A First-Principles Equation-of-State Table of Beryllium for High-Energy-Density Plasma Simulations

Y. H. DING

University of Rochester, Laboratory for Laser Energetics

Summary

An accurate equation-of-state (EOS) table of beryllium has been built from first-principles calculations for inertial confinement fusion (ICF) and high-energy-density–physics (HEDP) applications

- Based on density-functional-theory (DFT) calculations [combining Kohn–Sham molecular dynamics (KSMD) and orbital-free molecular dynamics (OFMD)], we have established a wide-range beryllium EOS table of density $\rho = 0.001$ to $\rho = 500$ g/cm^3 and temperature $T = 2000$ to 10^8 K
- The first-principles equation-of-state (FPEOS) table is in good agreement with the widely used *SESAME* EOS table (*SESAME* 2023)
- By implementing the FPEOS table into the 1-D radiation–hydrodynamics code *LILAC*, we studied the EOS effects on beryllium-shell target implosions; the FPEOS simulation predicts a higher neutron yield (~15%) compared to the simulation using the *SESAME* 2023 EOS table

TC13416

It is of great importance to calculate the EOS of beryllium for a wide range of conditions by using reliable methods

- In ICF applications, target designs are based mainly on the radiation–hydrodynamics simulations, where the materials will experience many different pressure (up to 10^5 Mbar) and temperature (up to 10^8 K) conditions;* accurate properties of beryllium under such extreme conditions are essential for ICF applications
- 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*
- Quantum molecular dynamics (QMD),** based on 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***

Combining orbital-based–DFT, KSMD, and OFMD, we can investigate wide-ranged EOS tables.

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TC13417

QMD calculations are based on DFT

- Total energy in terms of density

$$E = -\frac{1}{2}\sum_{n}^{Ne}\int \phi_n^*(\vec{r})\nabla^2\phi_n(\vec{r})d\vec{r} + \int n(\vec{r})V_{ne}(\vec{r})d\vec{r} + \frac{1}{2}\iint d\vec{r}d\vec{r}'\frac{n(\vec{r})n(\vec{r}')}{|\vec{r}-\vec{r}'|} + \int \mu_{xc}(n)n(\vec{r})d\vec{r}$$

- Minimize with respect to single-particle orbitals

$$\frac{\delta E}{\delta\phi_i} = \frac{\delta T}{\delta\phi_i(\vec{r})} + \left[\frac{\delta E_{en}}{\delta n_i(\vec{r})} + \frac{\delta E_{ee}}{\delta n_i(\vec{r})} + \frac{\delta E_{xc}}{\delta n_i(\vec{r})}\right]\frac{\delta n_i(\vec{r})}{\delta\phi_i(\vec{r})} = \epsilon_i\phi_i(\vec{r})$$

- The Kohn–Sham equations can be solved self-consistently

$$-\frac{1}{2}\nabla^2\phi_i(\vec{r}) + \left[V_{ne}(\vec{r}) + \int\frac{n(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}' + \mu_{xc}(n) + n(\vec{r})\frac{\delta\mu_{xc}(n)}{\delta n(\vec{r})}\right]\phi_i(\vec{r}) = e_i\phi_i(\vec{r})$$

$$(T + V_{eff})\phi_i(\vec{r}) = \epsilon_i\phi_i(\vec{r})$$

- Ion force for molecular dynamics $F = -\nabla_{\vec{R}}\langle\psi|\hat{H}|\psi\rangle = \frac{\partial}{\partial\vec{R}}(F_{ei} + F_{ii})$

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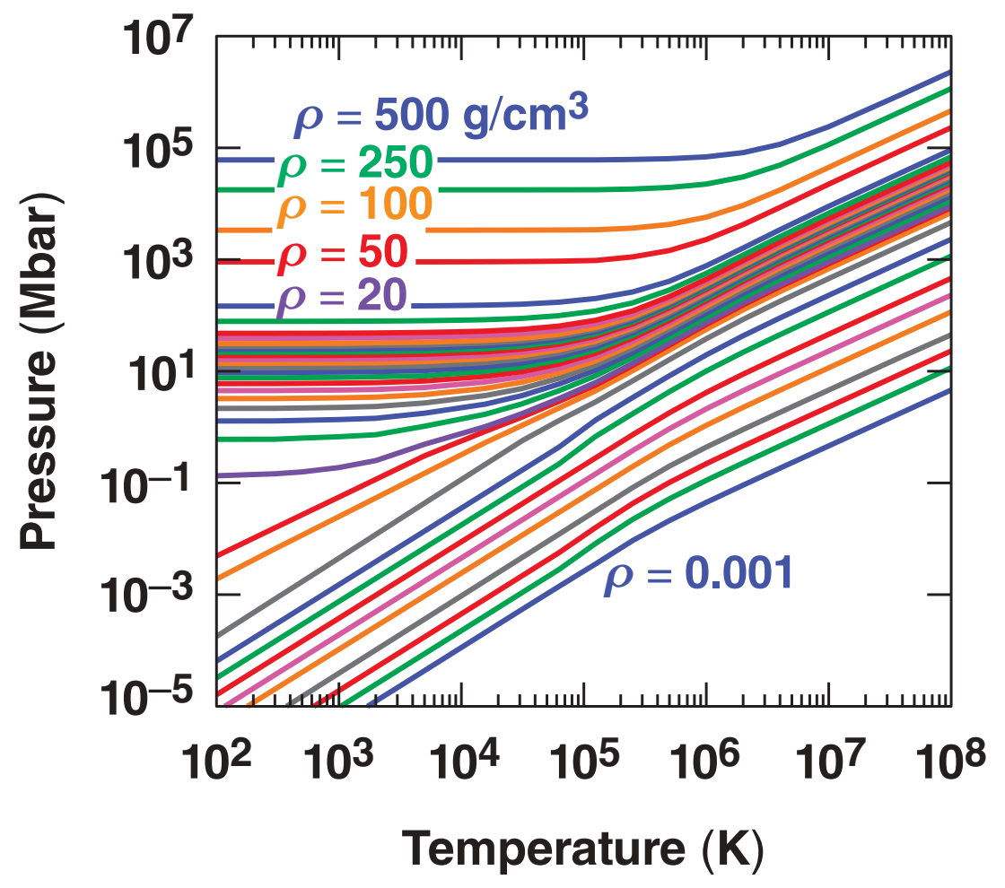
The FPEOS of beryllium has been calculated for densities and temperatures from $\rho = 0.001$ g/cm^3 to $\rho = 500$ g/cm^3 and $T = 2{,}000$ K to 10^8 K



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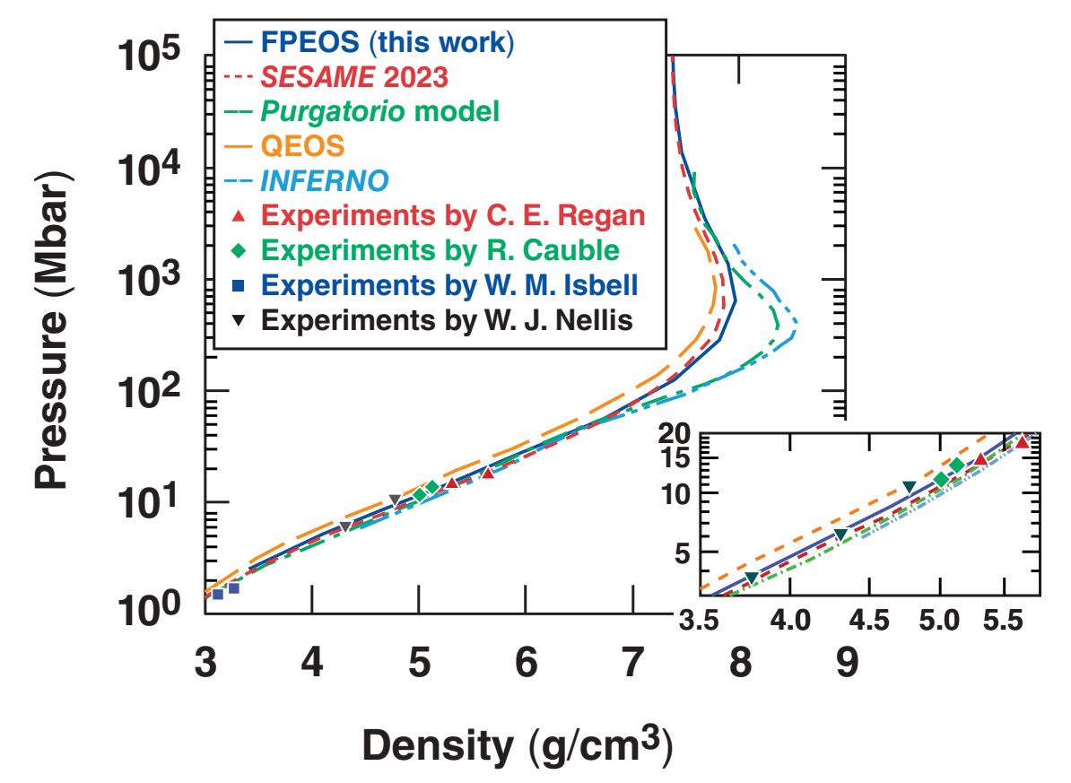
Y. H. Ding and S. X. Hu, Phys. Plasmas 24, 062702 (2017).

