperature profiles at $t = 2.2$ ns versus the target radius for two simulations. At this time, the first shock front was located at $R \sim 1436$ μm with the main shock behind it, which indicates that the shock was still propagating inside the Be layer. We can see that the FPEOS simulation predicts a slightly lower density ($\sim 2\%$) than the *SESAME* simulation since the FPEOS is slightly stiffer than *SESAME* EOS in the temperature region $T = 10^4$ to 10^5 K as we compared in Sec. II. The shock location in the FPEOS simulation is almost the same as in the *SESAME* case. The reason behind this phenomenon is that shock speed (V_s) depends on the shock density (ρ_s) through the formula of $V_s = \sqrt{P_s/\rho_0}/\sqrt{1 - \rho_0/\rho_s}$, from

FIG. 13. The density and temperature profile comparisons between the FPEOS (solid blue line) simulation and *SESAME* 2023 (dashed red line) simulation. At time $t = 2.2$ ns, the shock front is located at $R \sim 1446$ μm , which indicates that the shock is still propagating inside the Be layer.

which we obtain a very small difference ($\sim 0.7\%$) in shock speed. In addition, the hydro simulation with FPEOS predicts an $\sim 4\%$ lower temperature than the *SESAME* case. This will also result in a slightly smaller mass ablation rate of beryllium.

We also took a snapshot [in Fig. 14(a)] at $t = 10$ ns, where the shell was at the end of acceleration, and plotted both the density profile and the electron temperature profile as functions of the target radius. One sees from Fig. 14(a) that the peak density predicted by the FPEOS is $\sim 3\%$ lower than predicted by *SESAME* simulations. The temperature at peak density predicted by FPEOS was ~ 16.6 eV, while the *SESAME* prediction was ~ 15.7 eV—a difference of $\sim 6\%$. We can see that at the back surface of the shell, there are more significant temperature differences ($\sim 18\%$). Figure 14(b) plots density and ion temperature as functions of radius at the peak compression ($t = 12$ ns). In these situations, the differences between FPEOS and *SESAME* simulations are small even for peak density as with the temperature increase above $T > 10^6$ K.

Finally, we compared the overall target performance between the FPEOS and *SESAME* simulations, which indicated that the peak areal density of the FPEOS simulation was $\rho R = 1.60$ g/cm², only $\sim 1\%$ higher than the *SESAME* simulation, which reached $\rho R = 1.58$ g/cm². The FPEOS

FIG. 14. Same as Fig. 13 but for different implosion times: (a) $t = 10$ ns, where the shell is at the end of acceleration and (b) $t = 12$ ns, where it is at peak compression.

simulation also predicted a higher total neutron yield ($Y = 3.76 \times 10^{14}$), which is $\sim 15\%$ higher than the *SESAME* simulation, ($Y = 3.28 \times 10^{14}$). In summary, the EOS differences of beryllium between FPEOS and *SESAME* have small impacts on 1-D implosion simulations. The discrepancies of the main overall target performance between the two simulations are within 15%. We anticipate, however, that ICF/HED simulations using the *INFERNO* and *Purgatorio* models will result in much larger differences than the FPEOS simulations since the two EOS models give too soft a Hugoniot as seen in Fig. 2.

VI. CONCLUSION

We have used the two first-principles methods of KSMD and OFMD to calculate the EOS of beryllium for wide density and pressure conditions, from which we established the FPEOS table for beryllium. The densities of our calculations range from $\rho = 0.001 \text{ g/cm}^3$ to $\rho = 500 \text{ g/cm}^3$ and the temperatures range from $T = 2000 \text{ K}$ to $T = 10^8 \text{ K}$, which covers both WDM regime and the ideal plasma region. From the established FPEOS table of Be, we have derived its principal Hugoniot curve, which is investigated in detail by comparing it with several theoretical models and available experiments. We found that our FPEOS Hugoniot curve agrees quite well with experimental data. The Hugoniot pressure predicted by FPEOS is $\sim 10\%$ higher than the widely used *SESAME* 2023 table of beryllium in a low-compression region ($\rho/\rho_0 < 3$). With an increase in pressure, the Hugoniot pressure of FPEOS can be up to $\sim 30\%$ lower than *SESAME*. The peak compression ratio calculated by FPEOS is in good agreement with *SESAME* predictions with differences within $\sim 2\%$. However, the *INFERNO* and *Purgatorio* models predict a much softer Hugoniot curve in a higher-compression region. As for the off-Hugoniot condition, both the pressure differences and internal energy differences are within $\sim 20\%$ maximum between FPEOS and *SESAME* 2023 tables. To examine the EOS effects on HED plasma simulations, we used the 1-D radiation-hydrodynamics code *LILAC* to simulate an ICF implosion with a beryllium shell, using FPEOS or *SESAME* 2023, respectively. During the shell's acceleration process, the discrepancies in the density and temperature profiles between the two equations of state are less than 4%. At peak compression, the density and temperature differences can be up to 18% in maximum. The overall target performance is within $\sim 15\%$ in maximum between FPEOS and *SESAME* 2023 simulations. Even though we had no *INFERNO* and *Purgatorio* EOS models at hand, we expect from our previous experience that FPEOS simulations with a Be ablator will give much different results than the *INFERNO*/*Purgatorio* simulations because the two EOS models show too much ($\sim 10\%$) softening in their shock Hugoniot.

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