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Applicability of the Mie-Grüneisen Equation of State Model to Warm Dense Matter Conditions

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Abstract

The Mie-Grüneisen (MG) model provides a linear relation between thermal pressure (pressure relative to a reference temperature) and the corresponding thermal energy, which is widely used to interpolate and extrapolate equations of state (EOS) beyond experimental data. However, its applicability to warm dense matter (WDM) conditions, where strong coupling and ionization become significant, remains poorly constrained. Here we assess the validity of the MG approximation using first-principles simulations of representative materials—MgO, H, He, Si, CH₂ and others—spanning the condensed and WDM regimes. Combining finite-temperature density functional theory molecular dynamics (DFT-MD) with path integral Monte Carlo (PIMC), we compute consistent pressure and energy relations over a wide range of densities and temperatures. We show that the proportionality between thermal pressure and thermal energy is linear function of density but does depend on temperature, allowing us to build an effective Grüneisen parameter $\gamma(V, T)$. However, systematic deviations appear at high temperatures where ionization effects introduce significant temperature dependence in γ . These results establish the quantitative limits of the Mie-Grüneisen framework in the WDM regime and provide a benchmark for constructing wide-ranging EOS models relevant to inertial confinement fusion and planetary interior studies.

KEYWORDS:

Warm Dense Matter, EOS, DFT-MD, PIMC, High pressure, ICF, H, He, Si, C, CH₂, MgO, SiO₂, MgSiO₃

1 | INTRODUCTION

Understanding the behavior of matter under extreme conditions of pressure and temperature is central to a broad range of fields including geophysics, planetary science, inertial confinement fusion (ICF), and warm dense matter^[1] (WDM) research. In these regimes, direct experimental access to thermodynamic properties is often limited, making accurate theoretical and computational equations of state (EOS) indispensable.^[2,3] The EOS not only provides the relationship between density, temperature, pressure, and energy but also serves as a foundation

for determining secondary quantities such as sound velocity, specific heat, and related thermodynamic quantities that are essential to interpreting experiments and modeling dynamic compression processes, such as shock temperatures and thermal expansivity.

For this reason, wide-ranging EOS models are often constructed by combining data from static compression experiments, dynamic compression (shock) experiments, and first-principles simulations.^[4,5] However, the extrapolation of these data to off-Hugoniot or off-isentrope conditions requires additional simplifying assumptions. One of the most widely used models for this purpose is the Mie-Grüneisen (MG) formulation of the EOS, in which the thermal pressure difference is

approximated as

$$[P(V, T) - P(V, T_0)] \approx \frac{\gamma}{V} [E(V, T) - E(V, T_0)], \quad (1)$$

where

$$\gamma(V, T) \equiv V \left(\frac{\partial P}{\partial E} \right)_V = - \left(\frac{\partial \ln T}{\partial \ln V} \right)_S \quad (2)$$

is the Grüneisen parameter, which enters many thermodynamic relationships and characterizes processes such as ramp compression^[6] and how rapidly the temperature increases in the interior of a convecting planet or star. Here, $P(V, T_0) \equiv P_{\text{ref}}(V)$ and $E(V, T_0) \equiv E_{\text{ref}}(V)$ are the pressure and internal energy values along an isotherm of reference temperature T_0 , typically the cold curve ($T_0 = 0$) for solids and some high temperature for liquids. We can interpret Eq. (1) as a first-order Taylor expansion of the pressure as a function of energy along an isochore, provided that $\gamma(V) \approx \gamma(V, T_0)$ is independent of temperature. The success of the MG model stems from the empirical observation that pressure increases linearly with the internal energy of a material as temperature is increased along an isochore of volume V . The ratio γ/V is therefore assumed to be independent of temperature and, in some cases, independent of volume as well, such that the slope $(\partial P / \partial E)_V = \gamma_0 / V_0$ becomes constant for all volumes and temperatures ($\gamma_0 \rho_0 = \gamma \rho = \text{constant}$, where ρ is the mass density). Thus, the pressure at higher temperatures and the isentropic temperature profiles can be inferred for any volume V from a single measurement of γ , provided one can model the energy $E(V, T)$ accurately. This property has made the model a standard tool for estimating thermodynamic states that are inaccessible to experiment that are conducted in diamond anvil cells or with dynamic compression techniques.^[7–14]

The Grüneisen parameter is not only a fundamental quantity in theoretical descriptions of high-temperature and high-pressure materials, but it also plays a central role in interpreting experimental data. In studies of silicate liquids, such as MgSiO_3 at super-Earth mantle conditions,^[8,10,15] measurements of sound velocity combined with pressure-density compressibility along the Hugoniot curve allow direct determination of γ , which in turn constrains the adiabatic temperature profile of the material (see Eq. (2)). Moreover, in inertial confinement fusion (ICF) experiments, the Mie–Grüneisen EOS is widely used to model the off-Hugoniot response of ablator materials such as polystyrene and GDP.^[7] By combining Hugoniot measurements, sound velocity, and multiple-shock release behaviors, experimentalists can predict pressure and temperature states in subsequent shocks, assess hydrodynamic instabilities, the effect of material composition and phase changes on the EOS. Across these applications, the Grüneisen parameter provides a practical link between thermodynamic observables and material response under extreme conditions, guiding both interpretation of high-pressure experiments and the construction of EOS models that are valid over wide ranges

of density and temperature. These examples highlight the experimental relevance of the Mie–Grüneisen framework and motivate a detailed first-principles study of $\gamma(V, T)$ in the WDM regime, which can provide complementary insights to both planetary science and high-energy-density physics.

Nevertheless, the simplicity of the Mie–Grüneisen approach conceals important assumptions. It implicitly treats $\gamma(V)$ as a single-parameter description of anharmonic and electronic contributions to the thermal pressure, and assumes that these effects scale uniformly with internal energy. These approximations may fail in materials that undergo electronic excitation and ionization, typical of the warm dense regime. In such cases, deviations from the Mie–Grüneisen prediction are expected and they can significantly affect estimates of off-Hugoniot states, sound velocities, and energy transport properties, which in turn propagate into hydrodynamic modeling of fusion targets or planetary mantles.

In this work, we use previously published first-principles density functional theory molecular dynamics (DFT-MD) and path integral Monte Carlo (PIMC) equation-of-state data to critically assess the validity and limitations of the Mie–Grüneisen model. By analyzing fully consistent $P(V, T)$ and $E(V, T)$ relations for a series of compositions—metallic magnesium (Mg), ionic magnesium oxide (MgO), and enstatite (MgSiO_3)—we directly evaluate how well the Mie–Grüneisen form reproduces the thermal pressure obtained from DFT-MD simulations. We further analyze the volume and temperature dependence of the Grüneisen parameter. These comparisons allow us to quantify the intrinsic errors associated with the model and to identify regimes where its use remains valid versus where more complete EOS formulations are required. Beyond their methodological importance, these results have direct implications for the interpretation of shock and ramp-compression experiments and for the construction of wide-ranging EOS tables^[16] used in WDM and fusion research.

