Modeling of picosecond time evolution of clusters irradiated by FEL pulse

Vikrant Saxena[1], Zoltan Jurek[1], Beata Ziaja[1,2] and Robin Santra[1,3]
[1]*Centre for Free-Electron Laser Science, DESY, Notkestrasse 85, 22607 Hamburg, Germany*
[2]*Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland*
[3]*Department of Physics, University of Hamburg, 20335 Hamburg, Germany*

The recently developed x-ray free-electron lasers (FEL) open up new horizons in the experimental investigation of matter under extreme conditions. The study of FEL induced dynamics of clusters is an important step towards the understanding of the behavior of chemically more complex systems. The interaction of a FEL pulse with clusters depends on the cluster size. It creates either a positively charged ion cloud (in case of small clusters), or a quasi-neutral nanoplasma (in case of large clusters) [1]. The expansion dynamics in the two cases are entirely different. In the first case, the positively charged ion cloud explodes due to the unscreened electrostatic repulsion between ions, whereas in the second case the quasi-neutral nanoplasma expands slowly due to the thermal pressure. The expansion of quasi-neutral plasma into vacuum has been a subject of continuing research interest [2-7].

To understand the spectroscopic data of particles originating from the FEL induced cluster dynamics, long-timescale computer simulations are required. For particle-based approaches, this is computationally expensive. On the other hand, employing the hydrodynamics approach, after the free electrons in the sample have reached local thermodynamic equilibrium, significantly reduces the computational cost. Therefore, in the present work we explore the accuracy of a hydrodynamics approach by numerically investigating both expansion cases for spherically symmetric clusters. In the first case, we investigate the Coulomb explosion dynamics of a cold ion fluid. In case of nanoplasma expansion, a two-fluid approach (for a warm electron fluid intermixed with a cold ion fluid) is used. The hydrodynamic simulation results are compared with the corresponding molecular dynamics simulations. Advantages and limitations of both approaches are discussed.

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