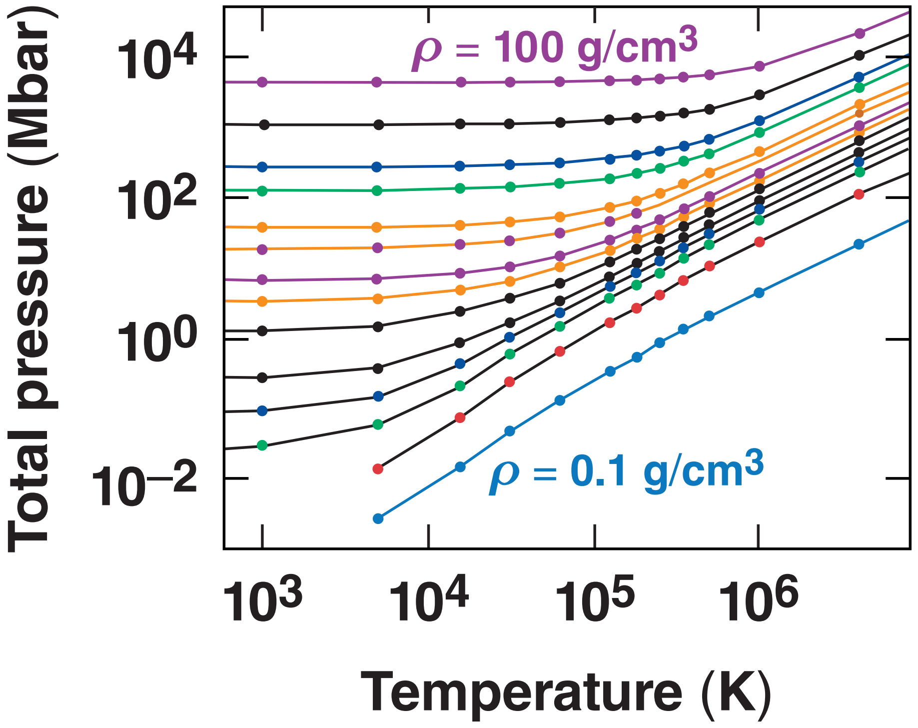
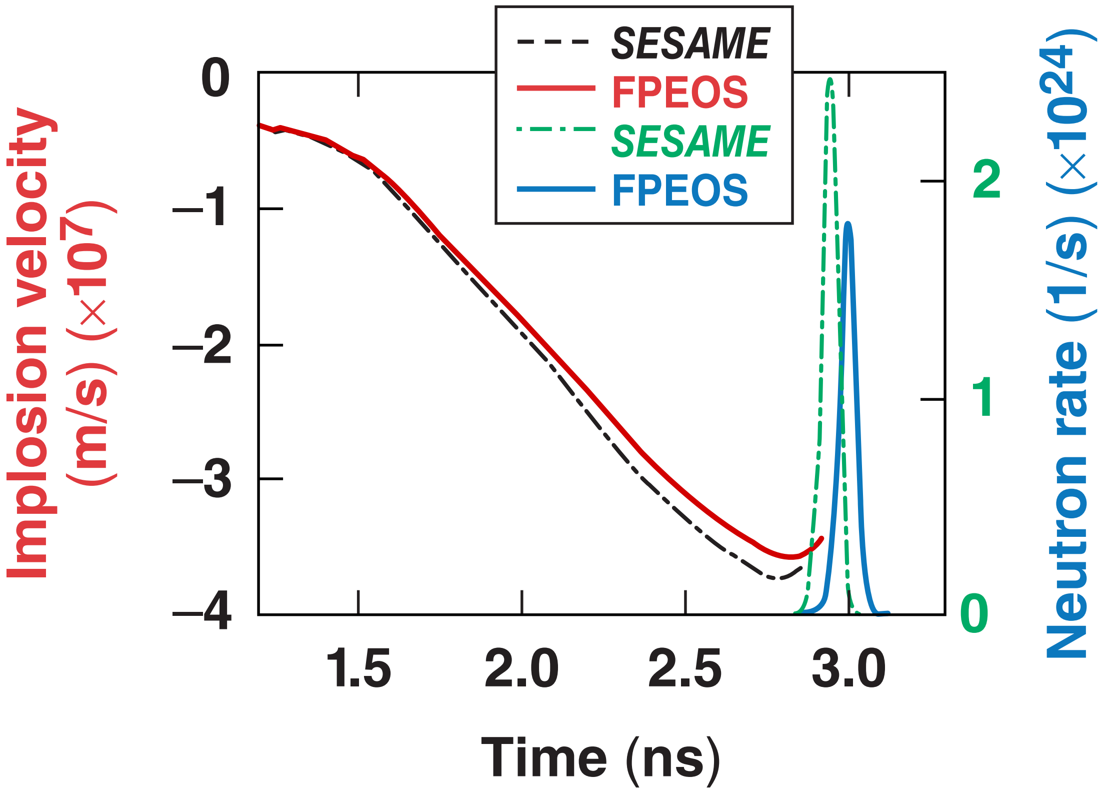
Extended Equation of State of Polystyrene Based on First-Principles Calculations





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Summary

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

- Combining the Kohn–Sham quantum molecular dynamics (QMD) and the orbital-free molecular dynamics (OFMD) methods, we have calculated the EOS of plastic CH under a wide range of plasma conditions (ρ = 0.1 to 100 g/cm^3 and T = 1,000 to 4,000,000 K)
- Significant differences have been identified in the low-temperature regime, when the first-principles equation-of-state (FPEOS) table of CH is compared with *SESAME*-EOS
- Hydrodynamic simulations of an ICF implosion using the FPEOS of CH showed an ~30% neutron reduction because of an ~5% slowdown of implosion velocity relative to the *SESAME* simulations

The mass ablation rate predicted by FPEOS is lower than the *SESAME* prediction.

