Modelling ultrafast non-equilibrium processes with molecular dynamics: a case study of laser excited tungsten

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We present a modelling capability for studying ultra-fast non-equilibrium processes with electron-ion coupling in classical large-scale molecular dynamics simulations. Our model uses real-space formulation in the framework of Langevin dynamics with spatial correlations[1,2] allowing to carry out non-equilibrium simulations such as, laser ablation, compression shock-wave, and collision cascade, that require to track millions of atoms. We have previously demonstrated our model in the study of radiation damage in multi-component alloy.[3,4]

In this study we study the an ultra-fast process driven by electron-phonon and phonon-phonon coupling at the fs level with both modelling and experiments[5]. A single crystal tungsten sample is excited by a fs-laser and MeV electrons are used to measure the time evolution of non-equilibrium state with diffuse electron scattering. Accompanying molecular dynamics simulations are carried out to gain insight into the detailed processes of laser excited tungsten. An excellent agreement between experiment and simulation validates the modelling approach for use in studies of ultra-fast processes in many areas, such as additive manufacturing, nuclear industry, and space technology.

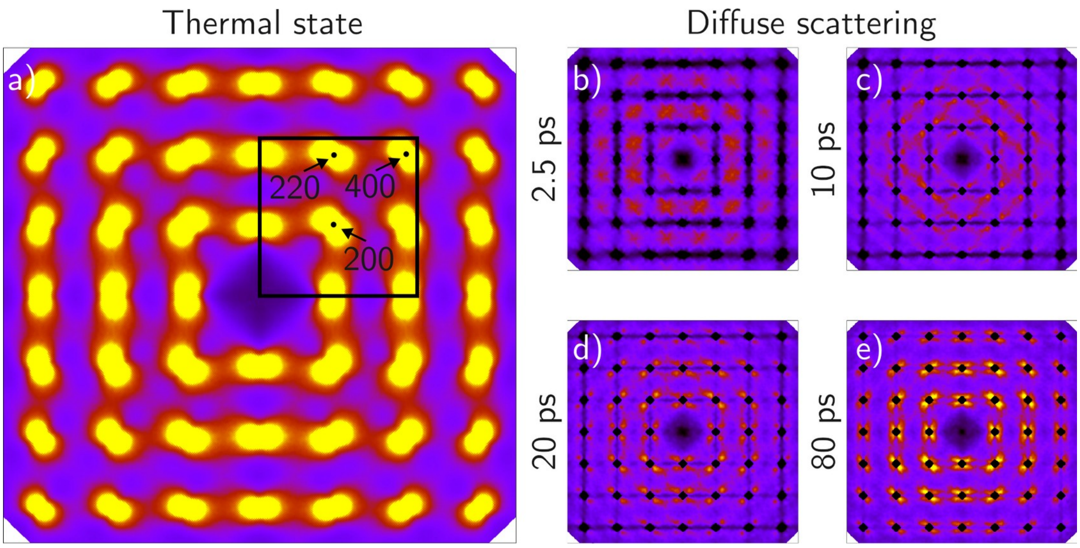

Figure 1: Simulated electron diffraction patterns of laser excited tungsten crystal. a) The thermal state at 300K used as the reference when calculating diffuse scattering plots. b)-e) Evolution of the diffuse scattering signal as the laser excited material heats from its initial state at 300K to the final state at around 600K. In the early stages of the process (b) the phonon modes near the edge of the Brillouin zone (indicated by the higher intensity) are excited due to the strong electron-phonon coupling of those modes. Subsequently at later times (c-d) the modes closer to Gamma points become excited. The thermal state representing the equipartition of the energy among the modes is finally achieved (e).

References

[1] A. Tamm, et al., *Phys. Rev. Lett.* **120**, 185501 (2018).
[2] A. Tamm, et al., USER-EPH package, http://github.com/LLNL/USER-EPH
[3] M. Caro, et al., *Phys. Rev. B* **99**, 174301 (2019)
[4] A. Tamm, et al., *Phys. Rev. B* **99**, 174302 (2019).
[5] M. Mo, et al., *Science Adv.* **10** eadk9051 (2024).