2 | METHODS

2.1 | Generating EOS from first-principle simulations

We build our EOS tables by performing simulations over a wide range of temperatures and densities using two complementary first principles methods: path integral Monte Carlo (PIMC) and finite-temperature Kohn–Sham density functional theory molecular dynamics (DFT-MD) simulations. Together, these methods provide a consistent description of a material from the condensed-matter regime to the warm dense and plasma states.

2.1.1 | Path Integral Monte Carlo Simulations

Path integral Monte Carlo calculations^[17–19] are the most appropriate and efficient first principles simulation techniques for a quantum system at high temperature where a substantial fraction of the electrons are excited. The PIMC approach is based on the thermal density matrix at temperature T , which can be written as a product of M density matrices at a higher temperature $M \times T$,

$$\hat{\rho} \equiv e^{-\beta \hat{H}} = \left(e^{-\tau \hat{H}} \right)^M. \quad (3)$$

$\beta = 1/k_B T$ plays the role of imaginary time and $\tau = \beta/M$ is the corresponding time step. At very high temperature where many-body correlation effects are weak excellent approximations exist for the thermal density matrix^[20,21]. Many-body correlations are then recovered by the matrix product in Eq. 3, which becomes an integral in imaginary time when one writes it in position space,

$$\langle \mathbf{R} | \hat{\rho} | \mathbf{R}' \rangle = \int d\mathbf{R}_1 \dots \int d\mathbf{R}_{M-1} \quad (4)$$

$$\langle \mathbf{R} | e^{-\tau \hat{H}} | \mathbf{R}_1 \rangle \langle \mathbf{R}_1 | e^{-\tau \hat{H}} | \mathbf{R}_2 \rangle \dots \langle \mathbf{R}_{M-1} | e^{-\tau \hat{H}} | \mathbf{R}' \rangle \quad (5)$$

where $\mathbf{R}_1$ through $\mathbf{R}_{M-1}$ represent the position vector of all particles as they travel in imaginary time from $\mathbf{R}$ to $\mathbf{R}'$. To evaluate the canonical partition function,

$$Z = \int d\mathbf{R} \langle \mathbf{R} | \hat{\rho} | \mathbf{R} \rangle, \quad (6)$$

only closed paths need to be considered while open paths are needed to compute the momentum distributions^[19,22–24] and other properties. Eq. 6 assumes the particles are distinguishable. For bosons and fermions one needs to project out the states of the corresponding symmetry, which is typically done by introducing a sum over permutations of identical particles, σ ,

$$Z_{B,F} = \frac{1}{N!} \sum_{\sigma} (\pm 1)^{\text{sgn}(\sigma)} \int d\mathbf{R} \langle \mathbf{R} | \hat{\rho} | \hat{\sigma} \mathbf{R} \rangle, \quad (7)$$

For fermionic systems, the permutations enter with alternating signs, which is a manifestation of the Pauli exclusion principle and leads the nearly perfect cancellation of positive and negative contributions, which is the well-known *fermion sign problem*. A direct evaluation with numerical methods leads to an exponential decay in efficiency with decreasing temperature and increasing particle number. D. Ceperley solved the sign problem in fermionic PIMC calculations elegantly but approximately by introducing the *fixed node approximation*^[25,26] that confines the paths to stay within the positive region that is spanned by an approximate trial density matrix. The approach is formally exact if the trial density matrix is exact, which is only known in a few cases like free particles. Here we employ trial density matrices that are constructed from Slater determinants of single-particle density matrices. This approach

becomes exact in the limit of high temperatures where electrons become completely ionized and weakly interacting. The first simulations were all performed to characterize the EOS of hot, dense hydrogen.^[27–32] Later simulations were performed for helium,^[33] carbon and H_2O ,^[34] nitrogen,^[35] oxygen,^[36] aluminum,^[37] and neon^[38] as the PIMC method was extended to simulate elements as heavy as silicon.^[39] In all cases the PIMC results complemented the results with DFT-MD calculations at lower temperature that we will discuss in the next section. The EOS tables for 21 elements and compounds^[40–44] were then combined into a first-principles EOS database,^[16] which invokes the ideal mixing approximation^[41] to compute the shock Hugoniot curves for arbitrary mixtures. Although for a long time it was assumed that the fixed node approximation was unavoidable for investigating fermionic systems of practical interest, it should be stated that significant progress has been made by performing direct calculations with positive and negative terms.^[45]

Recently Xiong and Xiong^[46] employed PIMC simulations of fictitious identical particles to interpolate thermodynamic properties between a bosonic system with $\xi = +1$ and fermionic system with $\xi = -1$ where ξ is base value in Eq. 7. Their approach has since been adapted to PIMC simulations in the regime of warm dense matter,^[47,48] where it allows one to perform very large simulations with up to 1000 particles under low degeneracy conditions.

All our PIMC simulations were performed using our code, CUPID, with periodic boundary conditions, explicitly treating both nuclei and electrons as quantum paths. We verified the convergence of energies and pressures with respect to time-step and system size, ensuring statistical uncertainties below 1% in the computed observables.

2.1.2 | DFT Molecular Dynamics at Finite Temperature

Under temperature–density conditions where electronic excitations are moderate and quantum degeneracy remains significant, we employed Kohn–Sham density functional theory molecular dynamics (DFT-MD) simulations^[49–51] to complement the PIMC results at higher temperatures. In this approach, the electrons are treated quantum-mechanically within the finite-temperature Mermin extension of DFT, while the ions evolve classically according to the forces derived from the instantaneous electronic density. Within the Born–Oppenheimer approximation, the ionic forces are obtained from the electronic ground-state free energy via the Hellmann–Feynman theorem. This combination provides a fully self-consistent description of the coupled electron–ion system.

All DFT-MD simulations were carried out with the VASP^[52] code using the projector-augmented wave (PAW) formalism.^[53,54] Depending on the material, we employed

the ground-state Perdew–Burke–Ernzerhof (PBE) generalized gradient approximation^[55] or the local density approximation (LDA) exchange–correlation functional,^[50] choosing LDA at high densities where local effects dominate. Electronic thermal excitations were included via the finite-temperature Mermin functional. The details of the parameters used for each material (number of atoms, simulation time, time step, plane-waves, k -points used, etc.) are described in detail in our earlier work.^[16]

By combining PIMC and DFT-MD results, we obtain a seamless equation of state for each material covering temperatures from the condensed phase to the fully ionized plasma regime. The overlap between the two methods provides a cross-validation region that ensures the internal consistency of the computed pressures and energies.