TC12148

Collaborators

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Accurate knowledge of material properties (EOS, opacity, and thermal conductivity) is required for ICF and HEDP simulations

- In the warm dense regime, strong coupling and electron degeneracy play an essential role in determining the material properties in high-energy-density (HED) states
- First-principles methods are needed to take these important effects into account to self-consistently understand material properties under extreme conditions
- First-principles studies on the EOS, opacity, and thermal conductivity of warm dense deuterium–tritium (DT)* have shown a significant impact on ICF simulations
- Self-consistent calculations of the material properties of ICF ablators (e.g., CH** or C***) are important for designing and understanding ICF and HEDP experiments

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*S. X. Hu *et al*., Phys. Rev. Lett. 104, 235003 (2010); Phys. Rev. B 84, 224109 (2011); Phys. Rev. E 89, 043105 (2014); Phys. Rev. E 90, 033111 (2014); Phys. Plasmas 22, 056304 (2015).
**S. Hamel *et al*., Phys. Rev. B 86, 094113 (2012).
***L. X. Benedict *et al*., Phys. Rev. B 89, 224109 (2014).

First-principles methods of QMD and OFMD can be combined for material-property calculations under extreme conditions

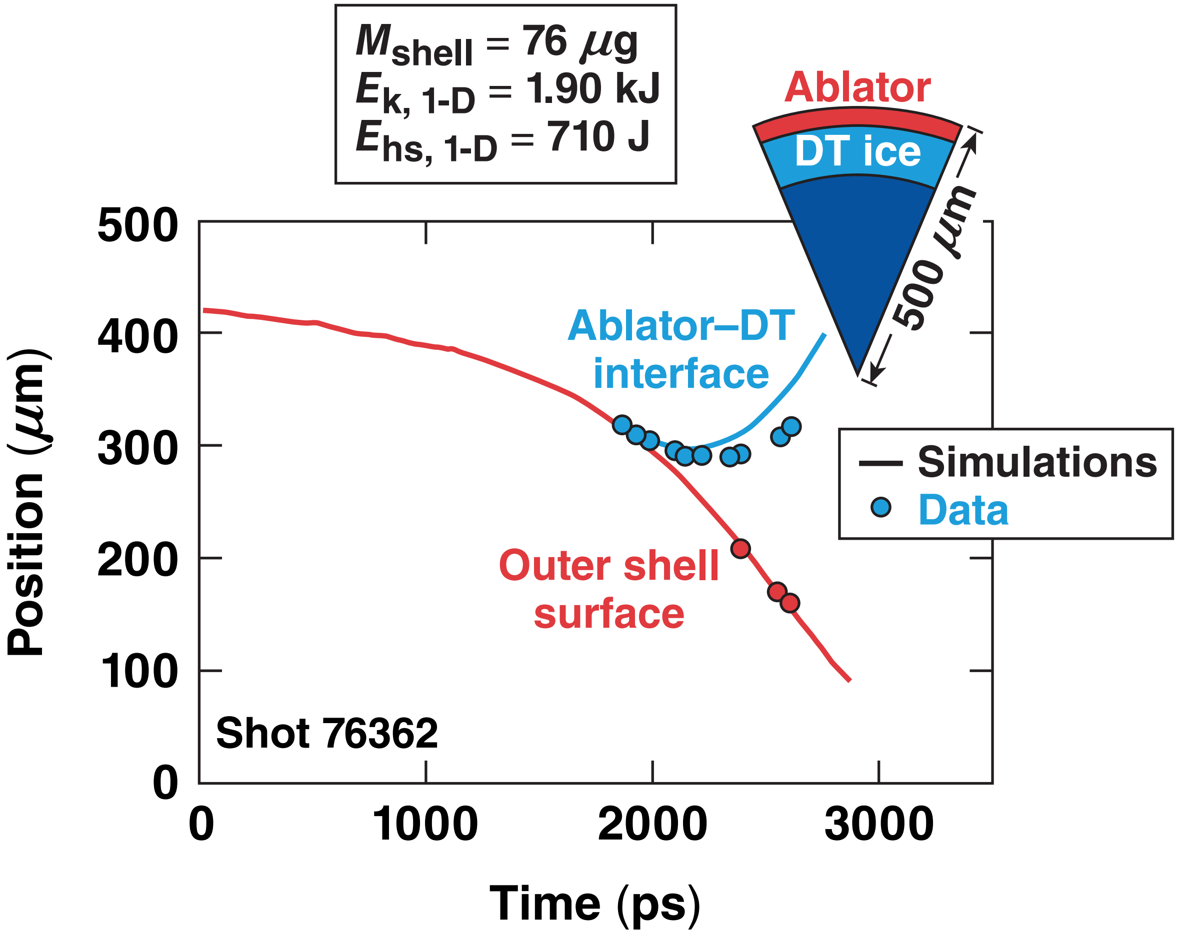
- QMD method is based on the Kohn–Sham density functional theory (DFT),* while OFMD uses Thomas–Fermi molecular dynamics**

- The QMD method can handle plasma conditions up to the Fermi temperature, while the OFMD can be used for high-temperature conditions

- A full range of density and temperature conditions can be investigated with the combined QMD–OFMD method

*W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).
**F. Lambert, J. Clérouin, and G. Zérah, Phys. Rev. E 73, 016403 (2006).

The mass ablation rate predicted by the *SESAME*-EOS of CH is higher than experimental observations*

