

Molecular Dynamics Simulations Reveal Hydrogen Streaming upon Release from Polystyrene Shocked to Inertial Confinement Fusion Conditions

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Shock release from inertial confinement fusion (ICF) shells poses a great challenge to radiation-hydrodynamic simulations because the kinetic effects and large Knudson numbers are beyond the regular single-fluid approximation and cannot be included in standard equation-of-state (EOS) models. This has been evidenced by a recent experiment¹ on polystyrene (CH), in which low-density plasmas (10^{19} to 10^{20} cm⁻³) released from a laser-shocked CH shell were observed to travel significantly ahead of what regular hydro-simulations predict. Further hydro-simulations were rendered to agree with experiments by *assuming* excessive pre-expansion at the rear surface of the CH shell before arrival of the shock. In this work, we take a novel route to elucidate the microscopic shock-release physics of CH by large-scale nonequilibrium molecular dynamics (MD) at the experimental conditions. Our results revealed species separation and hydrogen streaming out of CH upon shock release and provided excellent explanation to experimental observations. Such kinetic effect of species separation as revealed by our simulations is currently missing in single-fluid radiation-hydrodynamic simulations, which could have profound implications to ICF target designs.

CH is an important ablator material in ICF and high-energy-density experiments. In experiments, it can be shocked to warm-dense-matter states with multimegabar pressures and tens-of-electron-volt temperatures, while the unshocked regime remains under ambient conditions; after shock breakout, electron-ion recombination occurs and chemical bonding may be expected while the system is cooling down. The various pressures and temperatures and distinction between up- and downstream of the shock front challenge regular hydro-simulations that are based on the single-fluid approximation and MD simulations that use empirical potentials. Previous MD studies of hydrocarbons are limited to pressures up to ~ 200 GPa (Refs. 2–4). Recently, we have developed an approach that uses many-body reactive force fields, combines with first-principles ionization models, and greatly extends the regime of fidelity of the MD simulations to ~ 2100 GPa (associated shock velocity ~ 55 km/s, temperature $\sim 1.5 \times 10^5$ K), which is more than $10\times$ the maximum previous record. This approach is justified according to benchmark calculations of various atomistic models with up to several million atoms, which uniformly show small differences (3%–20%) in the Hugoniot EOS in comparison with those predicted by accurate first-principles calculations.⁵

By studying the time evolution of spatial and velocity distributions of hydrogen and carbon after shock breakout, we find that hydrogen atoms stream far ahead of carbon. In addition, the motion of both species is linear throughout the simulation, whereas hydrogen travels much faster than carbon, more so at the lower density of 10^{19} than at 10^{20} cm⁻³ [Fig. 1(a)]. In comparison with the experiment, the hydrogen velocities calculated from our MD simulations at both densities of 10^{19} and 10^{20} cm⁻³ compare favorably well with the measured values, while the carbon velocity along with its dependence on density is clearly off trend [Fig. 1(b)]. Furthermore, by exponentially fitting the hydrogen distribution profile at 10^{19} to 10^{20} cm⁻³, we estimated the plasma scale length and found that it increases tenfold from 2 to 10 ps [Fig. 1(c)].

We note that the above comparisons to experimentally measured plasma properties are based on the assumption that $\langle Z \rangle = 1$. While this provides a reasonable estimation for the upper bound of hydrogen ionization, we notice that the temperature remains above 10,000 to 30,000 K until after 10 ps. We have, therefore, performed average-atom model calculations⁶ using density functional theory for carbon and hydrogen plasmas at the temperature of 20,000 K and densities between 10^{19} to 10^{20} cm⁻³ to estimate a lower bound for the ionization. From these calculations, we have found $\langle Z \rangle$ to be approximately 0.5. Therefore, we have

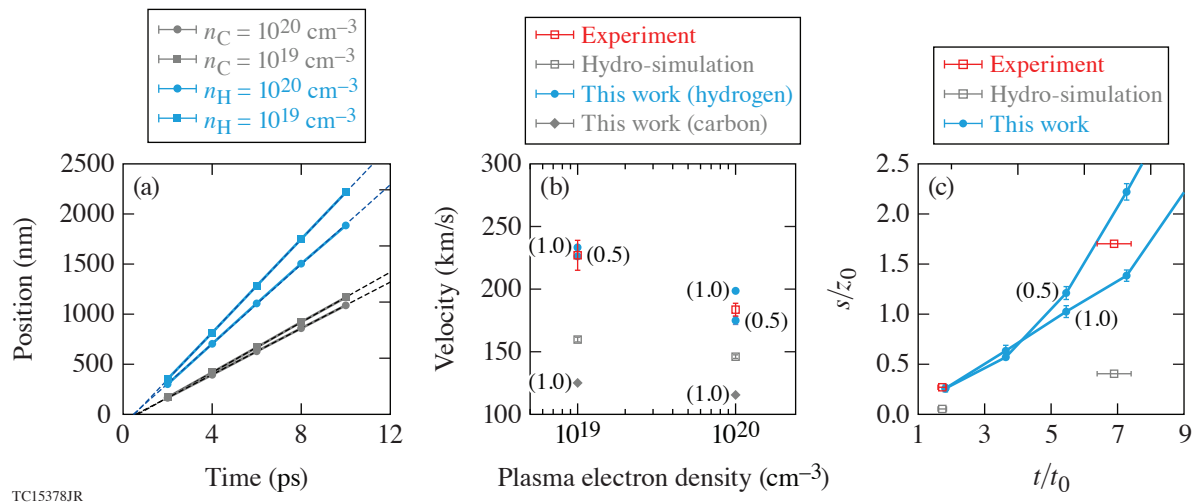


Figure 1

(a) Drifting of carbon and hydrogen, (b) plasma velocities, and (c) scale lengths (normalized by sample thickness z_0) as a function of time (normalized by shock duration t_0) at 10^{19} and 10^{20} cm^{-3} according to our simulations of shock-released CH and in comparison with experiment and regular single-fluid hydro-simulations from Ref. 1. The solid lines in (a) and (c) are guides to the eyes and the dashed lines in (a) are linear fits to the data. In (b) and (c), error bars denote the fit error; the labels of “1.0” and “0.5” indicate the estimated charge state $\langle Z \rangle$ for carbon or hydrogen.

considered the range of $\langle Z \rangle = 0.5$ to 1 to directly compare with the experimental results. For the lower bound of $\langle Z \rangle = 0.5$, the re-evaluated plasma velocity decreases slightly by 7 km/s at 10^{19} cm^{-3} and by 24 km/s at 10^{20} cm^{-3} , while scale length remains constant at 2 ps but increases by the amount of sample thickness (z_0) at 10 ps. Giving these ionization estimates, the hydrogen plasma velocities and scale lengths all match the experimental values very well (Fig. 1).

These results provide a clear microscopic picture of post-shock-release hydrogen streaming that offers an important factor to be considered in improving radiation-hydrodynamic simulations. We expect similar species-separation processes can occur during shock release of deuterium–tritium (DT) fuel in ICF implosions, especially for strong shocks. The other implication to ICF is the likely hydrogen streaming into the DT layer upon shock transits through DT/CH interfaces, which might induce atomic mixing, thereby reducing the final compression areal density.

This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0003856, the University of Rochester, and the New York State Energy Research and Development Authority.

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