LAMMPS AS A LIBRARY FOR THE THEORETICAL STUDY OF THE ROLE OF PHONONS IN ULTRAFAST DEMAGNETIZATION

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Ultrafast modification of the magnetism of materials by laser pulses has attracted significant attention since its discovery in 1996 [1] because of its potential applications in computing and data storage. The process involving the transfer of angular momentum between electrons, phonons, and magnons is a complex interaction of light and matter, and it is still only partly understood [2].

To allow us to investigate phonons evolution after a laser pulse, we implemented a simple approximation to modify molecular dynamics trajectory to enhance specific vibration modes. Using LAMMPS as a library feature [3], we created a framework that allows LAMMPS to handle data input, generate snapshots to be processed by our method and output the modified trajectory.

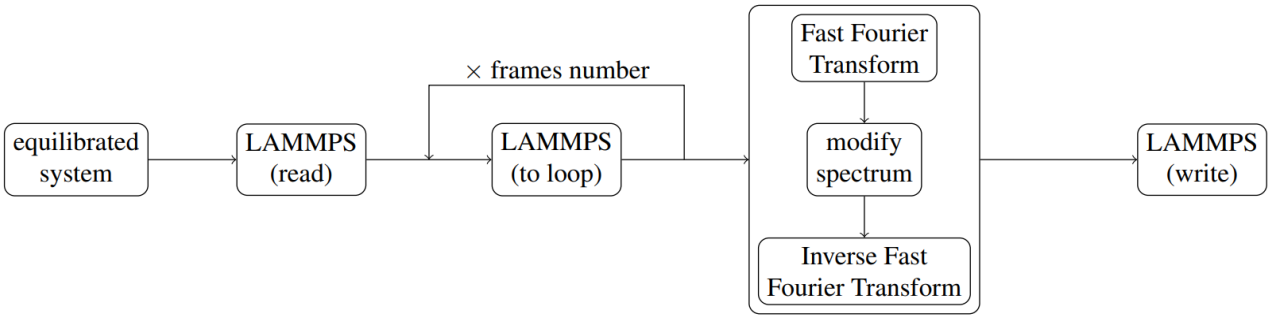

Fig. 1. A simplified schematic of the applied workflow.

Using the developed framework, we will study how phonons can contribute to re-establishing the equilibrium by carrying away the excess heat and angular momentum. We will evaluate the evolution of lattice vibrations from high temperatures of selected vibration modes towards an equilibrium using SNAP machine-learning interatomic potential (ML-IAP) [4]. Snapshots of the molecular dynamics trajectories will allow us to predict changes in the diffraction patterns and in electron energy loss spectra (EELS) in a time-resolved way [5,6].

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