

Computational and Experimental Evidence of Species Separation in CH Shock Release

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Materials shock release, such as that of the CH ablator into the DT fuel or that of DT ice into gas, is involved in different stages of inertial confinement fusion (ICF) and can affect performance but is challenging to quantify both experimentally and theoretically. Typically, the design of ICF experiments relies on single-fluid hydrodynamic simulations. On occasion, however, such simulations omit the microscopic chemistry and physics that play an important role. For example, Thomson-scattering experiments¹ have shown that the fractions of carbon and hydrogen species on the laser-ablation side of a CH₂ foil are different from the initial target composition. Another set of experiments² based on optical interferometry measurements of CH shock release found low-density plasmas at locations far ahead of hydrosimulation predictions. Interestingly, when considering radiation transport and pre-expansion at the rear surface of CH before shock arrival, improved agreements with experiments were reached.² Follow-up studies,³ however, indicate that inconsistency remains between simulation and experiments that used a gold shield to prevent radiation preheat.

Recently, S. Zhang and S. X. Hu employed a large-scale molecular-dynamics (MD) approach to simulate the release of strongly shocked CH polystyrene.⁴ They found species separation and hydrogen streaming ahead of carbon that produce low-density plasmas whose velocities and scale lengths both match experimental observations. This demonstrates MD as a promising approach for simulating nonequilibrium processes, such as shock release, under extreme conditions. One advantage of the MD approach is that any atomic level kinetic effect is explicitly taken into account. In addition, our calculations show that existing reactive force fields for CH can be readily used for high-pressure applications involving CH and produce post-shock equations of state that are similar to the known Hugoniot of CH in a broad range of pressures (deviations are less than 20% for pressures up to 135 Mbar).

We performed extensive MD simulations and designed new laser-driven experiments by considering different shock strengths to further clarify the microscopic shock-release physics of CH. Our experimental design prevents radiation preheat of the sample and employs a thin (~50-nm) Si₃N₄ foil to witness the release of shocked CH across a vacuum gap [Fig. 1(a)]. Interestingly, we observe VISAR (velocity interferometer system for any reflector) reflectivity changes before fringe shifts [Fig. 1(b)] and similarly for all glow-discharge polymer and CH experiments when shocked to above 550 GPa, but not in the experiments of pure diamond or beryllium. These observations are all consistent with our MD-predicted species separation and hydrogen streaming, which are clearly seen upon shock breakout and during the release of CH under strong shocks (350 GPa or higher) but absent for weak shocks (160 GPa or lower) [Figs. 1(c) and 1(d)]. Furthermore, our experiments show that the velocity of the Si₃N₄ foil jumps up earlier in the case of a stronger shock [Fig. 1(f)]. This is also consistent with our MD results, which show that species momentum ramps up (when hydrogen arrives) before jumping up (as carbon arrives) and that this momentum jumping happens at earlier times for stronger shocks [Fig. 1(e)].

