FIRST-PRINCIPLES STUDIES ON THE EQUATION OF STATE, THERMAL CONDUCTIVITY, AND OPACITY OF DEUTERIUM-TRITIUM AND POLYSTYRENE (CH) UNDER EXTREME CONDITIONS

S.X. Hu[1], L.A. Collins[2], V.N. Goncharov[1], S. Skupsky[1]
[1]Laboratory for Laser Energetics, University of Rochester, Rochester, NY, USA
[2]Los Alamos National Laboratory, Los Alamos, NM, USA
shu@lle.rochester.edu

Using first-principles molecular dynamics (FPMD) methods based on the density-functional theory (DFT), we have performed *ab-initio* calculations for the equation of state [1,2], thermal conductivity [3], and opacity[4] of deuterium-tritium in a wide range of densities and temperatures. Their impact on inertial confinement fusion (ICF) target designs has also been studied [5]. The static and transport properties of ICF ablator materials, such as polystyrene (CH), under warm-dense-matter (WDM) conditions are also crucial for ICF implosions. The strong coupling and electron degeneracy in WDM prevents the usual physics models from providing precise material properties of CH for ICF and high-energy-density-physics applications.

Using the DFT-based FPMD methods, we have performed EOS and thermal conductivity calculations of polystyrene for a wide range of densities (ρ = 0.1 g/cm^3 to ρ = 100 g/cm^3) and temperatures (T = 1000 to 4,000,000 K). Our FPMD results agree well with the existing Hugoniot experiments of polystyrene [6]. When compared with the widely used *SESAME*-EOS model, our first-principles-based EOS table showed up to an ~25% difference in pressure and energy, depending on the density and temperature conditions. It is also shown that our FP-based EOS predicts a stiffer Hugoniot at the maximum compression than the *SESAME*-EOS model suggested. Based on these extended first-principles EOS calculations, we have built a global EOS table of polystyrene using the free-energy model. In addition, we have calculated the thermal conductivity (κ) of warm-dense CH. The results indicate a significant increase in κ when compared to the Lee–More model used in our hydrocodes. Implementing the FP-based EOS and thermal-conductivity tables into our hydrocodes, we will explore and present how they may affect ICF target performance in integrated radiation–hydrodynamic simulations.

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