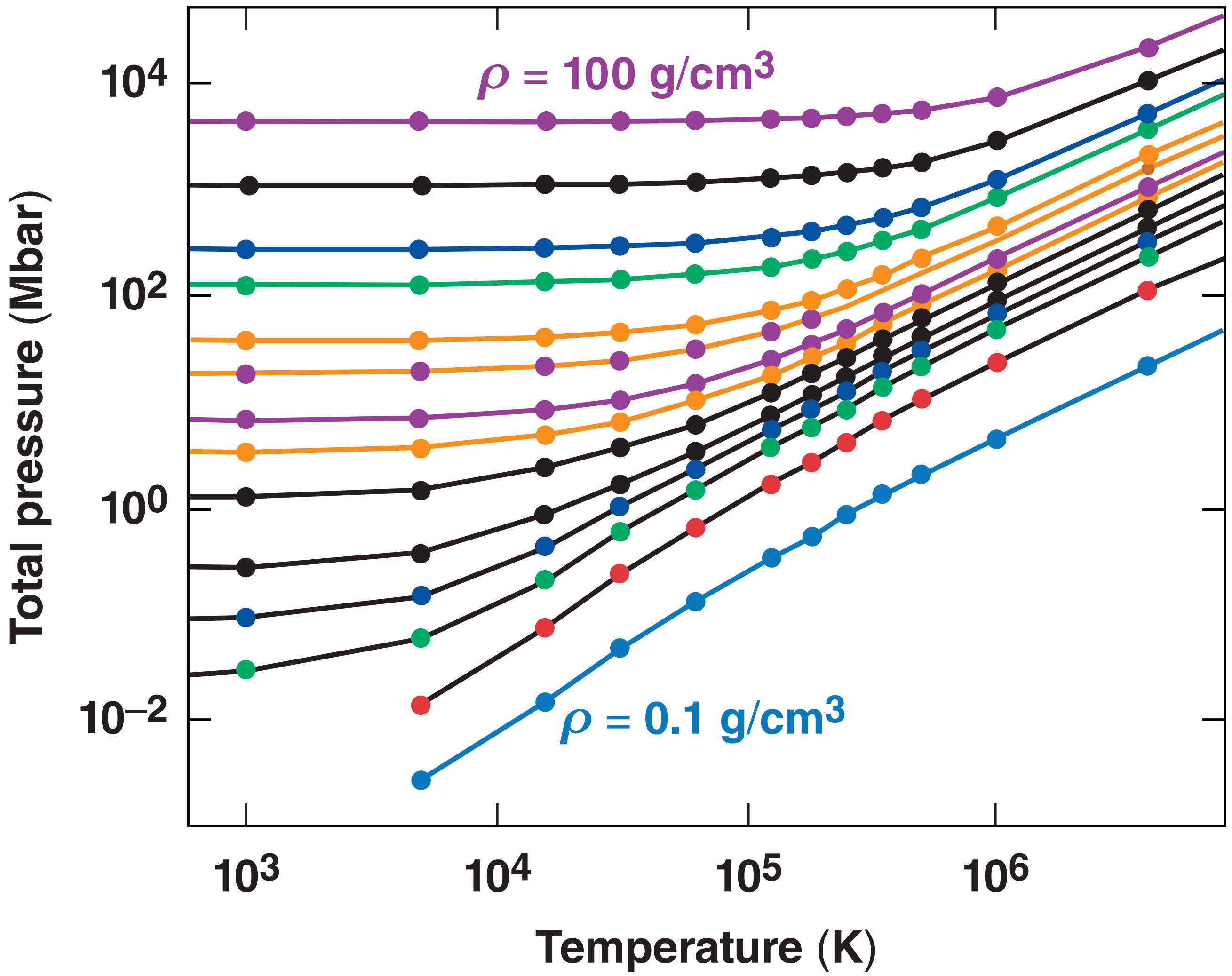


Would the FPEOS of CH give a better mass ablation rate toward experimental data?

E24015b

*D. T. Michel *et al*., Phys. Rev. Lett. 114, 155002 (2015).

The FPEOS of CH* has been calculated for densities and temperatures ranging from ρ = 0.1 to ρ = 100 g/cm^3 and T = 1,000 to 4,000,000 K



*S. X. Hu *et al.*, "First-Principles Equation-of-State of Polystyrene and Its Effect on ICF Implosions," to be submitted to Physical Review Letters.

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The calculated principal Hugoniot* of CH from FPEOS has been well compared with experiments