2.2 | Thermodynamic Models

The Mie–Grüneisen (MG) model provides a simple framework to describe thermal contributions to pressure and energy in condensed matter systems. In this model, shown in Eq. 1, the thermal pressure is assumed to be proportional to the thermal energy through the Grüneisen parameter, as expressed in

$$P_{\text{th}}(V, T) \approx \frac{\gamma(V)}{V} E_{\text{th}}(V, T), \quad (8)$$

where the thermal components are defined as

$$P_{\text{th}}(V, T) \equiv P(V, T) - P(V, T_0), \quad (9)$$

$$E_{\text{th}}(V, T) \equiv E(V, T) - E(V, T_0). \quad (10)$$

Here, T_0 is a reference temperature, typically the 0 K cold curve for solids or a chosen reference temperature for liquids. While the Grüneisen parameter γ generally depends on volume V , it is often treated as temperature-independent for simplicity.

Shock-compression experiments frequently rely on the relationship between the Grüneisen parameter, density, and sound speed. The Eulerian, adiabatic sound speed is given by

$$C_s = \sqrt{\left. \frac{\partial P}{\partial \rho} \right|_S}, \quad (11)$$

and can be used to connect measured Hugoniot states, described by the Rankine-Hugoniot equation,

$$H = (E - E_0) + \frac{1}{2}(P + P_0)(V - V_0) = 0, \quad (12)$$

to the Grüneisen parameter through the relation^[8,9,56,57]

$$\gamma(\rho) = 2 \frac{C_s^2 - \left. \frac{dP}{d\rho} \right|_H}{\frac{P}{\rho} - \left. \frac{dP}{d\rho} \right|_H \left(\frac{\rho}{\rho_0} - 1 \right)}, \quad (13)$$

which provides an experimental means to calculate $\gamma(\rho)$ from measured pressure–density data along the Hugoniot curve. These last two relations are exact from thermodynamics and

are essential for interpreting thermodynamic behavior under the extreme conditions relevant to ICF and planetary interiors.

Model 1: volume dependent γ

If the Mie–Grüneisen approximation of Eq. 8 is valid and γ is independent of temperature, then the ratio $P_{\text{th}}/E_{\text{th}}$ should remain constant along an isochore, depending only on volume. In this limit, the volume dependence of γ is often approximated by a simple linear form,^[58]

$$\gamma(V) = \gamma_0 + \gamma' \left(\frac{V}{V_0} - 1 \right), \quad (14)$$

where γ_0 and γ' are fitting parameters that do not depend on temperature. This formulation assumes that thermal effects can be described entirely through the volume dependence of γ and either an increase ($\gamma' > 0$) or decrease ($\gamma' < 0$) with increasing volume can be captured by a linear relationship.

For solids, one often relies on a different empirical relationship, $\gamma = \gamma_0(V/V_0)^q$, while liquids do not show such a strong dependence on volume and one prefers Eq. (14) instead.^[58]

Model 2: temperature and volume dependent γ

At sufficiently high temperatures, deviations from the MG approximation are expected, since electronic excitations can introduce a temperature dependence to γ . In such cases, the proportionality between P_{th} and E_{th} can be expressed as

$$\frac{P_{\text{th}}(V, T)}{E_{\text{th}}(V, T)} \approx a(T)\rho + b(T) \quad (15)$$

where $\rho = m/V$ is the density and m the mass per formula unit. By equating the empirical proportionality in Eq. (15) with the Mie–Grüneisen relation of Eq. (8), one obtains a temperature-dependent Grüneisen parameter,

$$\gamma(V, T) \approx V [a(T)\rho + b(T)] = a(T)m + b(T)V, \quad (16)$$

which allows γ to vary with both V and T .

To explicitly incorporate temperature effects, we adopt the temperature-dependent expression for $\gamma(V, T)$ given by Eq. (16). While this formulation improves empirical agreement at high temperatures, it is not strictly thermodynamically consistent. Expanding the pressure in powers of the energy difference gives

$$P(V, E) = P(V, E_0) + \frac{\gamma(V, T_0)}{V} [E(V, T) - E(V, T_0)] + \frac{1}{2V} \left(\frac{\partial \gamma}{\partial E} \right)_{V, T_0} [E(V, T) - E(V, T_0)]^2 + \mathcal{O}(\Delta E^3), \quad (17)$$

which shows that P_{th} is not strictly proportional to E_{th} when γ depends on E or T . Despite this limitation, such temperature-dependent models often yield a more accurate description of materials under extreme conditions than purely volume-dependent formulations and we can still use Eq. (1) with this temperature-dependent γ .

We will employ both approximations in the following section to develop practical models for the Grüneisen parameter.

Debye-Hückel plasma model

In the weak coupling limit, the thermodynamic functions of a plasma can be approximated by the Debye-Hückel screening model that introduces the parameter,^[59]

$$\kappa^2 = \frac{4\pi}{Vk_B T} \sum_i Z_i^2 N_i, \quad (18)$$

that takes into account all N_i particles with charge Z_i in volume V . The Debye screening radius is given by $r_D = 1/\kappa$. The Debye correction to the pressure and the internal energy per unit volume are given by,

$$P_D = -k_B T \frac{D}{3}, \quad (19)$$

$$E_D = -k_B T D \quad \text{with} \quad D = \frac{\kappa^3 V}{8\pi} \quad (20)$$

Debye-Hückel model thus predicts γ for an ideal, nondegenerate plasma to be,

$$\gamma(V, T) = \frac{2 + \frac{DV}{3N}}{3 + \frac{DV}{N}}, \quad (21)$$

that depends on V and T . The temperature dependence enters via D and κ . With increasing DV/N , as screening effects increase, this function decreases from the ideal gas value of $\gamma_{\text{ideal}} = 2/3$, which explains the high-temperature behavior of our PIMC results that we will discuss in the next section.

3 | RESULTS

We begin by examining how pressure and energy vary with temperature at fixed density, relative to a reference isotherm, using the EOS of MgO as an example.^[40] From our EOS, we use the pressures $P(V, T)$ and energies $E(V, T)$ obtained from our first-principles simulations to define the thermal contributions relative to a reference temperature of $T_0 = 20,000$ K.

