Abstract Submitted
for the DPP20 Meeting of
The American Physical Society

Modelling of diffusive interface broadening between materials at warm dense conditions in support of XFEL experiments.[1] TOMORR HAXHIMALI, Lawrence Livermore Natl Lab, ROBERT RUDD, JAMES GLOSLI, CATHERINE BURCKLEN, TOMMASO PARDINI, STEFAN HAURIEGE, Lawrence Livermore National Laboratory — Transport processes in warm dense matter such as diffusion remain poorly understood with considerable scatter between models and the absence of experimental data. We present results of modeling of diffusive interface broadening between diffusion couple materials in plasma generated in x-ray free electron laser (XFEL) experiments. A novel x-ray scattering technique developed recently at LLNL to measure the interdiffusion in liquids leverages the high intensity of XFELs to provide highly sensitive measurements on picosecond time scales. It will be extended to provide highly sensitive measurements on picosecond time scales, matching warm-dense-matter diffusion processes which are directly accessible to atomistic simulation. For the experimental design we have used existing interdiffusion models relevant to warm dense matter conditions. In a few cases we directly simulate these experiments using a fully atomistic approach at the actual length and time scales. The motion of ions is simulated via the screened Coulomb potential based on a Thomas-Fermi-Poisson description of the electrons. The simulation results will be used to compare to the experiment and to improve upon existing theories and to test our atomistic model.

[1]This work was performed under the auspices of the US Dept. of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344.

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Date submitted: 01 Jul 2020 Electronic form version 1.4