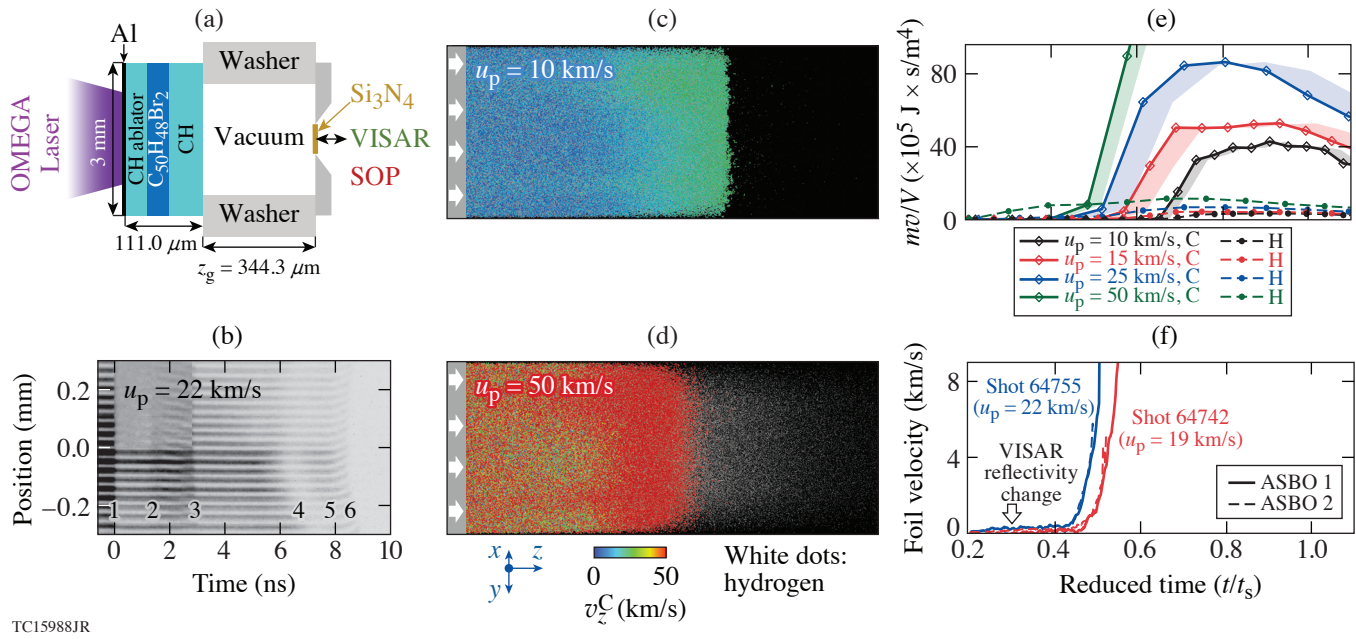


Figure 1

(a) A schematic of the target design and (b) a representative VISAR image of our CH shock-release experiment. An aluminum overcoat and a brominated CH layer are used to prevent radiation preheat of the CH sample. The upper half of the Si₃N₄ foil is coated with titanium. In (b), the numbers “1” to “6” denote the times that the laser turns on, first visibility of the shock front, shock breakout of the CH sample, the reflectivity change of the Si₃N₄ foil, fringe shift indicating motion of the foil, and blackout of fringes, respectively. [(c),(d)] Snapshots of our MD simulations during the release. Carbon atoms are color coded according to their z-component velocities, and hydrogen atoms are shown as white dots. Species separation is clearly observable for strong shocks but absent for weak shocks. (e) Species momentum at the position of a “witness foil” and (f) experimentally measured foil velocities after breakout of shocks with different strength. Time in (e) and (f) is originated from the moment of shock breakout and reduced by the scaling factor $t_s = z_g/u_s$, where z_g is the thickness of the vacuum gap and u_s is the velocity of shock upon breakout. In (e), shaded areas denote the estimated uncertainties in time bounded by the post-shock and first-principles⁵ Hugoniot values of u_s . In (f), the time of VISAR reflectivity change in shot 64755 is indicated with an arrow; u_p is the particle velocity in experiments or piston velocity in simulations. ASBO: active shock breakout.

We also quantified the effect of hydrogen isotopes on CH shock release by comparing the results from CH, CD, and CT calculations. We found lighter hydrogen isotopes stream farther away from carbon, while the spatial velocity profiles of different species are similar. This results in higher momentum and energy (by one to two orders of magnitude) of the lighter species/isotopes at the release front of the heavier species. Such differences in streaming rate of different isotopes could lead to degradation of the final compression in ICF experiments, as well as discrepancies between hydrodynamic predictions and experiments.

To understand the effect of radiation preheat on the shock release, we simulated preheated CH by considering samples with different thicknesses. Our calculations show species velocities increase with both the cell size and the degree of preheat, more so for hydrogen than carbon. We also found that the scale length of the species increases with cell size but is not sensitive to preheat. By extrapolating these results to the experimental sample size with 10% thermal expansion (as predicted by hydrodynamic simulations with radiation transport³), we can expect the velocity and scale length of the carbon species (or electrons if considering average ionization $\langle Z \rangle \sim 1$) to become comparable to those measured in experiments,² which would reconcile the findings from hydrodynamic simulations. Under our established understanding of species separation, however, we must expect that hydrogen runs ahead at much faster velocities and longer scale lengths than carbon. Therefore, we conclude that pre-expansion, if it occurred in the experiment conducted by Haberberger *et al.*,² would be much less than 1 μm. This is in clear contrast to hydro-predictions and can be tested by future experiments.

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