Figure 1 illustrates the effect of temperature on the EOS of liquid MgO. The upper panel shows pressure as a function of volume for two representative isotherms, $T_0 = 20,000$ K and $T_1 = 250,000$ K, highlighting the thermal pressure contribution at different volumes. The lower panel shows the corresponding relationship between pressure and energy along the fixed-volume path $V = 6.25 \text{ \AA}^3/\text{f.u.}$, that is, along an isochore. According to the Mie-Grüneisen relation (1), the thermal pressure at constant volume is expected to increase linearly with the thermal energy, with the slope given by $\gamma(V)/V$, which is what we observe in Fig. 1 (lower panel). This confirms that, at least over the temperature range spanning from 20,000 K and 250,000 K, the proportionality between P_{th} and E_{th} is a

reasonably good approximation. However, it is not immediately clear whether this linear behavior persists at significantly higher temperatures, where ionization effects could induce curvature to the $P(E)$. Second, it is not obvious how strongly $\gamma(V)/V$ itself varies with volume. In the next section, we systematically analyze these dependencies using all available EOS data, extracting the slope $P_{\text{th}}/E_{\text{th}}$ at different volumes and temperatures to assess the validity and limitations of the Mie-Grüneisen approximation for liquid MgO.

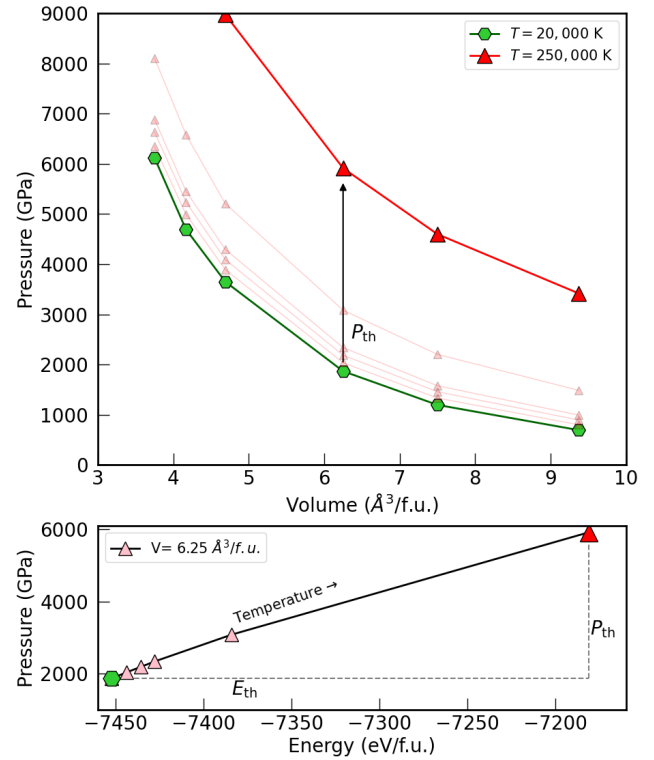


Figure 1 Upper panel: Pressure as a function of volume for isotherms of MgO between $T_0 = 20,000$ K and $250,000$ K. Lower panel: Pressure as a function of internal energy along the $V = 6.25 \text{ \AA}^3/\text{f.u.}$ isochore.

3.1 | Temperature dependence

We next consider all available values of $P_{\text{th}}(V, T)$ and $E_{\text{th}}(V, T)$ from our EOS^[40] relative to the reference isotherm at $T_0 = 20,000$ K. The ratio between these quantities, $P_{\text{th}}/E_{\text{th}}$, is shown in Fig. 2 as a function of density for several temperatures. This ratio is a proxy for γ/V , according to Eq. (8). If the Mie-Grüneisen approximation were exact, $P_{\text{th}}/E_{\text{th}}$ would be independent of temperature. Instead, we observe a weak but systematic variation with temperature.

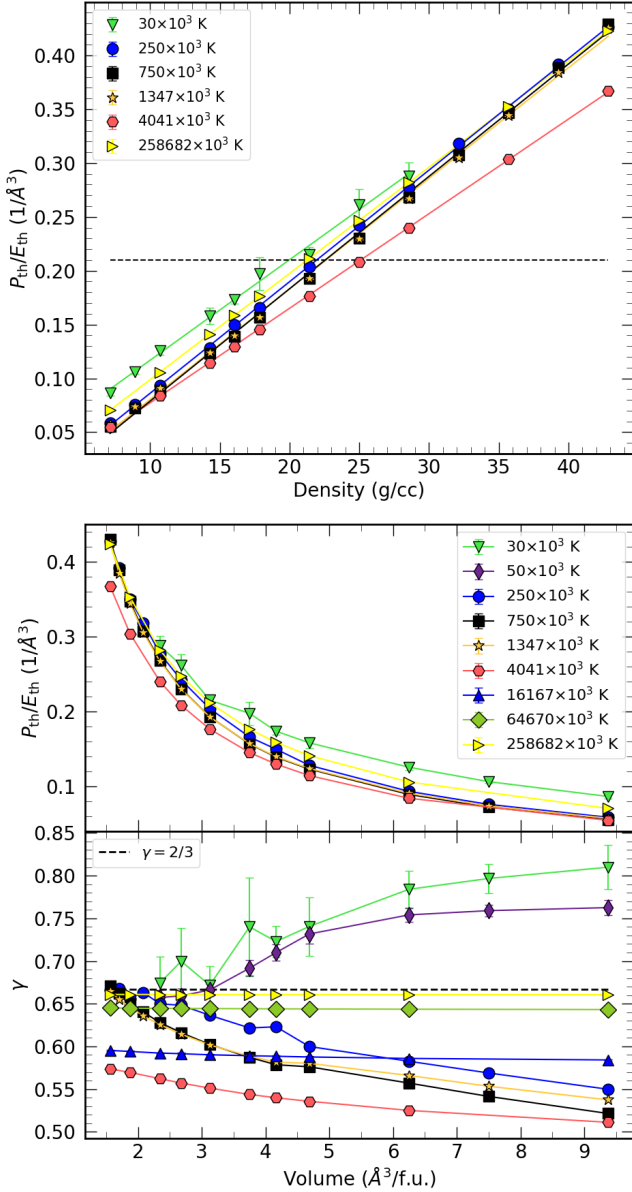


Figure 2 Top panel: Thermal pressure divided by thermal energy of MgO^[40] as a function of density for different temperatures. A linear fit $P_{\text{th}}/E_{\text{th}} = a(T)\rho + b(T)$ is shown with solid lines; small deviations from perfect straight lines arise from numerical smoothing of the underlying data. Bottom panels (shared x-axis = volume): Upper panel: $P_{\text{th}}/E_{\text{th}}$ as a function of volume; Lower panel: the approximated Grüneisen parameter γ computed from Eq. (8). The ideal-gas value $\gamma = 2/3$ is indicated by a horizontal dashed line.

