Advanced Simulation and Computing

Los Alamos NATIONAL LABORATORY

News and Operational Highlights

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PREDICTIVE CAPABILITIES

Presenting a new Phase Transformation Kinetics Model for Metals

Some metals undergo solid-solid phase transformations at high pressure, wherein the crystal structure changes. Such changes are often accompanied by a sudden reduction in volume. Examples include the transition of alpha-phase iron to epsilon-phase iron at pressures of around 13 Gigapascal (GPa) and the transition of body-centered tetragonal beta-phase tin to gamma-phase tin at roughly 9.4 GPa. Under high rate loading, such as shock compression, these types of phase transitions complete at even higher pressures because of the time the phase transition takes to "react" to the applied loading. However, the underlying dynamics are not well understood. Therefore, PEM is developing the theory and new models to fill this gap.

This gap is reflected in the phase transformation kinetics model currently implemented in LANL's hydrocode FLAG. The model is a very simple phenomenological model that lacks the necessary physics to precisely predict the time-resolved free surface velocity of shock-loaded beta tin across its phase transition to gamma tin. To add this capability to FLAG, PEM developed, from theory, a new kinetics model that enables the predictive capabilities needed. Specifically, given initial material properties and loading conditions, the new model can predict the duration of time a phase transformation takes to complete. It can also predict the "overshoot" pressure, i.e., the pressure at which the phase transition starts and ends as a function of loading conditions (such as pressure rate if ramp loading is considered). This new model will soon be implemented into FLAG.

Figure 1 shows some results for the alpha to epsilon iron transition using our preliminary research code, which implements the simpler case of ramp loading , where the metal is compressed at a constant pressure rate (i.e. pressure increases linearly with time, which greatly simplifies some of the equations). Good agreement with experiment shows the new model's flexibility, which is missing in the currently implemented model. The parameters that are fit to experiment describe details such as the material's microstructure, and an in principle can be calculated using molecular dynamics simulations using molecular dynamics simulations to make the model fully predictive.

For more information, contact DJ Luscher (djl@lanl.gov), PEM Program Manager. We acknowledge the technical contributions of Daniel N. Blaschke, Abigail Hunter, and Dean Preston, with support from the EOS project.

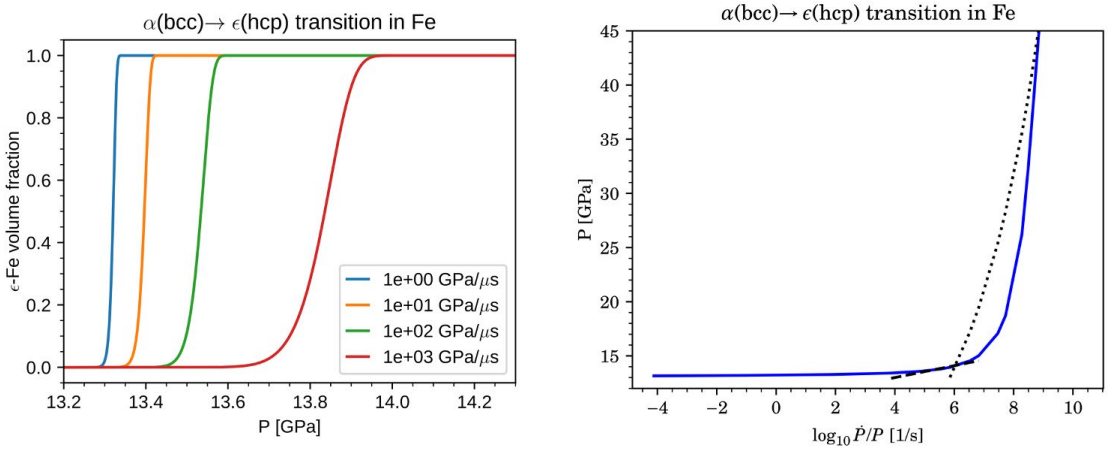

Figure 1 On the left, the epsilon Fe volume fraction is shown as a function of ramp pressure for constant loading rates of 1, 10, 100, and 1000 GPa/microsecond at. On the right, predictions (blue curve) are compared to experimental data from Smith et al. 2013 (dashed / dotted curves which Smith et al. fitted to their data measured at Lawrence Livermore National Laboratory). Specifically, the onset pressure of the phase transition is shown as a function of strain rate (approximated by pressure rate over pressure).

MATERIALS

Development of Interatomic Potentials Aids in Materials Discovery for Extreme Environments

Many applications important to the NNSA mission require metal alloys to survive thermal and mechanical extremes. The tradeoffs in material properties associated with conventional alloys are generally well understood in the context of these extreme environments. The discovery of new materials promises to enable technology advancements beyond what can be achieved with standard alloy compositions.

High entropy alloys (HEAs) and multi-principal element alloys (MPEAs) are designer materials of much interest because of their remarkable ability to combine high strength and ductility. A HEA is a complex metal alloy comprising five or more elements in near-equal proportions, designed to maximize atomic diversity and configurational entropy, resulting in unique mechanical and thermal properties such as high strength, toughness, and resistance to wear, corrosion, and oxidation. MPEAs are similar to HEAs but can be comprised of three or more elements in near-equal proportions.

Because HEAs and MPEAs are mixtures of multiple elements, the composition space that must be explored to optimize properties is large. This means that examining the design space to discover optimal HEA/MPEA compositions using experimental methods alone is intractable. Atomistic modeling using classical molecular dynamics can help accelerate the identification of compositions that are well-suited for experimental characterization. This modeling approach enables specified numbers of atoms from multiple elements to be placed in high-entropy configurations and then computes the resulting material properties and deformation mechanisms. The accuracy of these calculations depends on the quality of the interatomic potentials used to compute the energy and resulting forces associated with configurations of atoms.