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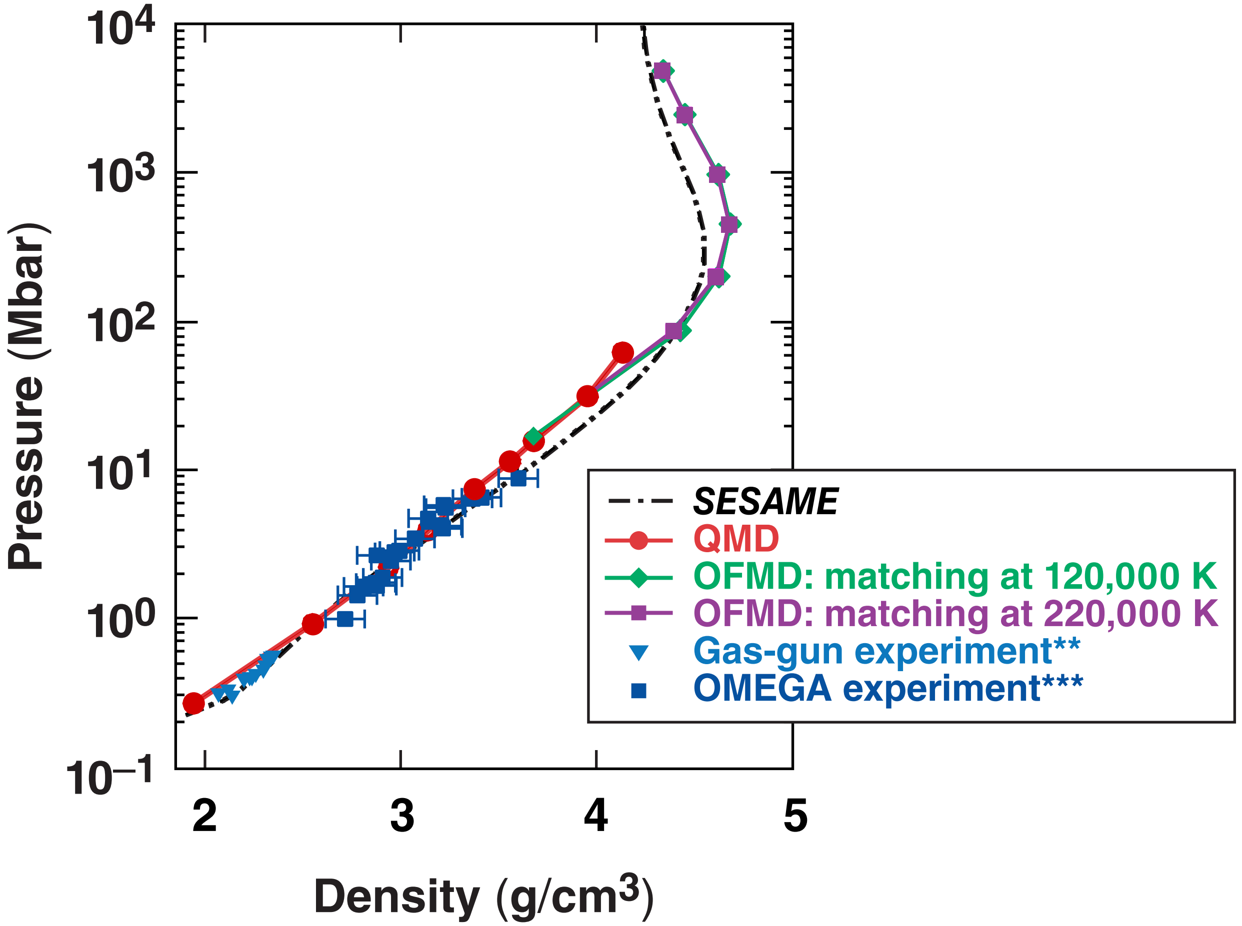
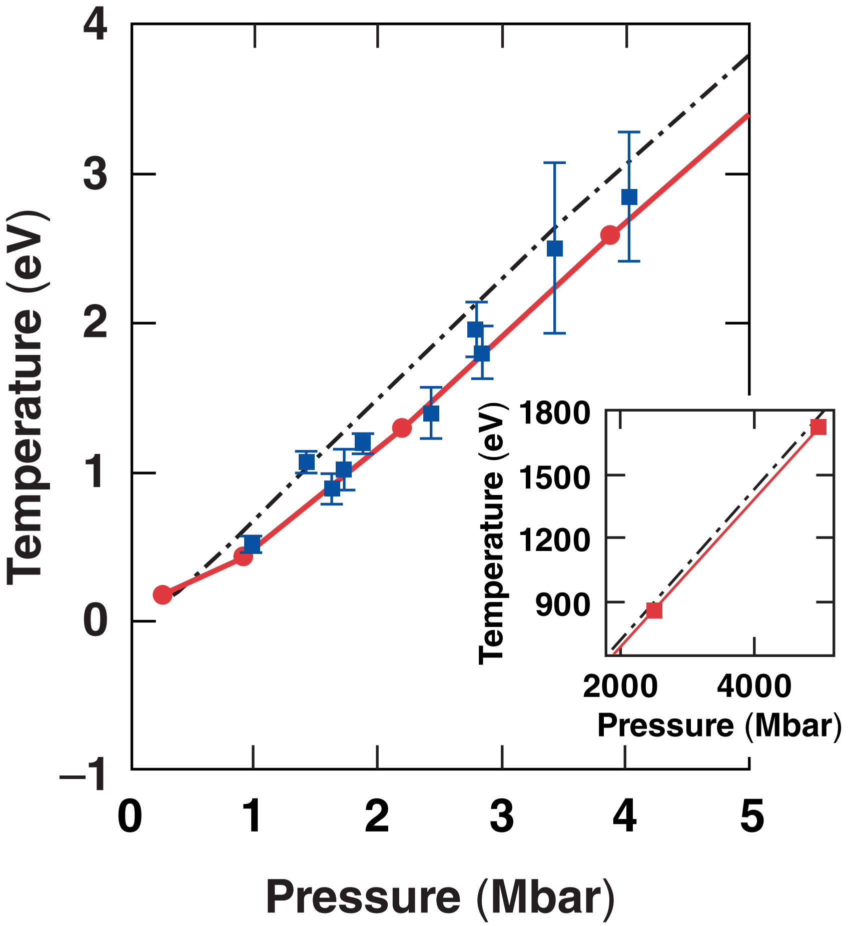