The upper panel of Fig. 2 shows that $P_{\text{th}}/E_{\text{th}}$ varies almost linearly with density, so Eq. (15) is a good approximation at any temperature. We can therefore use the fitted coefficients $a(T)$ and $b(T)$ as an effective description of the Grüneisen

parameter in the Mie–Grüneisen framework by assigning the ratio in Eq (15) to $\gamma(V, T)/V$. Thus, the Grüneisen parameter for liquid MgO takes the form of Eq. (16). The parameters $a(T)$ and $b(T)$, listed in Table 1, therefore provide a convenient way to reconstruct $\gamma(V, T)$ across the sampled range of densities. The fitted parameters $a(T)$ and $b(T)$ encapsulate how

Table 1 Linear fit parameters to the EOS of MgO of $(P_{\text{th}}/E_{\text{th}}) = a(T)\rho + b(T)$ along different isotherms.

T (K)	$a(T)$ [1/amu]	$b(T)$ [$1/\text{\AA}^3$]
30 000	0.0155	0.0233
50 000	0.0151	0.0215
250 000	0.0172	-0.0176
750 000	0.0173	-0.0257
1 347 305	0.0171	-0.0224
4 041 916	0.0146	-0.0108
16 167 663	0.0148	-0.0021
64 670 651	0.0160	-0.0003
258 682 602	0.0164	-0.0001

the effective $\gamma(V)$ evolves with both compression and temperature. The slope $a(T)$, with units of $(1/\text{amu})$, quantifies how sensitively the ratio $P_{\text{th}}/E_{\text{th}}$ increases with density and therefore reflects the degree to which thermal pressure stiffens under compression. In contrast, the intercept $b(T)$, expressed in $(1/\text{\AA}^3)$, measures the residual value of γ/V in the low-density limit. At low and moderate temperatures ($T < 10^6$ K), $a(T)$ remains nearly constant, suggesting that $\gamma(V)$ is weakly dependent on temperature and that the thermal response of the liquid is well captured by a single Mie–Grüneisen parameter. As temperature increases, both $a(T)$ and $b(T)$ show small systematic variations, indicating modest deviations from the linear model as the material approaches the warm dense regime where electronic excitations and partial ionization alter the pressure–energy relationship. As we see in the bottom panels of Fig. 2, and as we have seen for other materials such as MgSiO_3 ,^[42] γ tends decrease with volume (increase upon compression) at the highest temperatures before becoming independent of both pressure and temperature when it reaches the ideal gas limit $\gamma \rightarrow 2/3$.

In Fig. 3, we assess the validity of the Mie–Grüneisen approximation for several materials (H,^[60] He,^[61] Si,^[62] CH_2 ^[63]) by computing the Grüneisen parameter through $\gamma = V \left. \frac{\partial P}{\partial T} \right|_V / \left. \frac{\partial E}{\partial T} \right|_V$, which is thermodynamically equivalent to its definition in Eq. (2). Within the MG framework, γ should exhibit the same volume dependence for all temperatures. However, we observe variations in $\gamma(\rho)$ with temperature, which reveals deviations from the linear proportionality between P_{th}

and E_{th} in Eq. (8), which corresponds to the presence of an explicit temperature dependence of γ .

The $\gamma(V)$ functions of all materials show somewhat similar temperature dependencies. With increasing temperature, $\gamma(V)$ initially decreases, goes through a volume dependence minimum before increasing again and approaching from below the high temperature limit of $2/3$ for an ideal gas. The regime where $\gamma(V)$ increases is well described by the Debye-Hückel model (see Sec. 2.2).

At moderate temperatures, these four materials exhibit an increase of the Grüneisen parameter with density along the isotherms, indicating that γ grows as the system is compressed (γ decreases with volume). This trend gradually weakens with increasing temperature where the Debye-Hückel model applies. Helium shows a distinctive pattern: at low temperatures, γ initially rises with density, reaches a maximum, and then decreases at higher densities, reflecting a non-monotonic evolution of γ . Only at temperatures above $\sim 6 \times 10^4$ K, helium reverts back to the monotonic trend with volume observed in the other materials.

The CH_2 system displays a contrasting trend. At the lowest temperatures, γ already exceeds $2/3$ and increases with density. As temperature increases, the entire set of curves shifts downward nearly uniformly, indicating that γ decreases with temperature at each density and reaches a pronounced minimum near 2×10^6 K. Beyond this point, a turnover occurs: at even higher temperatures, the curves rise again and progressively flatten, approaching the ideal-gas limit. Such behavior suggests complex coupling between the ionic and electronic contributions to the thermal pressure in CH plasmas, in contrast to the smoother behavior of the monatomic systems.

Overall, Fig. 3 shows that the Grüneisen parameter $\gamma(V, T)$ depends on temperature and that the rate of change with volume along each isotherm is different. Within the Mie-Grüneisen framework, γ is expected to depend primarily on volume but to remain approximately independent of temperature at fixed V . Therefore, the spread among isotherms in this figure directly reflects deviations from that assumption. For most of these materials, the low-temperature curves exhibit a clear increase of γ with density, consistent with the empirical form $\gamma(V) \propto (\rho_0/\rho)^q$ often used for solids. As temperature rises, the isotherms tend to collapse, indicating that γ becomes nearly temperature-independent and approaches the ideal-gas limit $\gamma \rightarrow 2/3$. Thus, rather than requiring γ to be constant, the figure demonstrates that γ retains a pronounced volume dependence at low temperatures while progressively losing its temperature dependence as ionization drives the system toward the ideal-gas regime.

3.2 | Performance of models

If we assume that γ does not depend on temperature (Model 1), which is not the case for temperatures significantly higher than our reference isotherm, $T_0 = 20,000$ K, we can use Mie-Grüneisen model in Eq. (14) to try to predict pressures at much higher temperatures T using a temperature-independent γ , given that we know the energies $E(V, T)$ from our EOS. In Fig. 4, we show pressure as a function of energy for liquid MgO along several isochores obtained from our original EOS, together with the pressures predicted from the Grüneisen model using the parameters obtained from the isotherm $T_1 = 250,000$ K in Table 1, namely

$$\gamma(V) = 0.0172 \text{ amu}^{-1} m - 0.0176 \text{ \AA}^{-3} V, \quad (22)$$

which implies that $\gamma' = -0.0176 \text{ \AA}^{-3} V_0$ and $\gamma_0 = 0.6932 - 0.0176 \text{ \AA}^{-3} V_0$ in Eq. (14), since $m = 40.3044$ amu for one MgO formula unit. This fitted Grüneisen parameter represents a case where γ decreases linearly with volume (increases upon compression) as we can see in Fig. 2. The results demonstrate that the model reproduces the pressures within an acceptable accuracy over a wide pressure range, but often outside the error bars of our simulations. In other words, by utilizing only the P - V - E information from a single isotherm $T = T_1$ (in addition to the reference isotherm at $T_0 = 20,000$ K), we are able to predict pressures not only at intermediate temperatures $T_0 < T < T_1$ but also at substantially higher ones ($T \gg T_1$) to a reasonable degree.