The calculated principal shock Hugoniot of beryllium from FPEOS has been compared with other theoretical models and experiments



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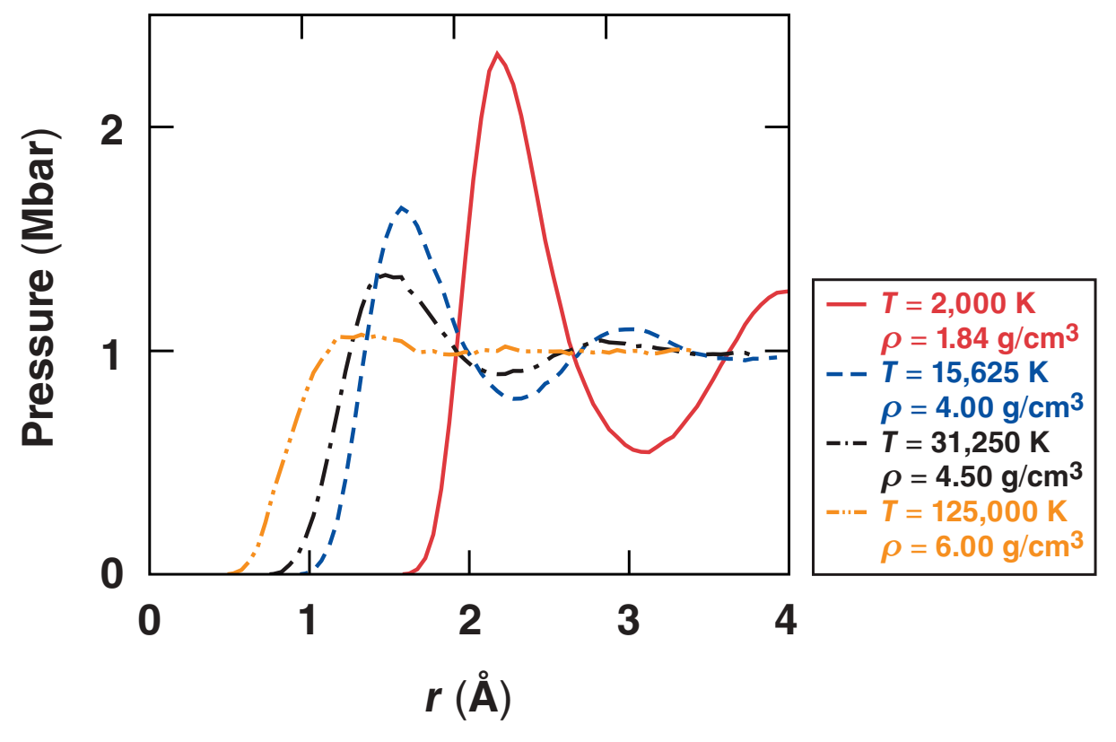
The ion–ion pair correlation function shows the structure change of Be along the principle Hugoniot curve



The peaks in the pair correlation $g(r)$ gradually disappear along the principle Hugoniot curve, which indicates the structure change from solid to liquid state.

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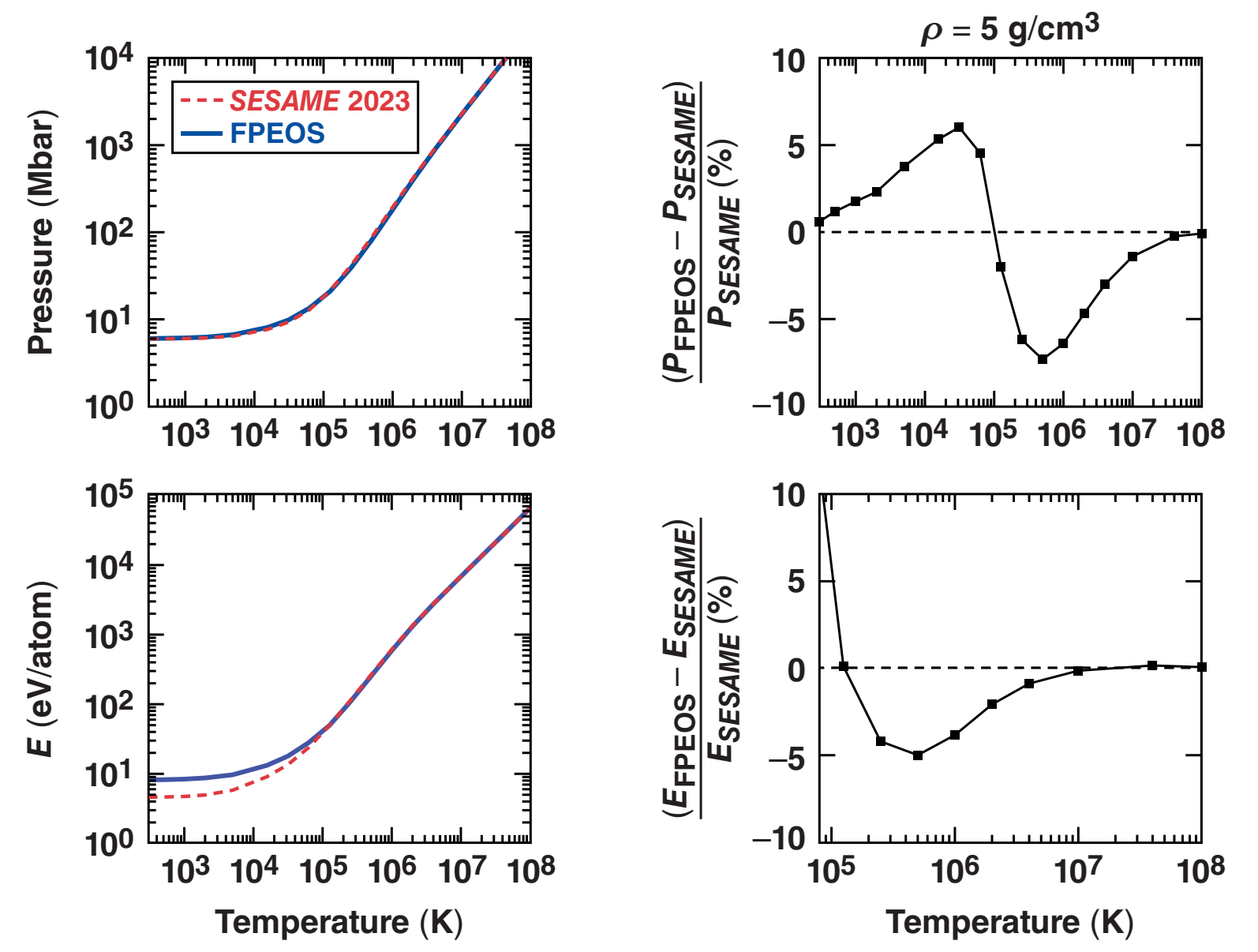
The off-Hugoniot equation-of-state comparison between FPEOS and *SESAME* at certain densities