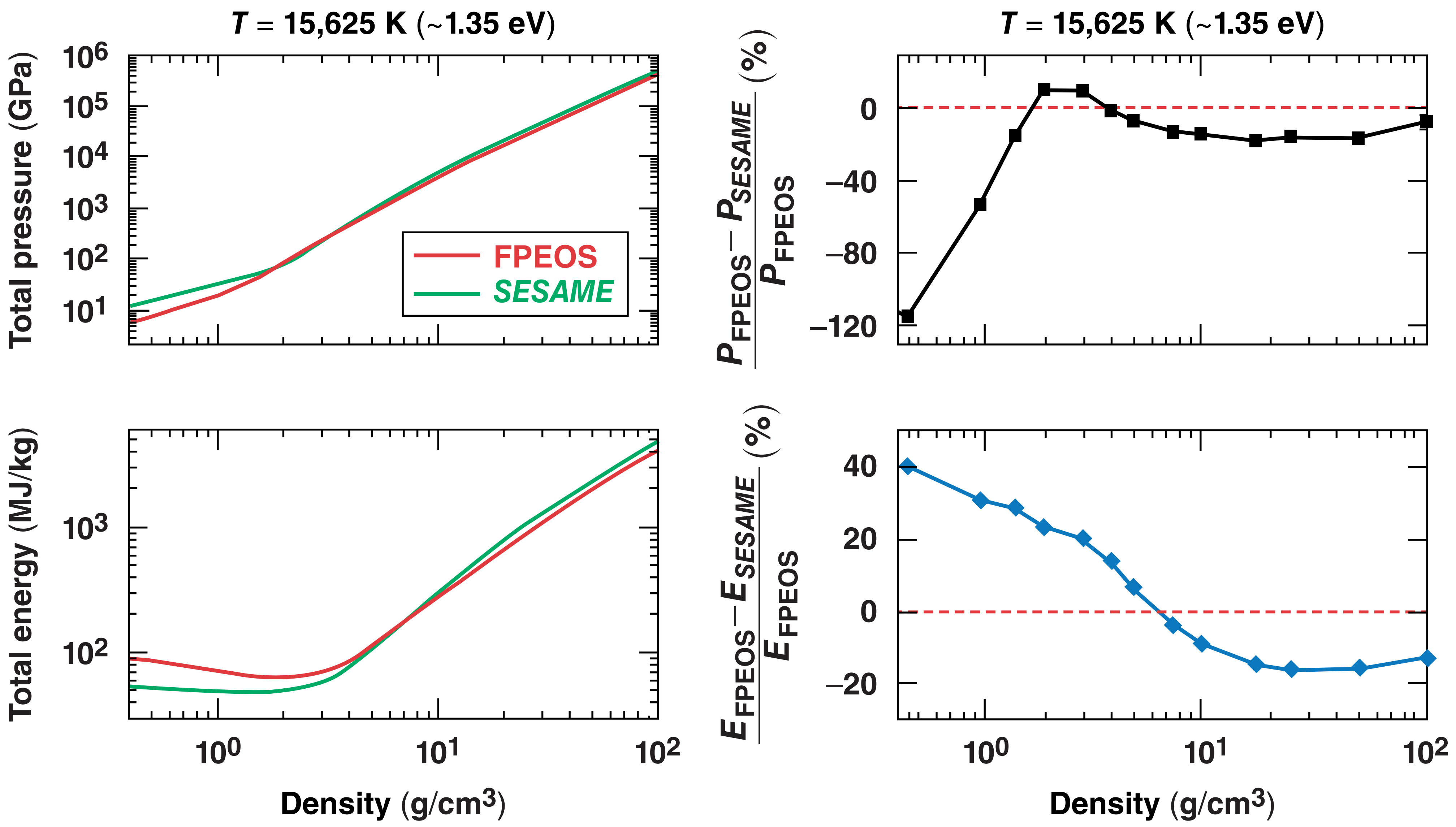


The Hugoniot temperature predicted by FPEOS is in better agreement with experiment!

*S. X. Hu, T. R. Boehly, and L. A. Collins, Phys. Rev. E 89, 063104 (2014).
**S. P. Marsh, ed. LASL Shock Hugoniot Data, Los Alamos Series on Dynamic Material Properties (University of California Press, Berkeley, CA, 1980).
***M. A. Barrios *et al.*, Phys. Plasmas 17, 056307 (2010).

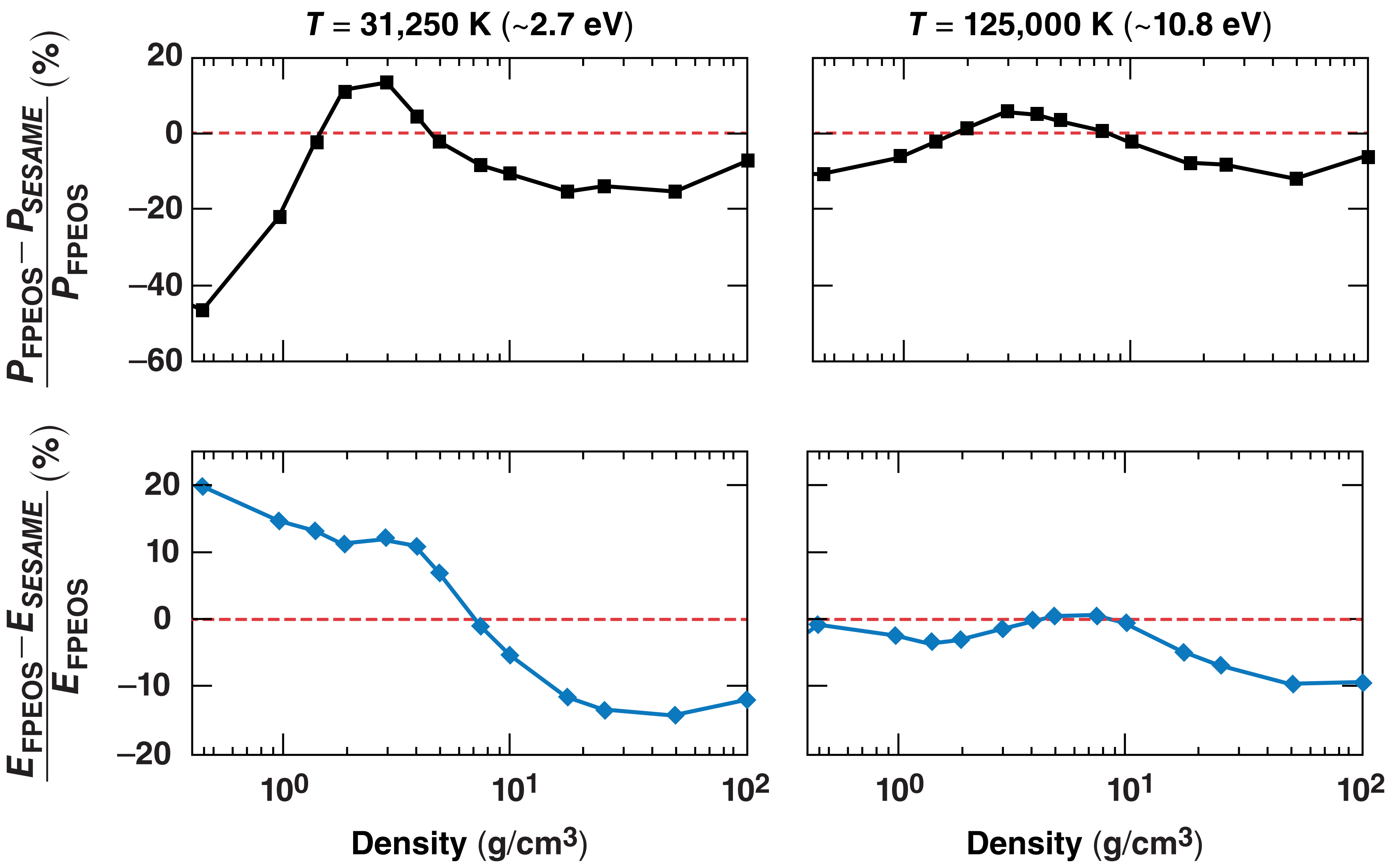
TC12152

Off the principal Hugoniot, a comparison of CH-FPEOS with *SESAME* shows a large difference in the low-*T* and low-ρ regimes