At higher temperatures, however, systematic deviations from the Mie-Grüneisen prediction begin to emerge, as we show in Fig. 5. These discrepancies become more noticeable once thermal excitations and partial ionization of the L and K electronic shells contribute significantly to the total pressure,^[40,64] violating the assumption that γ depends only on volume. In this regime, the simple Grüneisen form becomes insufficient, and a more complete description must explicitly account for temperature-dependent electronic effects. Thus, in an attempt to incorporate the effects of temperature on the Grüneisen parameter, we have considered a temperature-dependent Grüneisen parameter from Eq. (16) (Model 2, Sec. 2). While this model is thermodynamically inconsistent, because Eq. (17) implies that P_{th} is not proportional to E_{th} by the Grüneisen parameter, this model leads to at least some reasonable improvement over Model 1. We show the differences between Model 1 and Model 2 in Fig. 5. As we can see in the figure, while Model 1 already starts showing significant deviations beyond $T_1 = 250,000$ K, Model 2 is able to bring the predicted pressures into closer agreement with the EOS data in a wider temperature range but inevitably leads to strong deviations at the highest temperatures.

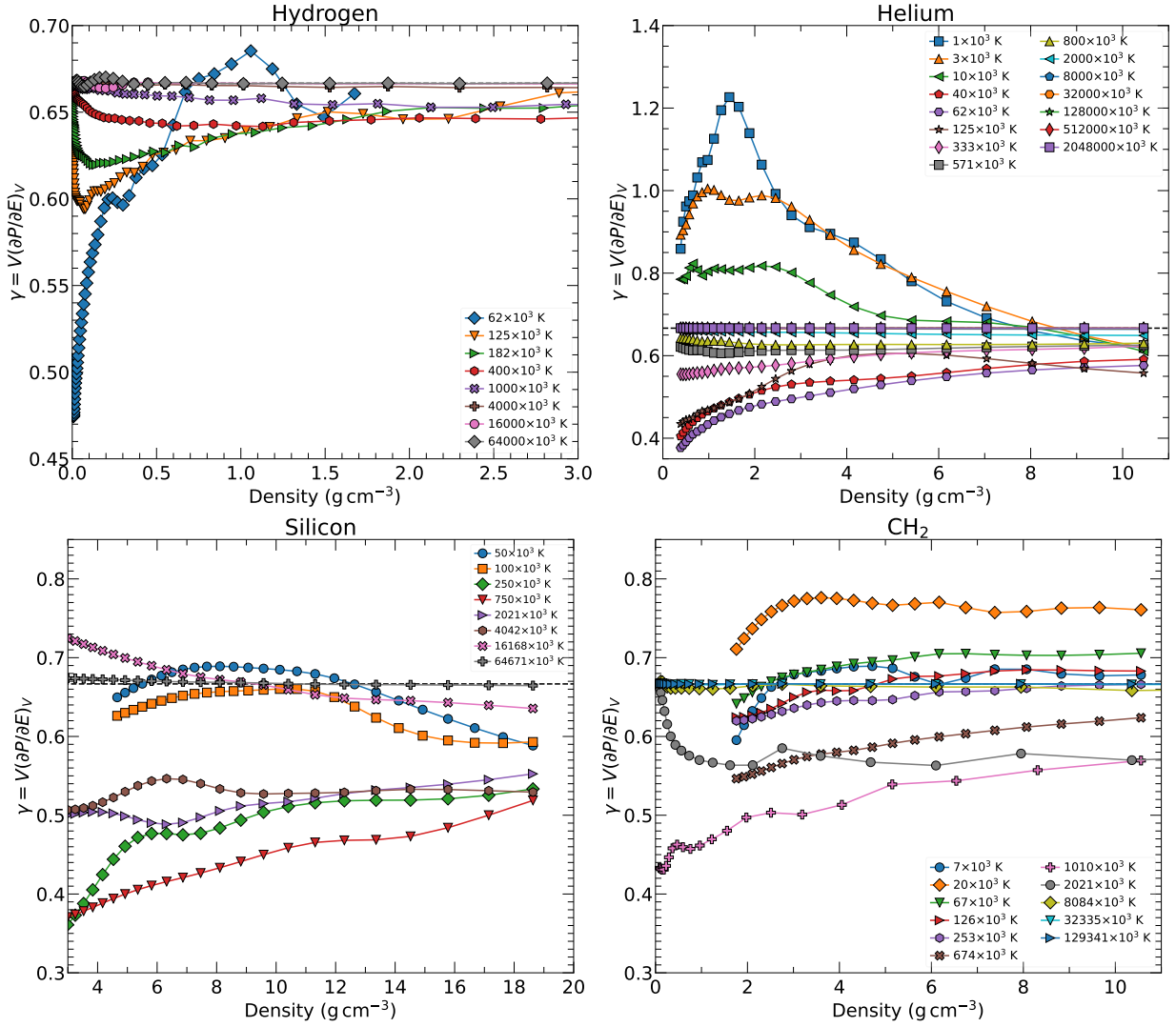


Figure 3 Grüneisen parameter from Eq (2) is plotted as a function of density for several isotherms of hydrogen, helium, silicon, and CH_2 . Under the Mie–Grüneisen model 1 ($\gamma = \gamma(V)$ without T -dependence), the curves at different T would collapse onto a single $\gamma(V)$ profile; deviations between isotherms indicate a nonzero $\partial\gamma/\partial T$. The horizontal line at $\gamma_{\text{ideal}} = 2/3$ marks the ideal, non-degenerate gas.

3.3 | Hugoniot curve and sound speed

When materials are dynamically compressed by shock waves, they reach states along the shock Hugoniot curve. The Eulerian sound speed in Eq. (11) is directly related to the Grüneisen parameter through Eq. (13). Experimentally measured sound speeds under shock compression can thus be used to infer the Grüneisen parameter as a function of density via Eq. (13), which in turn allows the construction of isentropic profiles when combined with Eq. (2).

To compute the sound speeds, we employed our FPEOS code^[16] to generate a family of isentropes for each material. Along each isentrope, the adiabatic sound speed was evaluated

directly from the thermodynamic derivative in Eq. (11), obtained numerically from a spline fit to the $P(\rho)$ isentropes. We show hydrogen (H) as an example in the top panel of Fig. 6, where the resulting sound speed C_S is plotted as a function of pressure along the isentropes. Each isentrope intersects the principal Hugoniot, also obtained from FPEOS, at a distinct pressure and density. These intersections, highlighted in the figure as filled symbols, define the sound speed at a Hugoniot state. Collectively, they trace the sound speed along the Hugoniot, as shown in the bottom panel of Fig. 6. The same procedure was repeated for helium, silicon, CH_2 , MgSiO_3 , and other materials, enabling a consistent comparison of the sound speed behavior across different materials and thermodynamic conditions.