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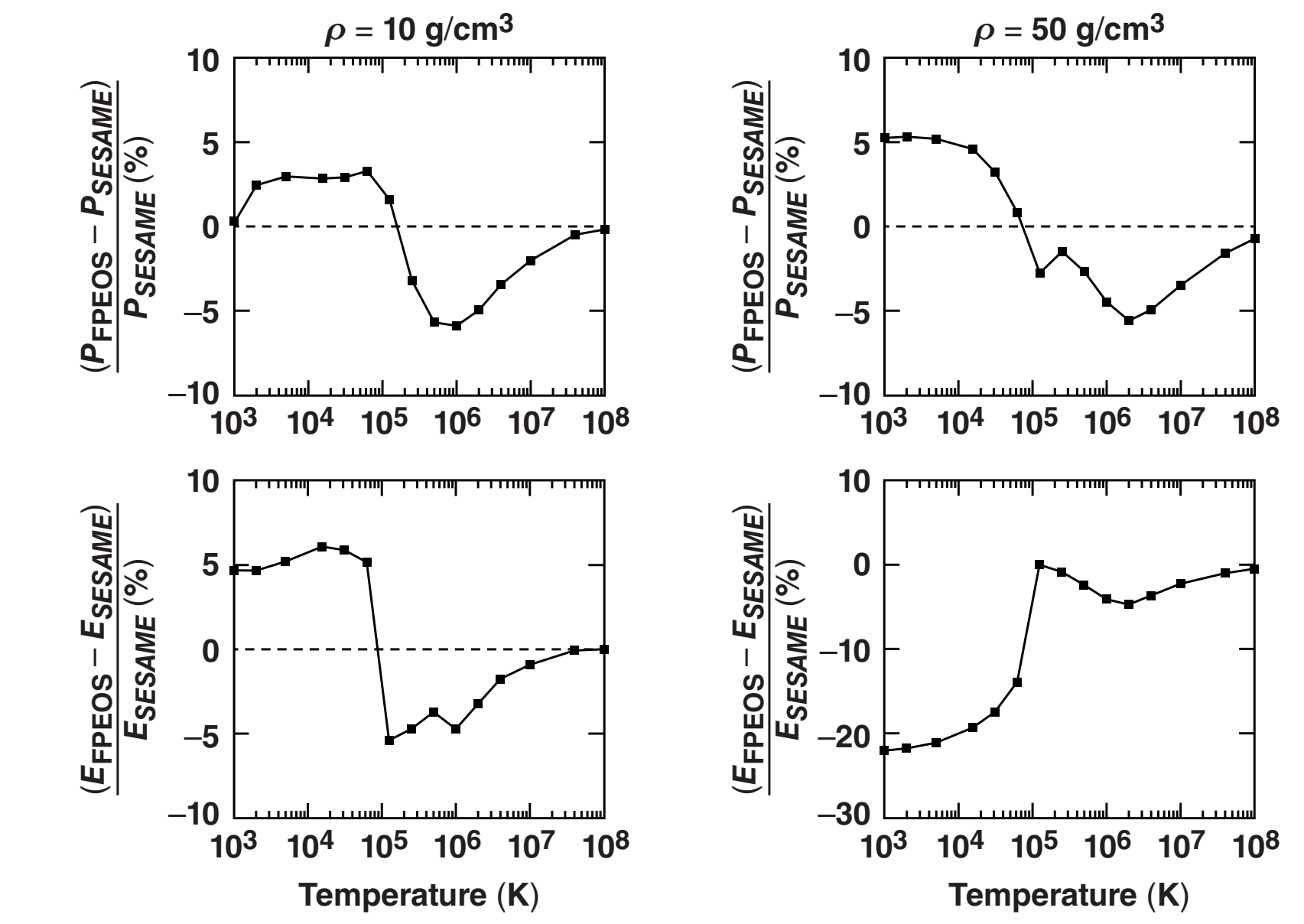

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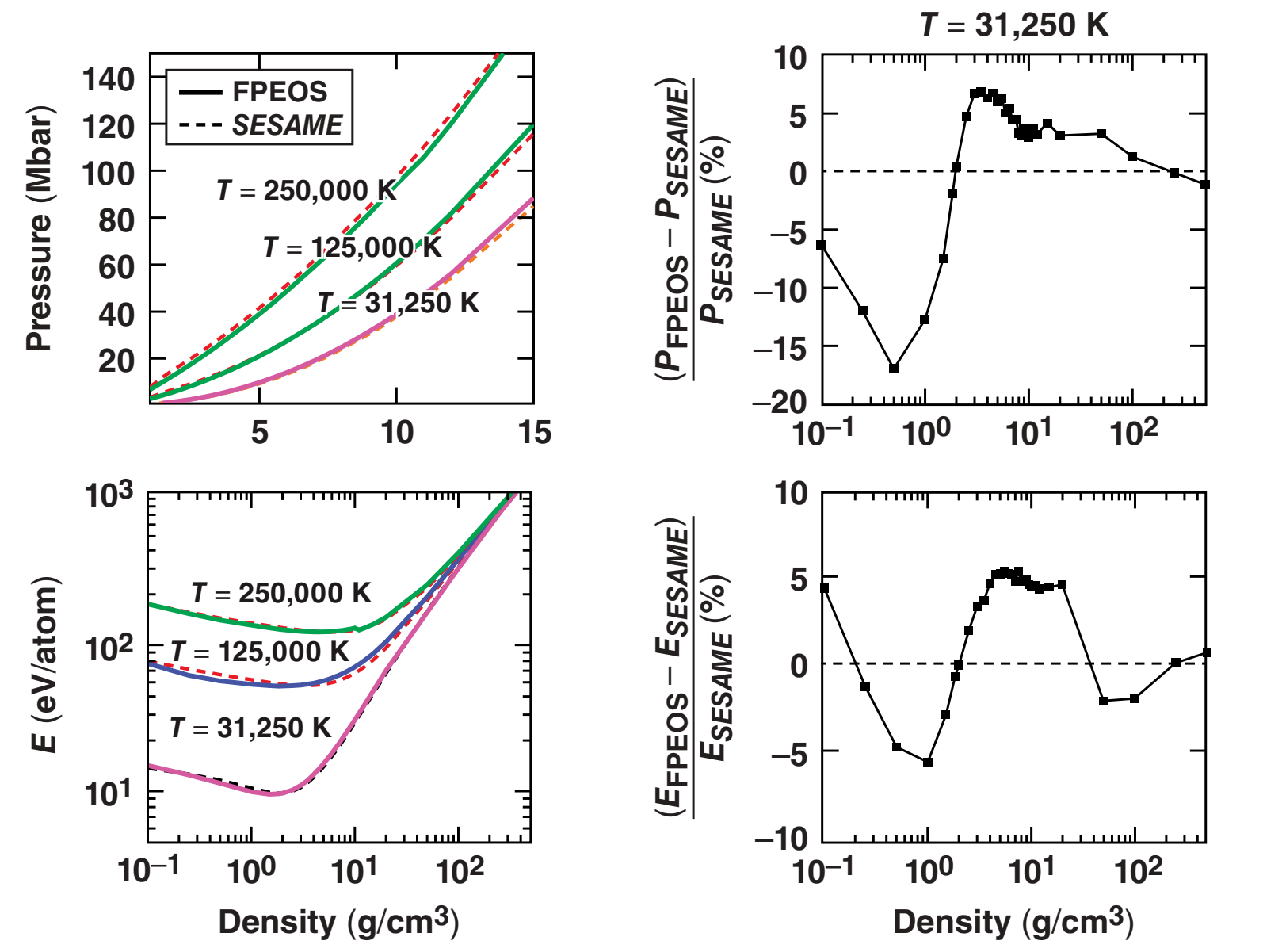

