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A Molecular Dynamics Post-Processor JAMES HAWRELIAK, BRUCE REMINGTON, HECTOR LORENZANA, DANIEL KALANTAR, EDUARDO BRINGA, JAMES BELAK[1], KAI KADAU, TIMOTHY GERMANN, PETER LOMDAHL, LANL, JUSTIN WARK, JON SHEPPARD, KATARINA ROSOLANKOVA, University of Oxford, HUW DAVIES, AWE — With the development of tera-scale computing facilities, modeling material behavior can now be done on the atomic scale. Non-equilibrium molecular dynamic simulations can calculate the position and interaction of millions atoms in a simulated material. By post-processing the simulation output files using Fourier transform techniques, it is possible to extract the long scale length ordering in the MD simulations. These techniques can be used on MD simulations of materials such as iron, titanium or copper to determine crystal structure and lattice kinetics as the crystal is strained. From the post-processed analysis a direct link can be made to the experimental measurements made using x-ray diffraction.

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