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A Coupling Simulation Integrating Molecular Dynamics and Particle-in-Cell Methods for Accurate Intense Laser-Target Simulations

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The irradiation of an intense laser on thin targets generate energetic ions in experiments, which has also been replicated using particle-in-cell (PIC) simulations. However, the ion energies obtained in simulations are sometimes significantly higher than the experiments. This discrepancy was also noticed in a recent experiment involving the ultra-intense JKAREN laser (without plasma mirrors)[1]. In the corresponding PIC simulations, assumptions regarding the target expansion due to the pre-pulse had to be factored, as corrections, to obtain the experimental energies. Thus, modelling the pre-pulse is essential; but the conventional hydrodynamic pre-pulse simulations are not possible due to the ultra-thin nature of the targets. Currently, there exists no framework to successfully integrate the pre-pulse simulation with the main pulse, especially for thin targets, since the scales and the physics of the simulations involved are vastly different. In this study, we propose a coupling scheme to integrate the pre-pulse; simulated through the molecular dynamics (MD) approach, with the main pulse simulated using the PIC method. The intensity of the laser pre-pulse is usually $< 10^{11}$ W cm^{-2}, even for a laser like JKAREN (I $= 10^{21}$ W cm^{-2}) without plasma mirrors. In this regime, the atomic physics is dominant and hence the use of MD for pre-pulse simulation is reasonable. Following the experiment[1], a 3D graphene target was created in MD (using LAMMPS) and irradiated (energy deposition) by an experimentally obtained pre-pulse profile, leading to the target's deformation. A section of the deformed target is then imported to the 2D PIC environment (EPOCH) through a density interpolation scheme and is simulated for the main pulse conditions[1]. The ion energy spectrum thus obtained is in good agreement with the experiment as compared to the previous results suggesting that the proposed method realistically captures the physics behind the experiment without assuming target pre-expansion.

References

[1] Kuramitsu, Y *et al.* Robustness of large-area suspended graphene under interaction with intense laser. *Sci Rep* **12**, 2346 (2022).