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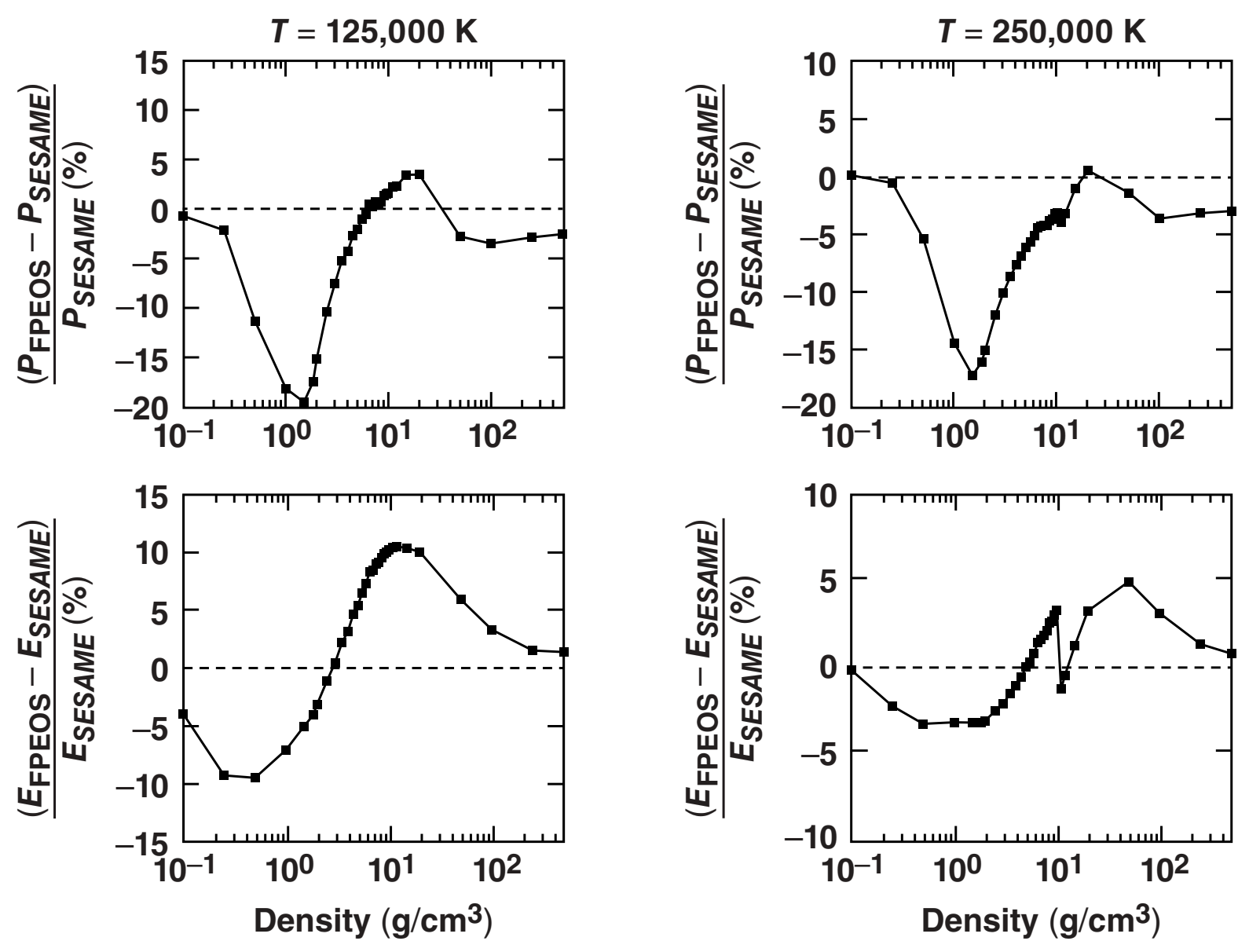

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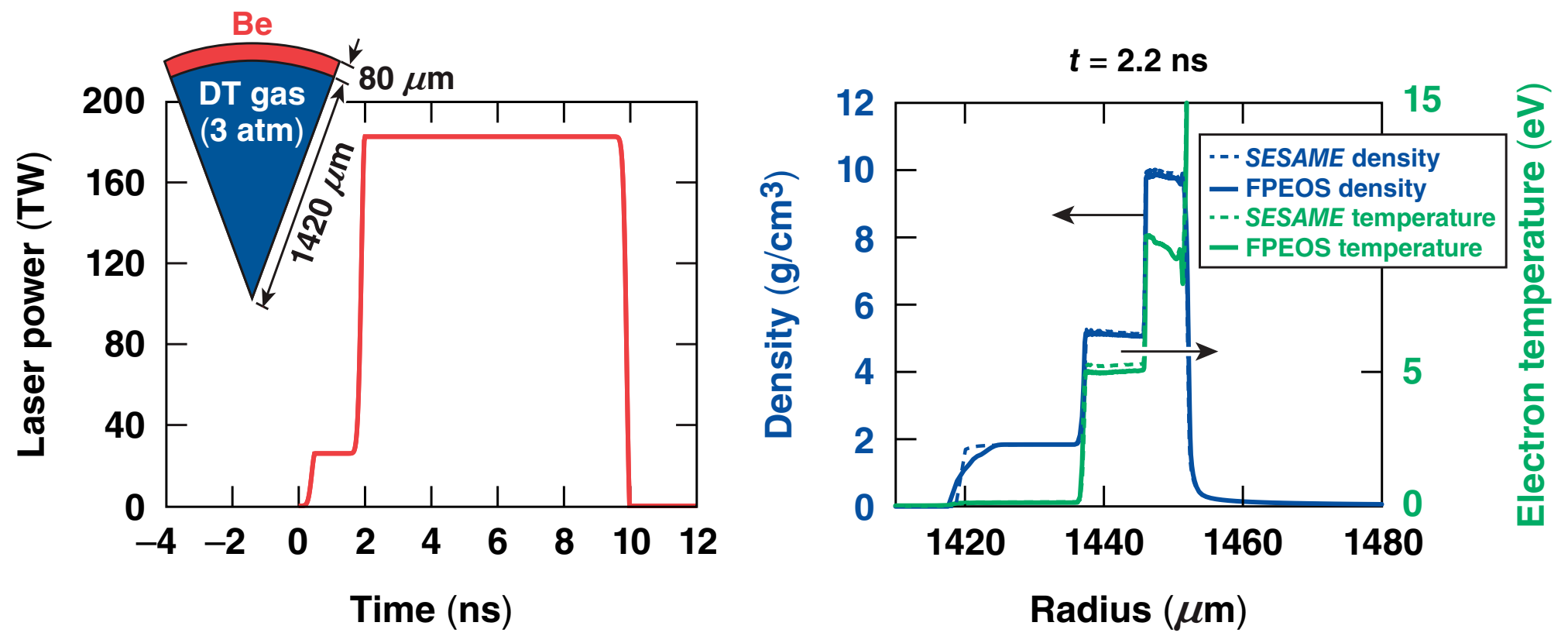
In the WDM regime the difference is most significant (20%).

The effects of beryllium FPEOS on high-energy-density (HED) plasma simulations



For DT, gas two simulations used the same FPEOS table and the first-principles opacity table.