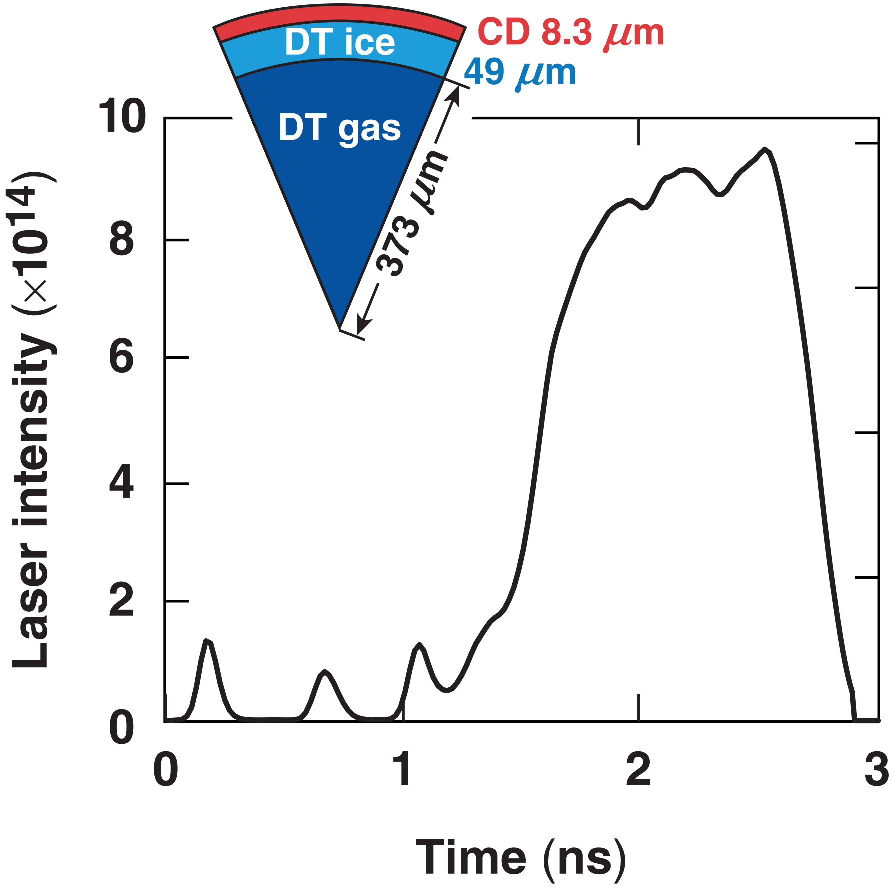
TC12153

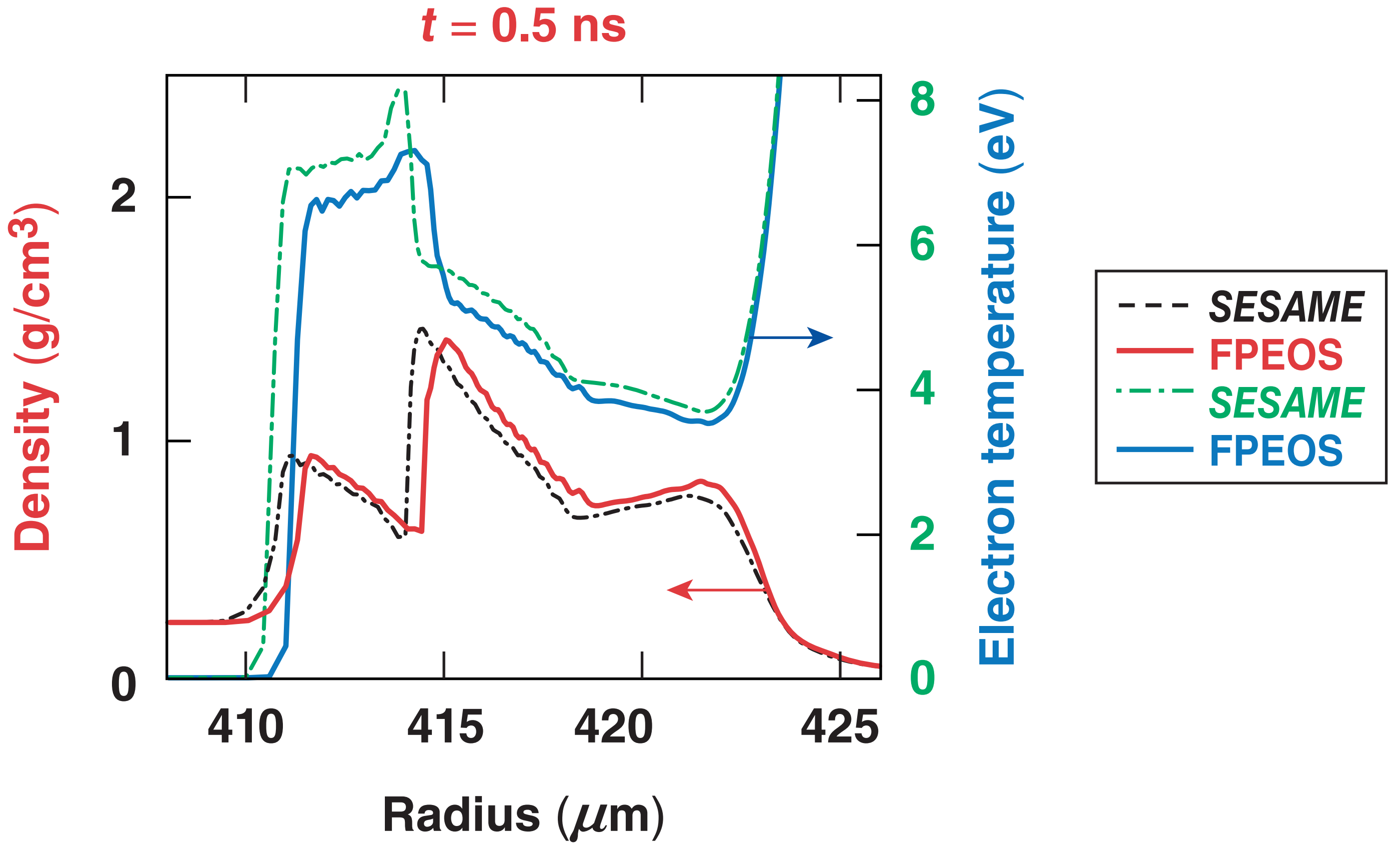
When the plasma temperature increases, the difference between FPEOS and *SESAME* becomes smaller (~10% range)



