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Atomistic simulation of systems driven through phase transitions by hot electron distributions XUKUN XIANG, JENNI PORTMAN, FARAN ZHOU, CHONG-YU RUAN, FREDERIQUE PELLEMOINE, DON MORELLI, PHILLIP DUXBURY, Michigan State Univ — A variety of pump-probe experiments are emerging to monitor the ultrafast structural response of materials. Typically a hot electron distribution is generated by an ultrafast laser pulse or by high energy particle beams, such as swift heavy ions. The hot electron distribution then thermalizes relatively quickly, on timescales in the 100fs range, while the lattice response is slower. Structural probes such as ultrafast electron diffraction or ultrafast x-ray diffraction, are able to image the structural response typically on timescales of 100fs to nanoseconds. In this presentation we discuss the results of simulations to elucidate this ultrafast structural response when materials are driven through a phase transition. Results for titanium, graphite and phase-change materials (such as $Ge_2Sb_2Se_5$) will be presented.

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