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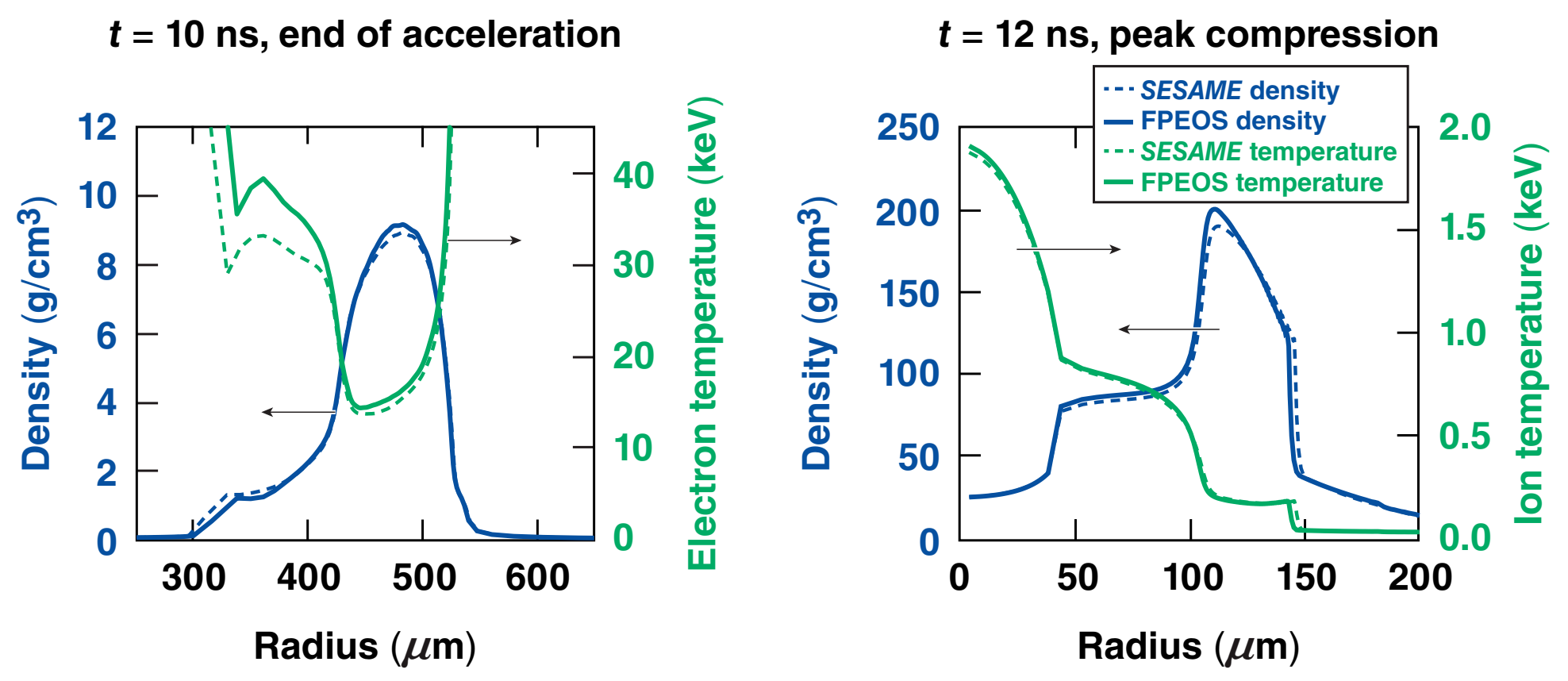

The FPEOS simulation also predicted a higher total neutron yield (y = 3.76 × 10^{14}), which is ~15% higher than the *SESAME* simulation, (y = 3.28 × 10^{14}).

TC13425

UNIVERSITY of ROCHESTER

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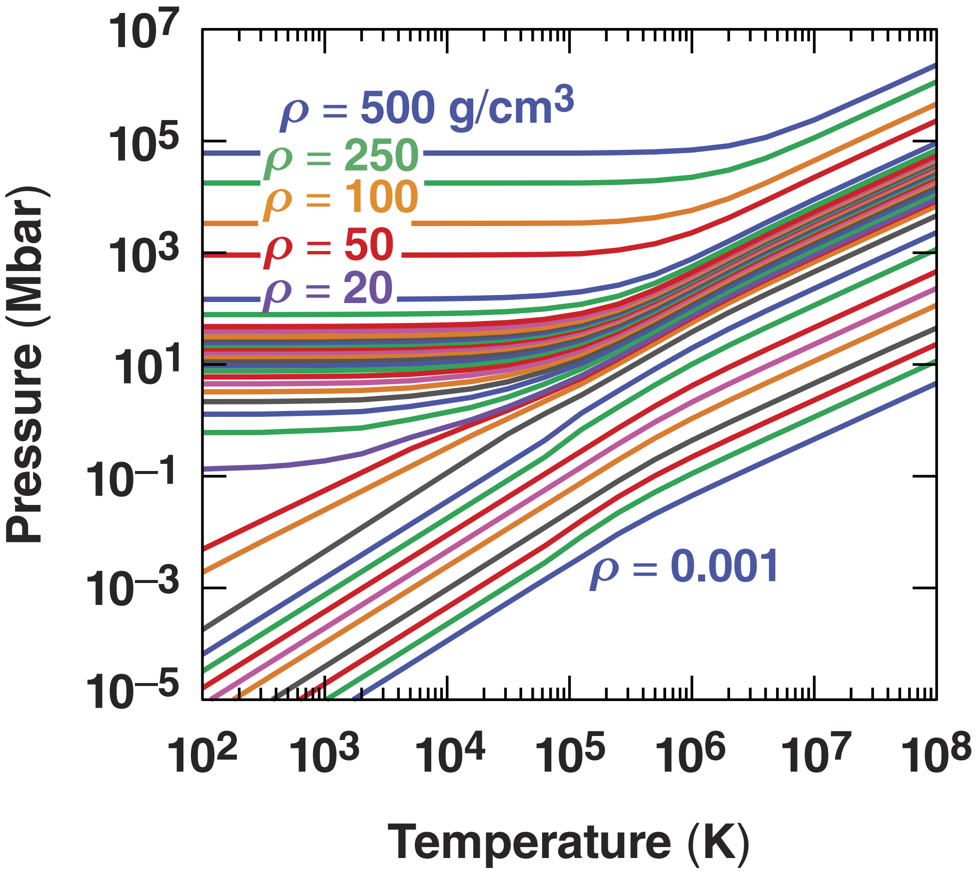

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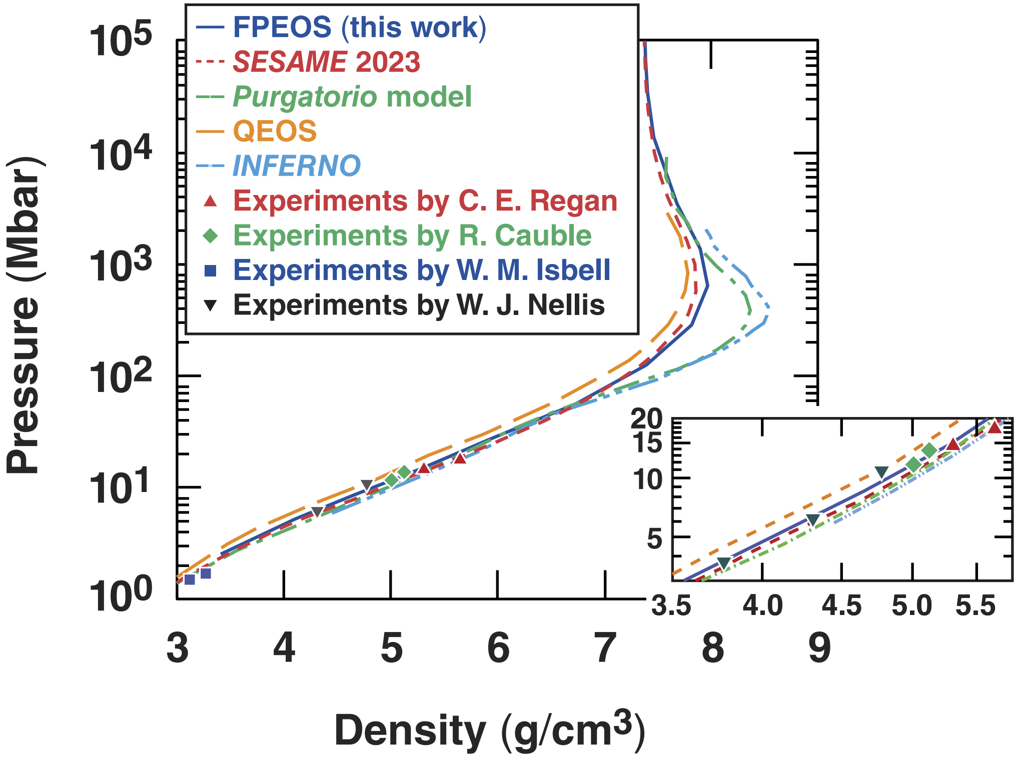