TC12154

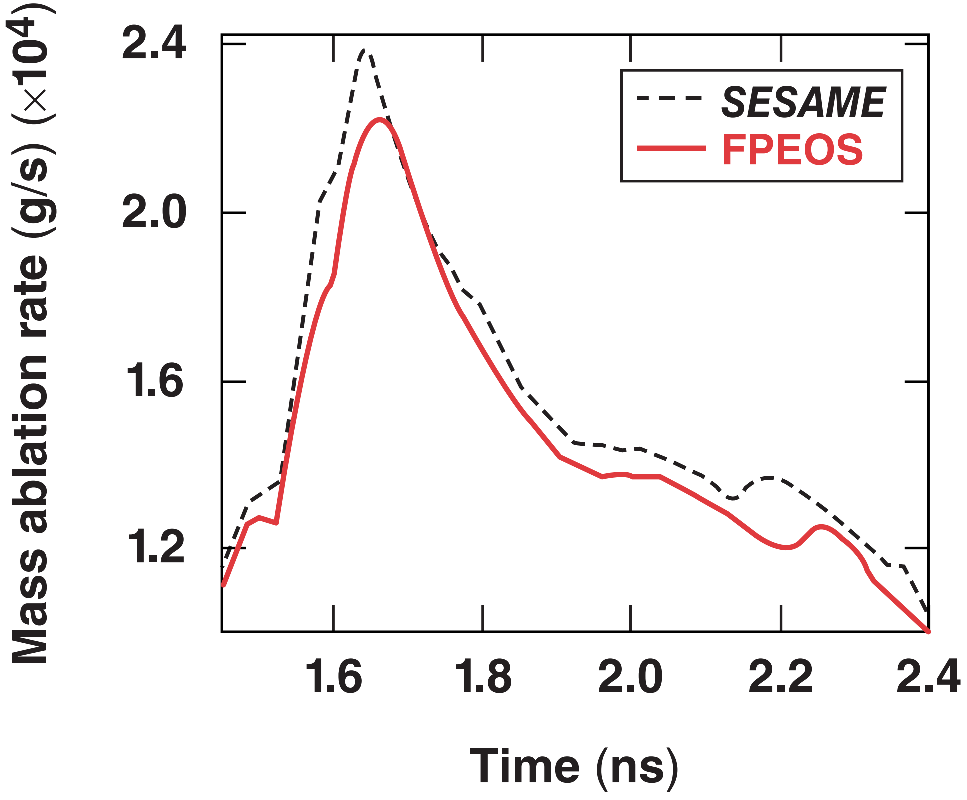
Low-temperature (<10-eV) plasma conditions are routinely accessed in low-adiabat ICF implosions

