Ultrafast laser induced solid-solid phase transitions in tungsten

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Electronic excitation by ultrafast laser irradiation leads to a significant modification of the electron density within an effectively cold underlying lattice. While in this cold plasma state the atoms experience very different forces than those present in the ground state. These forces may lead to coherent atomic motion and induce structural changes, such as non-thermal melting, on a sub-picosecond timescale. Here we show the appearance of soft phonon modes along the \( \Sigma \) line of the Brillouin zone in bcc tungsten at high electronic temperatures using finite temperature DFT based on the formalism of Mermin. The softening is sufficient to remove the barrier to transformation to both the fcc phase via the tetragonal Bain path and the hcp phase via the hexagonal Burgers path implying such a transformation will occur rapidly. We present the first dynamical simulation of a laser induced ultrafast martensitic solid-solid phase transition in a metal using \textit{ab initio} molecular dynamics simulations, which predict that tungsten will follow the tetragonal Bain path to transform into the fcc phase. The phase transformation is shown to be reversible as when the electronic temperature is reduced tungsten becomes bcc again.