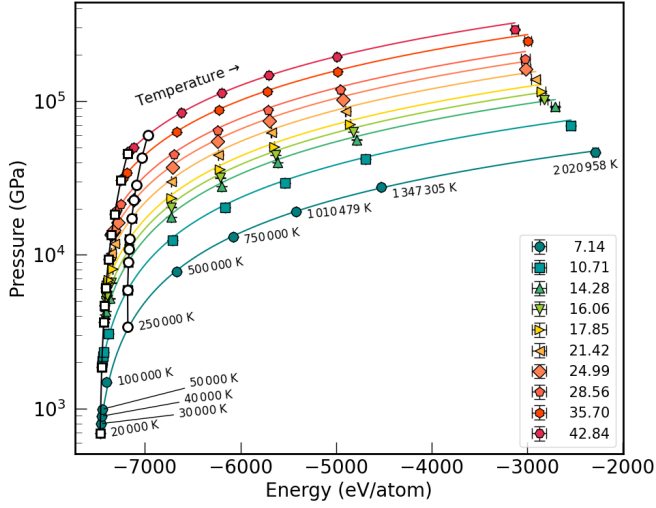


Figure 4 Pressures of the MgO liquid predicted using Eq. (8), assuming $\gamma(V) = 0.0172 \text{ amu}^{-1}m - 0.0176 V \text{ \AA}^{-3}$ (solid curves), where $m = 40.3044 \text{ amu}$. Symbols represent different densities, expressed in g cm^{-3} in the legend, where data points are taken directly from the MgO equation of state^[40], starting at the initial values $P(V, T_0)$ and $E(V, T_0)$ on the left. The open symbols represent the isotherms $T_0 = 20,000 \text{ K}$ and $T_1 = 250,000 \text{ K}$ used to infer the pressures at other conditions, represented by the solid curves.

In Fig. 6, the sound speeds of H, He, and CH_2 are noticeably higher than those of the denser materials across the entire pressure range, reflecting their lower average atomic masses and higher compressibilities. By contrast, the sound speeds of C, LiF, MgO, SiO_2 , and MgSiO_3 exhibit similar magnitudes and trends, consistent with their comparable stiffness at high pressures. The nearly linear trends observed in log-log space suggest a power-law dependence of the form $C_s \propto P^\alpha$, with α close to 0.45 for most materials. Our predicted sound speeds for MgO along its Hugoniot show remarkable agreement with the experimental measurements of McCoy *et al.*^[65].

We next use Eq. (13) to infer the Grüneisen parameter along the Hugoniot curve from the computed sound speeds and pressure-density slopes obtained from the FPEOS model. The resulting values of γ are shown in Fig. 7 as functions of both pressure and density. At low pressures and densities, the values of γ calculated from Eq. (13) exceed the ideal gas limit value $2/3$, except for H and He. This is also consistent with our estimates shown in Fig. 2. Most materials reveal a consistent qualitative trend: γ decreases with increasing density along the Hugoniot, reaches a minimum, and then increases asymptotically towards $2/3$ as they reach full ionization (upper panel of Fig. 7). This minimum is associated with the onset of K-shell ionization, after which it rises again and asymptotically approaches the ideal-gas limit along the Hugoniot curve.

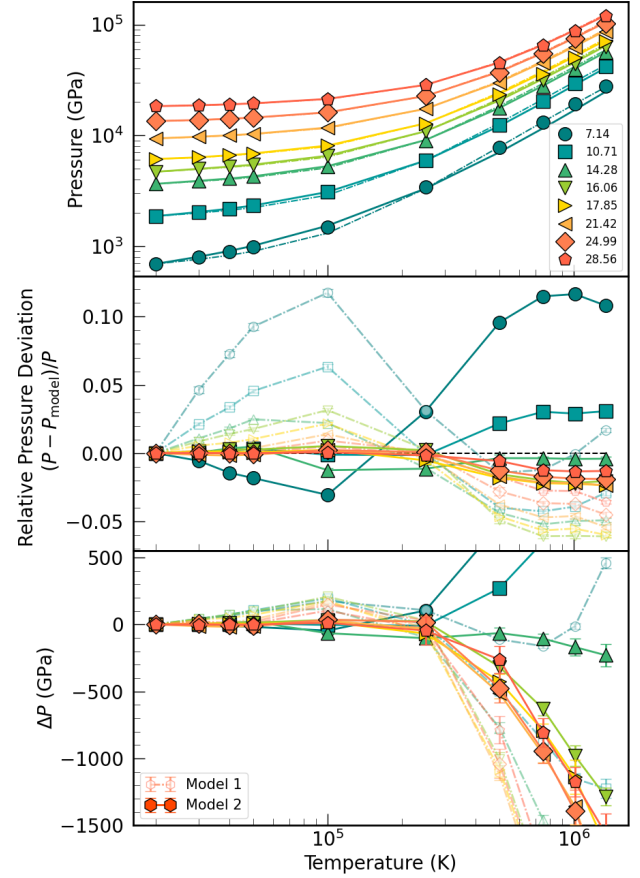


Figure 5 Top panel: Comparison between the predicted pressures of Model 1 (transparent, dash-dotted curves) and Model 2 (solid curves), which represent $\gamma(V)$ and $\gamma(V, T)$, respectively, with EOS data points of MgO shown as solid symbols representing each density, expressed in g cm^{-3} in the legend. Middle panel: Relative pressure deviation for both models along the same isochores, highlighting deviations between predictions and data. Bottom panel: Absolute pressure difference $\Delta P = P_{\text{model}} - P_{\text{EOS}}$ for both models.

Since the compression ratio can decrease with increasing pressure when the L- or K-shell ionization is complete (around $T \sim 10^6 \text{ K}$), it is preferable to plot the Grüneisen parameter along the Hugoniot curve as function of pressure instead because trends in $\gamma(\rho)$ can be difficult to interpret in ionization regime (lower panel of Fig. 7). For MgO, the excellent agreement between our computed sound speeds and experimental measurements^[65] demonstrates that Eq. (13) yields accurate predictions of the Grüneisen parameter along the shock Hugoniot curve. For SiO_2 , our computed Grüneisen parameter along the Hugoniot curve does not fully reproduce the experimental trend reported by Ocampo *et al.*^[66] who observed an increase of γ with density up to $\rho \sim 5 \text{ g/cm}^3$. At higher densities,