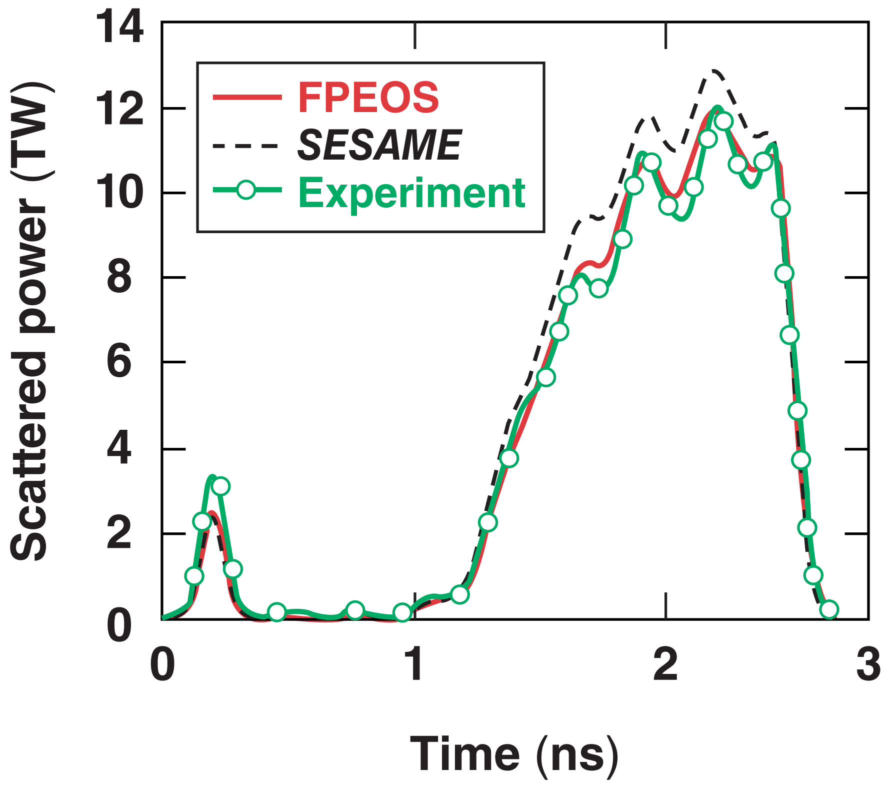




TC12155

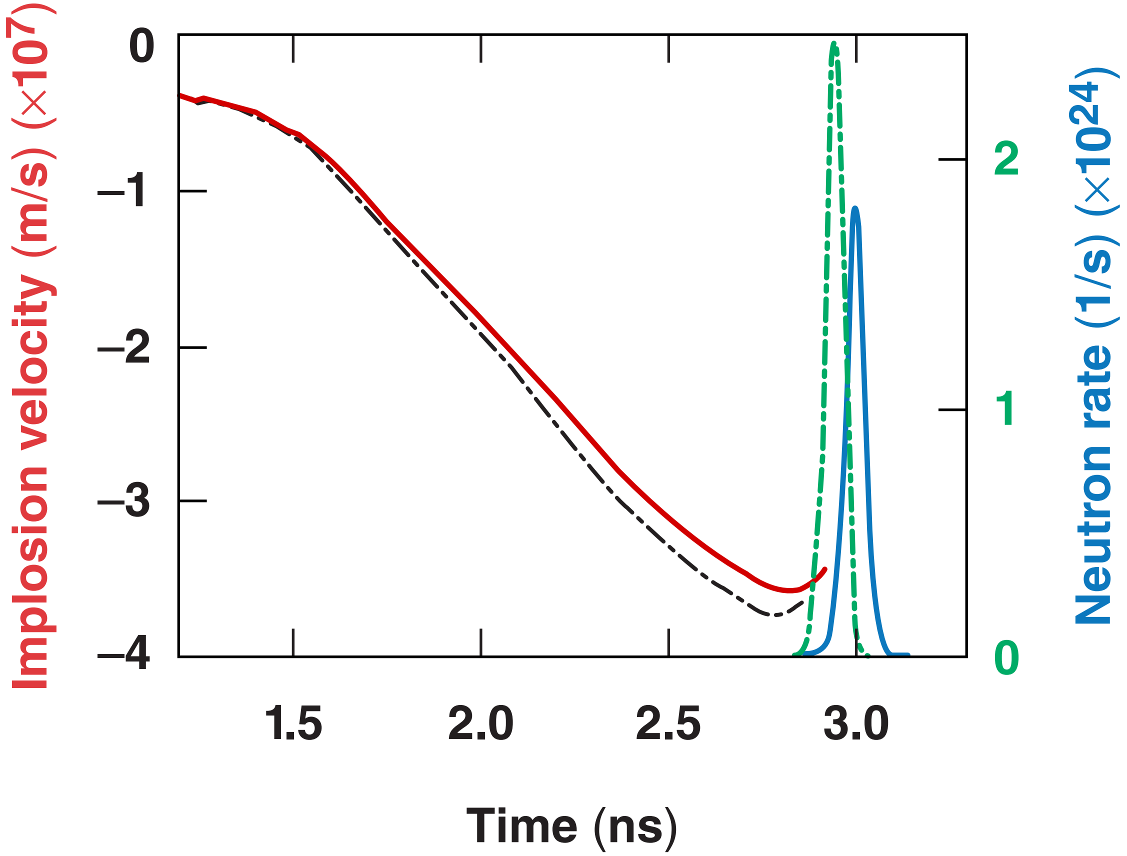
Hydro simulations with FPEOS predict a lower mass ablation rate and better agreement of scattered lights with experiment

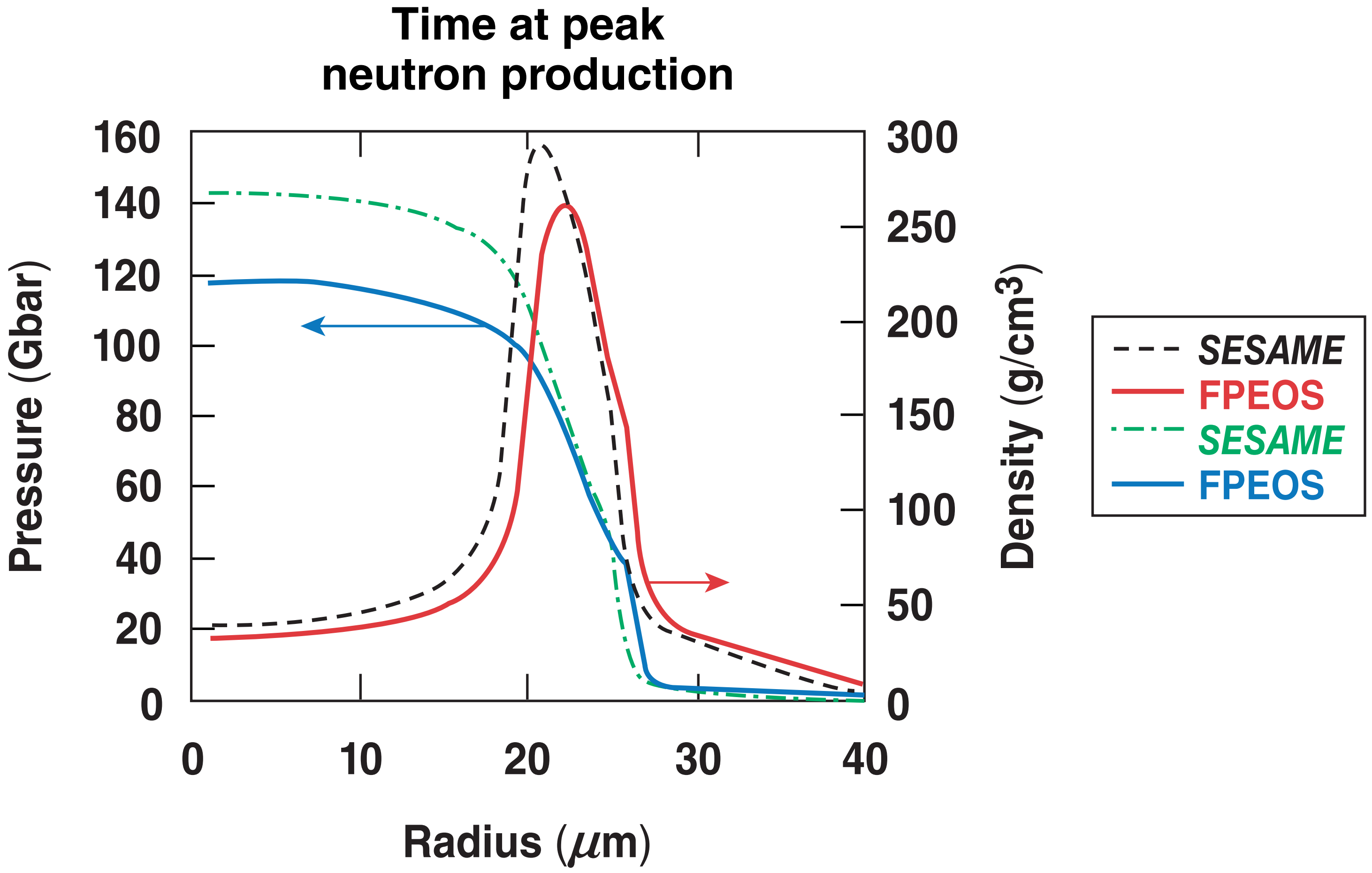




TC12156

The FPEOS simulation has predicted an ~5% decrease in implosion velocity and an ~30% reduction in neutron yield





Yield = 1.5×10^{14}; $\langle T_i \rangle_n$ = 3.6 keV; ρR = 261 mg/cm^2; P = 142 GBar (*SESAME*)
Yield = 1.1×10^{14}; $\langle T_i \rangle_n$ = 3.4 keV; ρR = 250 mg/cm^2; P = 118 GBar (FPEOS)

TC12158

Summary/Conclusions

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

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TC12148