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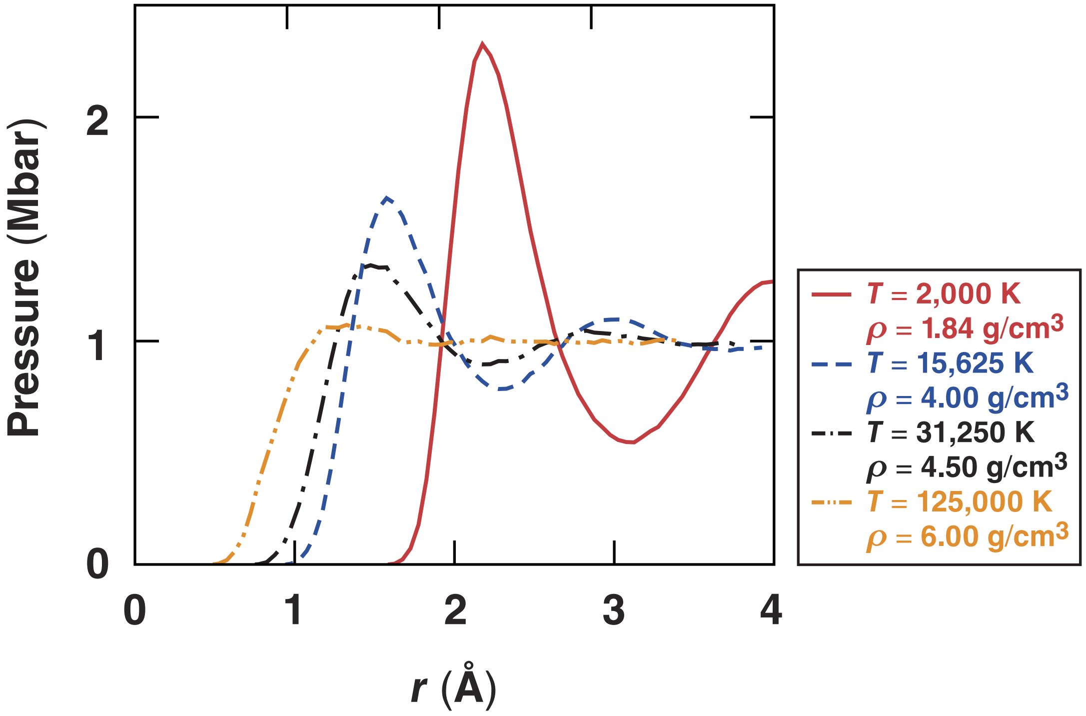

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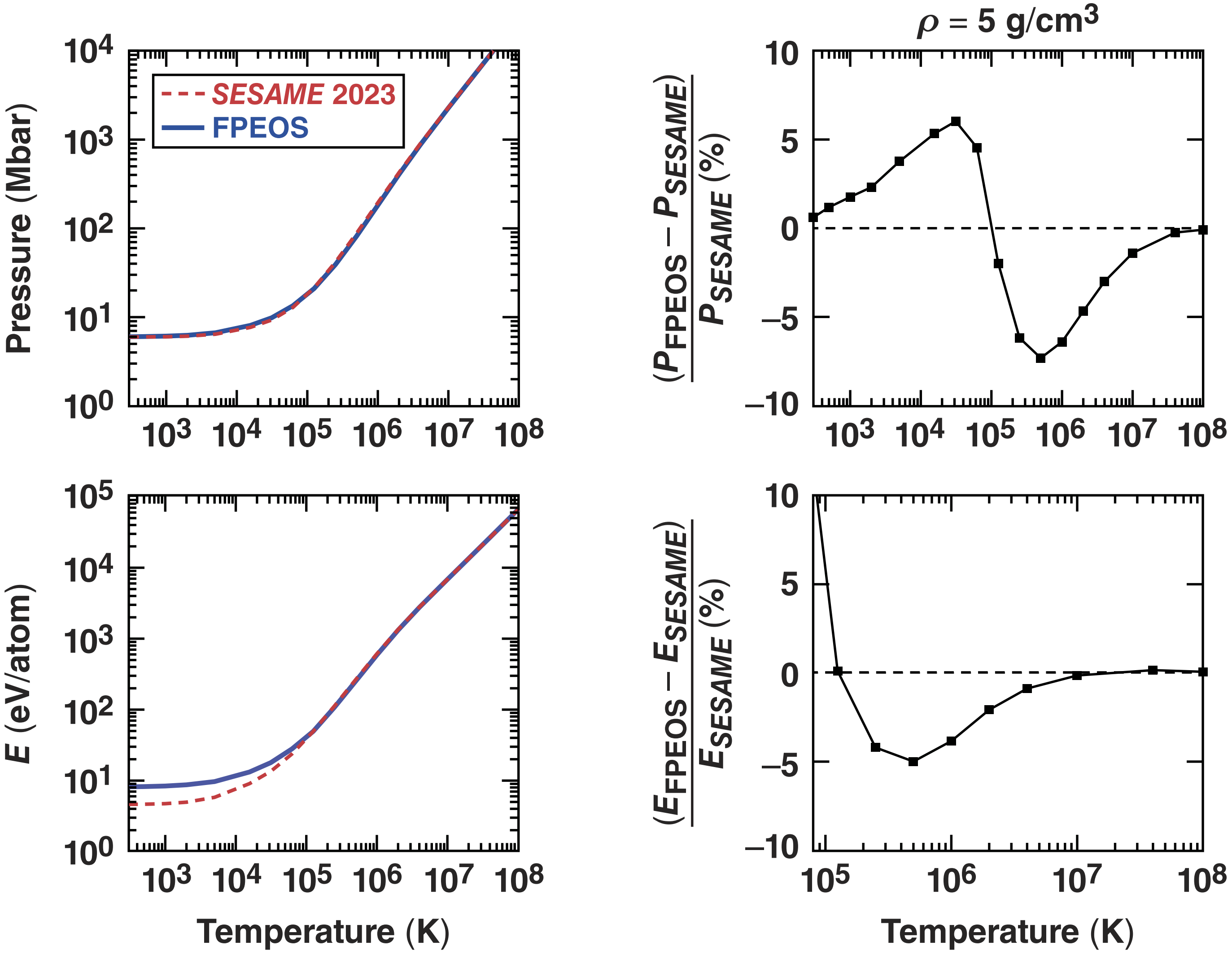

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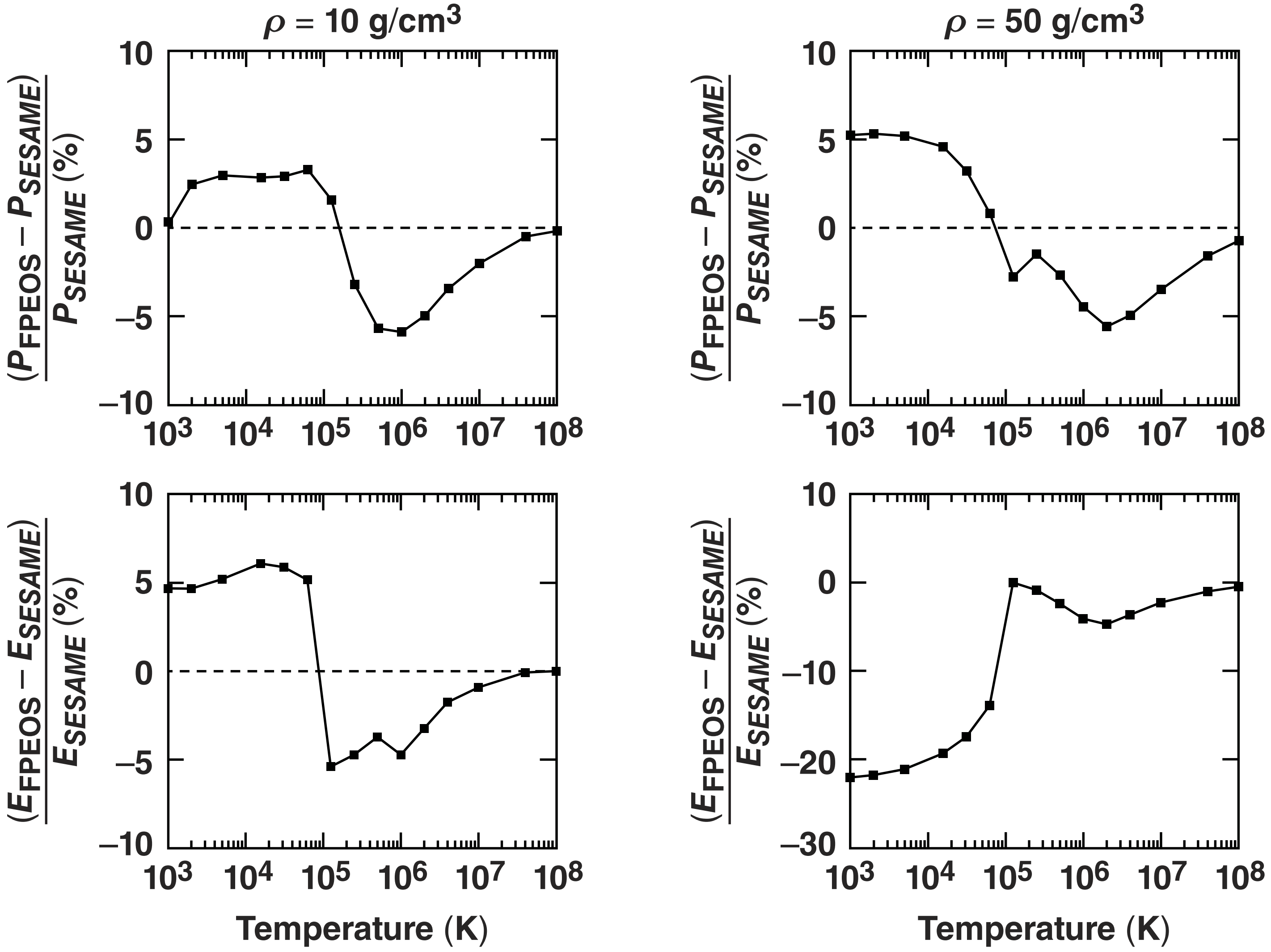