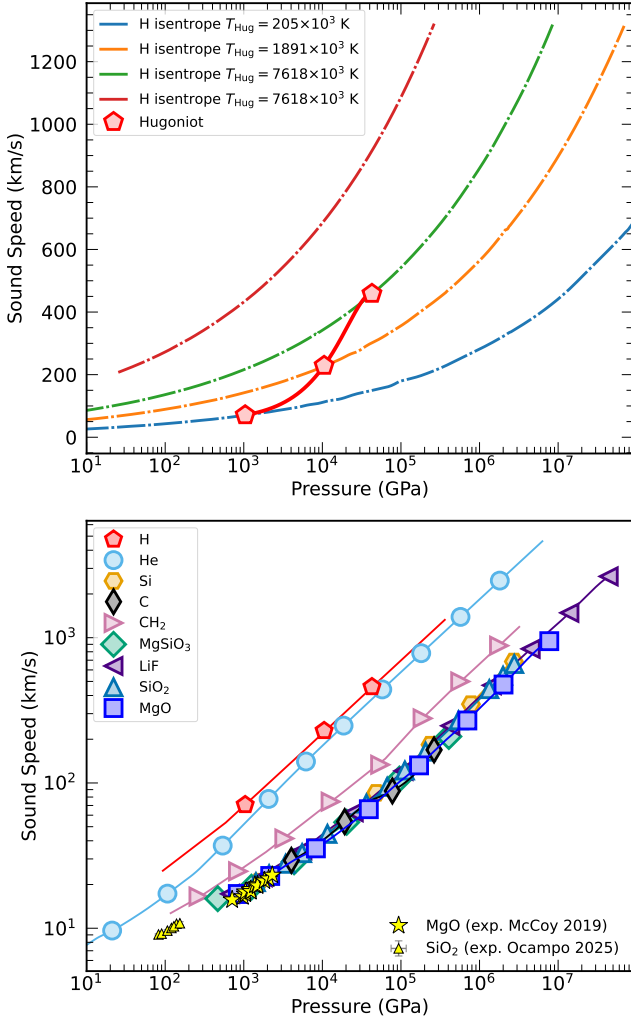


Figure 6 (Top) Sound speed along isentropes of hydrogen obtained from the FPEOS model. The semi-transparent filled symbols indicate their intersections with the principal Hugoniot, defining the sound speed at a Hugoniot state. (Bottom) Sound speed along the principal Hugoniot of various materials, derived from their respective intersections with the isentropes. The EOS of SiO₂ and corresponding sound speeds were obtained from a linear mixture of Si and O using FPEOS.^[16] Experimental data for shock-compressed MgO from McCoy *et al.*^[65] are also shown for comparison.

McCoy *et al.*^[67] reported a decrease of γ with increasing density along the principal Hugoniot curve of SiO₂. A turnover in $\gamma(P)$ emerges when both experimental datasets are combined, which can be fitted with the model provided by Ocampo *et al.* Since our SiO₂ calculations do not include densities below 6 g/cm³, they cannot constrain the existence or location of such a turnover in $\gamma(P)$. More generally, while γ does not necessarily decrease along isotherms, it typically decreases with

pressure along the Hugoniot for many materials. The applicability of Hugoniot-derived $\gamma(\rho)$ values to off-Hugoniot states depends on the extent to which the Grüneisen parameter varies with temperature for a given material.

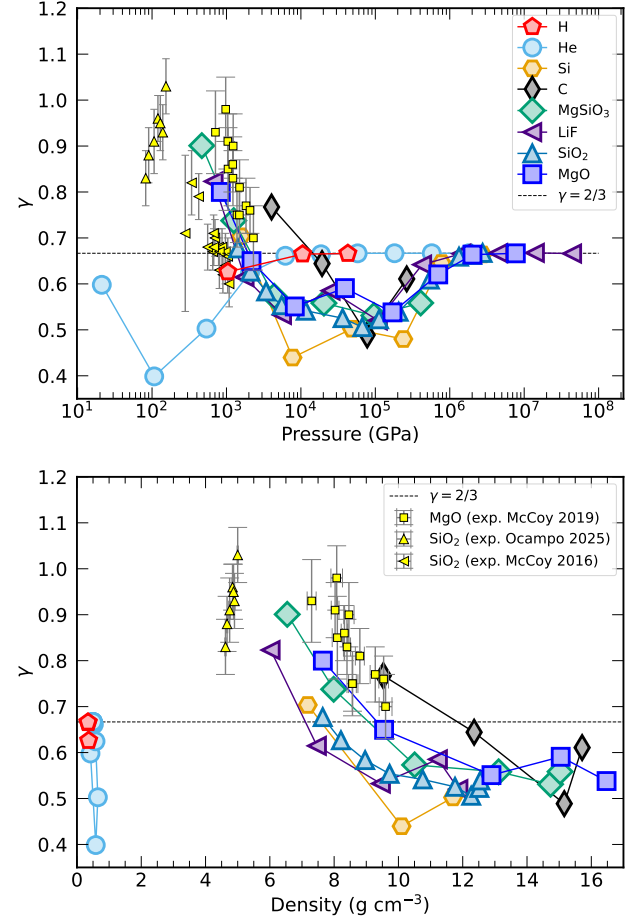


Figure 7 Grüneisen parameter along the principal Hugoniot as a function of (top) pressure and (bottom) density, computed from the sound speeds and pressure-density slopes obtained from FPEOS. Experimental data for MgO from McCoy *et al.*^[65] and for SiO₂ from Ocampo *et al.*^[66] and McCoy *et al.*^[67] are shown for comparison. The EOS of SiO₂ and corresponding sound speeds and values of γ (up triangles) were obtained from a linear mixture of Si and O using FPEOS.^[16] The turnover of γ at intermediate pressures reflects K-shell ionization, after which it converges toward the ideal-gas limit $\gamma = 2/3$.

4 | CONCLUSIONS

Our results demonstrate that even within the strongly coupled, partially ionized regime relevant to warm dense matter, the pressure and internal energy retain an approximately linear relationship over a wide range of densities and temperatures. This near-linearity supports the use of a Mie–Grüneisen-type formulation for thermal pressure in first-principles EOS models, with $\gamma(V)$ capturing the dominant dependence on compression. Deviations from exact proportionality between P_{th} and E_{th} quantify the breakdown of the traditional Mie–Grüneisen assumption, particularly as materials approach full ionization or undergo structural and electronic transitions.^[68]

Furthermore, the present framework provides a systematic method to extract an effective $\gamma(V, T)$ directly from first-principles data, allowing one to assess its variation along both isotherms and isentropes without invoking empirical mixing or analytic fits. This approach therefore bridges the gap between microscopic EOS calculations and macroscopic thermodynamic models, offering a physically consistent way to incorporate finite-temperature effects into hydrodynamic and planetary-interior simulations.

Data Availability All datasets and analysis scripts used in this study, including tabulated sound speeds, Hugoniot curves, values of the Grüneisen parameters along isentropes and Hugoniot curves, and the data underlying all figures, are publicly available at the repository https://github.com/fgonzcat/Mie-Gruneisen_EOS_WDM.git.

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