Recent work by ASC-PEM developed a multi-component Modified Embedded Atom Method (MEAM) potential for HEAs consisting of a mixture of niobium, tantalum, titanium, vanadium, and zirconium (i.e., NbTaTiVZr, including all subsets such as NbTaTiV). Niobium, tantalum, and vanadium each exhibit body-centered cubic (BCC) symmetry of their atomic lattice, while zirconium and titanium stabilize in a hexagonal close-packing geometry at room temperature and BCC at elevated temperatures. BCC crystal symmetry is an atomic lattice arrangement with one atom positioned at each corner of a cube and an additional atom located at the center of the cube. This geometry results in a high-symmetry structure that is often associated with materials having high strength and resistance to deformation.

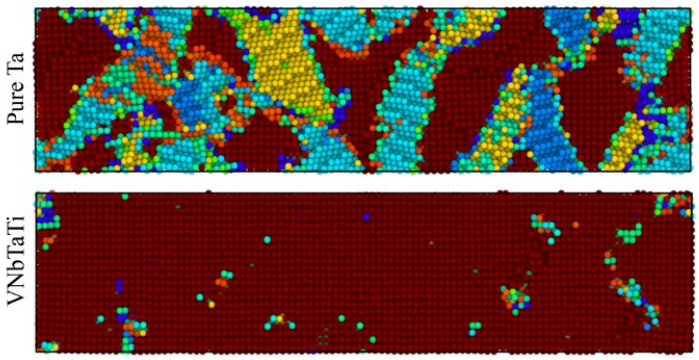

Figure 1 Molecular dynamics simulations using a newly developed interatomic potential exhibit the formation of deformation twins nucleating in the conventional BCC Ta (top) and no twins in the MPEA NbTaTiV (bottom).

Using the newly developed interatomic potential, molecular dynamics simulations of selected NbTaTiVZr and NbTaTiV compositions exhibited deformation behavior that was dominated by edge dislocations, unlike pure BCC elements (e.g., Ta) in which screw dislocations prevail. Although this work specifically focused on the deformation behavior of a subclass of HEAs, it developed a foundation for the high-throughput development of new, accurate interatomic potentials, which will enable application of molecular dynamics to a broad range of materials modeling problems, including understanding deformation mechanisms in alloys with multiple impurities (e.g., from manufacturing or aging).

For more information, contact DJ Luscher (djl@lanl.gov), PEM Program Manager. We acknowledge the technical contributions of Mashroor Nitol and Saryu Fensin and several other collaborators.

HIGH PERFORMANCE COMPUTING SYSTEM SCHEDULING

LANL Applies Advanced Simulation Methods to Optimize HPC Platform Performance

The Advanced Simulation and Computing program operates large HPC platforms for the purposes of conducting 1D, 2D, and 3D simulations for the Stockpile Stewardship program. A recent study evaluated the tradeoffs that affect system performance with a focus on optimizing platform availability for scientific calculations while minimizing maintenance interruptions. This approach allows for more informed decisions regarding HPC system scheduling and resource allocation, particularly in environments with complex supercomputing needs.

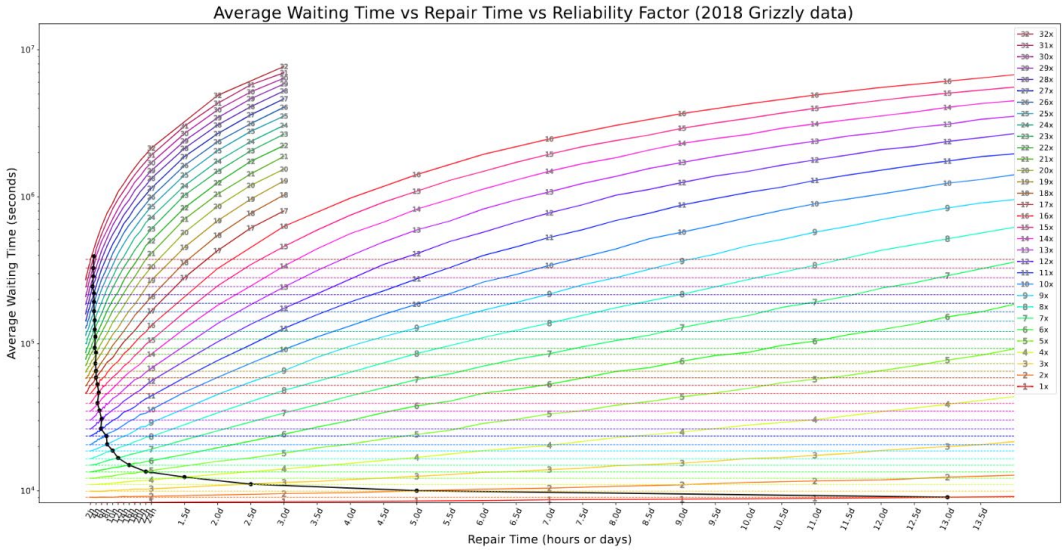

Figure 1 Graph showing various job wait periods and system repair times versus reliability as the performance of the HPC system improves.

To evaluate tradeoffs, LANL and Coastal Carolina University created a simulation using real-world failure data to perform parameter sweeps more efficiently and then examined how different repair times and node reliability impacted the system's operational effectiveness. Based on this simulation data, LANL found actionable insights for HPC operations and user support to optimize HPC cluster performance. The insights identified will improve annual assessment reports needed to certify the stockpile.

For more information, contact **Jason Hick** (jhick@lanl.gov), FOUS Program Manager. We acknowledge the work of Nathan DeBardeleben, Vivian Hafener, and Steve Senator of HPC division; Leslie Horace of Georgia Institute of Technology; and Craig Walker and William Jones of Coastal Carolina University.