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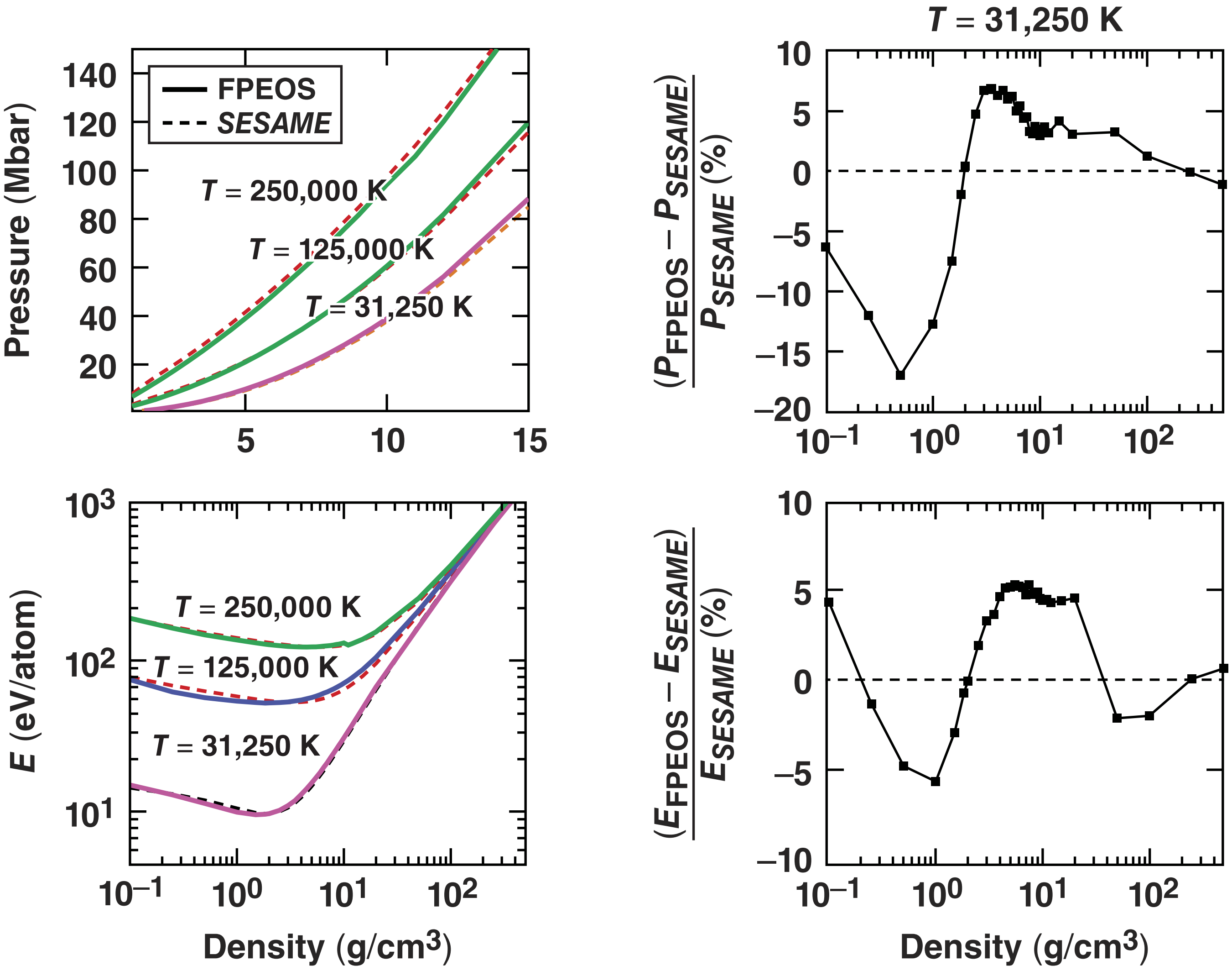

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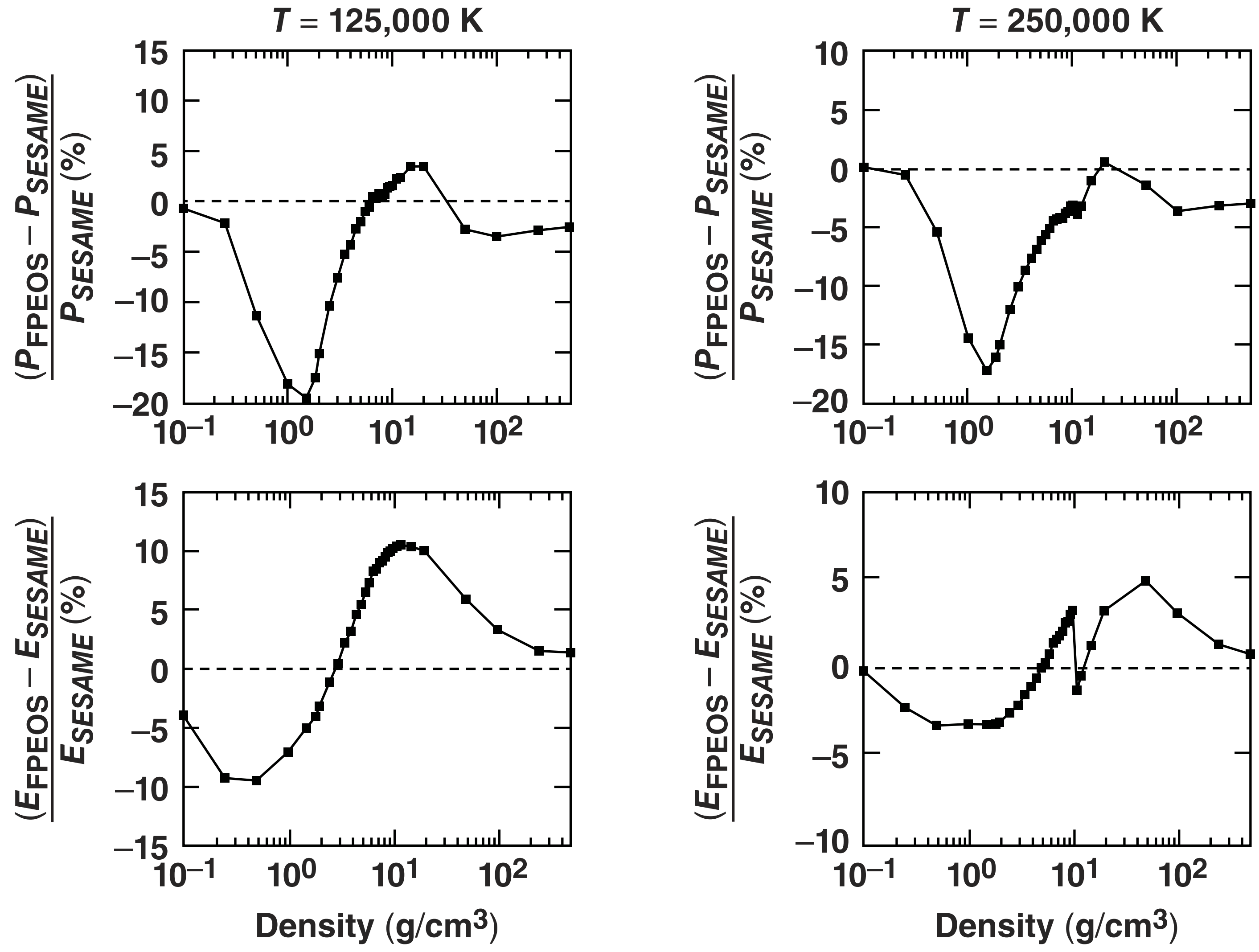

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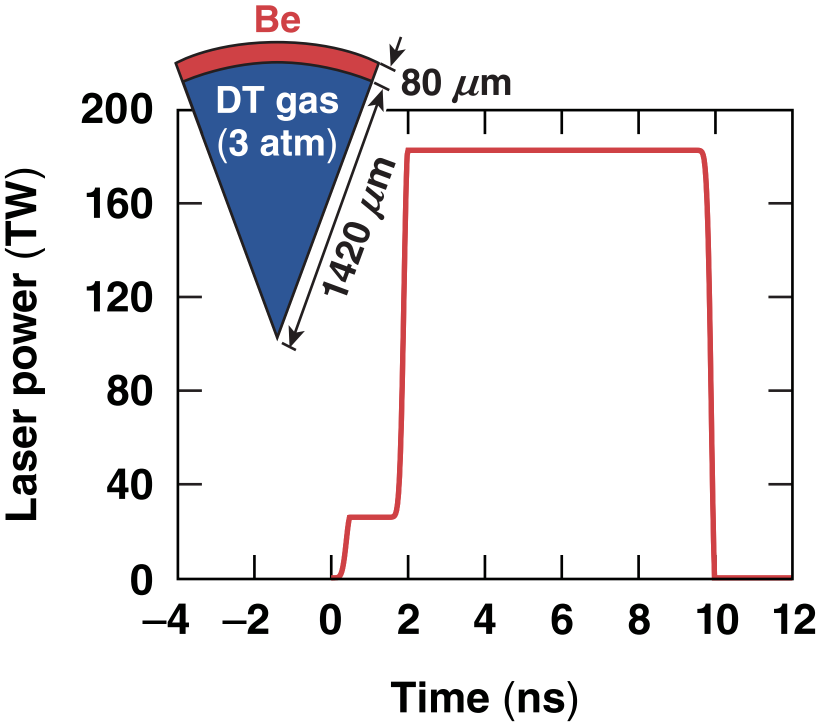

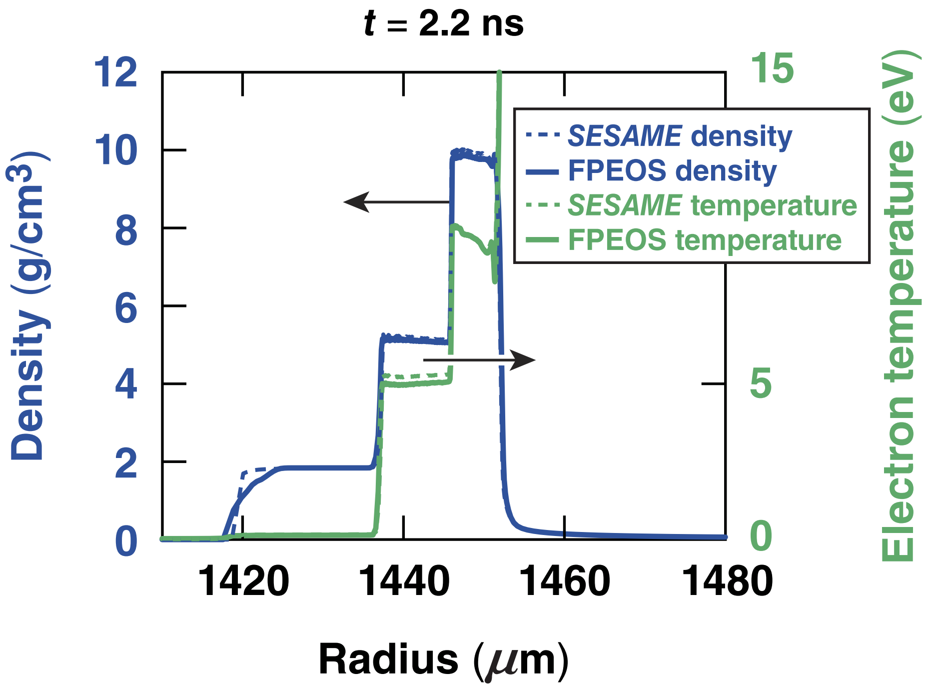

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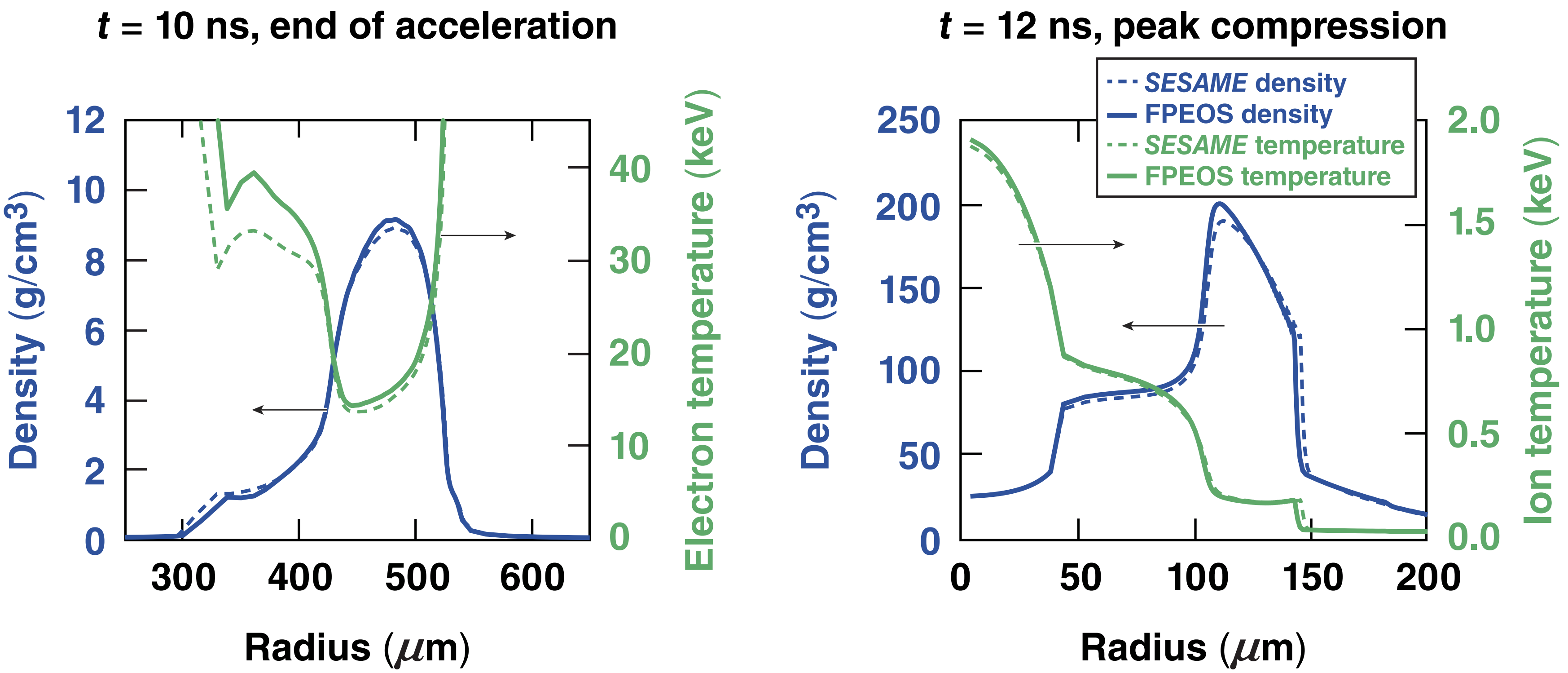

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