NOVEL METAL–CARBON MATERIALS

Allocation: Exploratory/50 Knh
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EXECUTIVE SUMMARY

We used the Blue Waters supercomputer to model novel metal–carbon materials called covetics, which are metals that are combined with carbon in a new way. Experimental results have shown that covetics have superior mechanical, thermal, and electrical properties compared to base metals. However, the role of the added carbon on materials performance is still not well understood. A goal of this project is to improve our understanding of covetics.

This project focused on copper covetics. The objectives were: (1) to build atomistic models using the Large-Scale Atomic Molecular Massively Parallel Simulator [2] (LAAMPS) molecular dynamics code to obtain a fundamental understanding of the material response of covetics and to provide inputs for continuum models; and (2) to develop experimentally-based continuum-level finite element and micromechanics models of covetics (using the Abaqus [4] software package) to create predictive tools for their bulk properties. Blue Waters is necessary because such multiscale modeling requires very high computational resources due to the hierarchical structure of these materials.

RESEARCH CHALLENGE

Experimental results have shown that covetics exhibit superior multifunctional properties compared to corresponding base metals, including improved mechanical properties, higher thermal and electrical conductivities, and higher corrosion resistance, making them excellent candidates for various technological applications. However, they need to be more fully studied and understood before they can be widely accepted and used commercially.

METHODS & CODES

Covetics are metals infused with carbon (up to 10 wt%) in amounts far exceeding the solubility limits predicted by phase diagrams. The metal is combined with carbon in a new way, which leads to a strong carbon–metal bond. To understand the nature of this bond, we performed powerful atomistic simulations. Atomistic simulations are computational techniques that can provide unique insights on materials characteristics and mechanisms that shape the material response. The most common methods in use are Monte Carlo algorithms, Molecular Dynamics (MD), and Density Functional Theory (DFT).

We conducted DFT calculations on covetics by assuming various copper–carbon configurations and studying lowest energy states. Our simulations were guided by high-resolution transmission electron microscopy observations that an epitaxial rearrangement of a lattice structure forms in the covetics and that the carbon forms alternating layers of graphene between atomic planes of metal. We extended these studies to other geometries of graphene ribbons intercalated between metal layers. We are studying the most promising lowest-energy candidates determined in these simulations on larger systems.

We also employed MD modeling, which has not been used previously on covetics. MD allows us to study larger material volumes due to relatively reduced computational cost compared to DFT and is critical in studying experimentally observed structures. We used LAMMPS classical molecular dynamics code, which has a modular design; the community code model allows users to extend the code at the source level. LAMMPS uses message-passing and spatial domain decomposition techniques and is highly efficient on large-scale computational platforms. LAMMPS' extreme level of parallel scalability (Fig. 1) was previously demonstrated on Blue Waters [3].

Stresses and their corresponding strains within the elastic limit are related by elastic constants. In this work, we calculated the elastic constants after relaxing the geometry for systems with and without carbon. In addition, we are studying structural

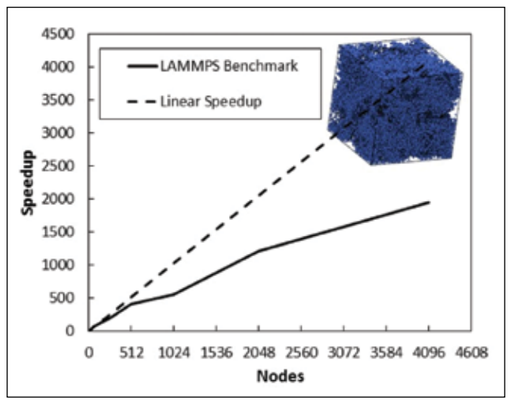

Figure 1: The Lennard–Jones benchmark runs on Blue Waters XE6 nodes. The parallel speedup curve is plotted for a fixed-sized test case (strong scaling test) with 200 million atoms.

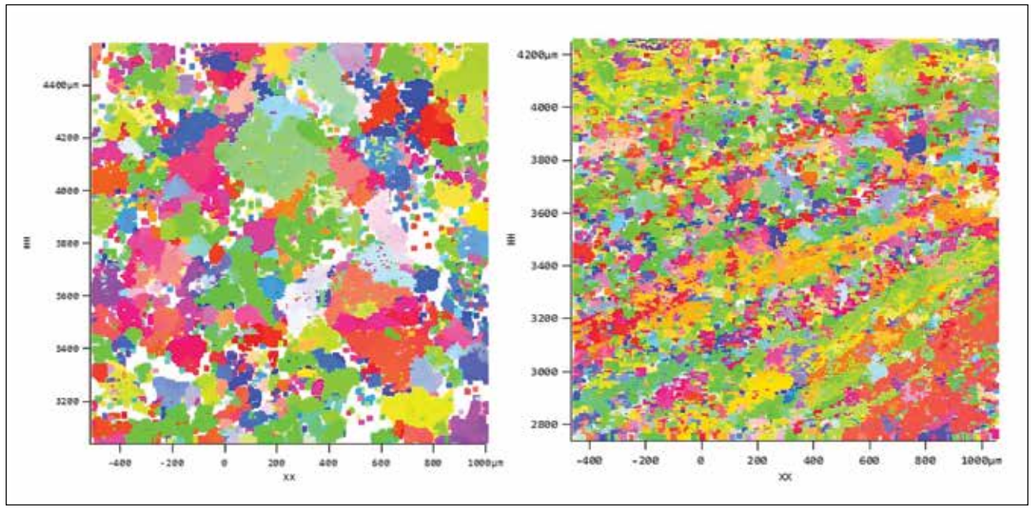

Figure 2: Orientation maps from white beam Laue diffraction for 0 wt% C (left) and 3 wt% C (right) copper–carbon covetics.

transformations occurring in the system (such as dislocations and void formation) for the most stable systems.

Our approach to creating continuum models involves computational modeling of a bulk mechanical response of copper covetics. To model the macroscopic mechanical response, we incorporated details from the micro scale (grain level) obtained from scanning electron microscopy, electron backscatter diffraction (SEM–EBSD), and X-ray microdiffraction imaging into the finite element program (Fig. 2). Data on texture, crystal orientations, and grain shapes obtained by SEM–EBSD and local mechanical properties measured by nanoindentation serve as inputs for such computational models.

We also modeled elastic and plastic materials responses by carrying out Finite Element Method (FEM) simulations with Abaqus, a commercial software package. Combined nonlinearities arising from inelastic material properties and geometric nonlinearities from large deformations leads to increased ill-conditioning of the global stiffness matrices. This makes the FEM analysis of 3D models difficult even using the latest high-performance computing platforms. To solve such a problem within each quasi-static timestep, a system of nonlinear equations must be linearized and solved in Abaqus with a Newton–Raphson iteration scheme, which requires several linear solver solutions or global equilibrium iterations. For this work, we used the direct multifrontal solver in Abaqus/Standard with hybrid Message-Passing Interface/Threaded parallelization.

RESULTS & IMPACT

This research is still in progress. However, our initial atomistic and continuum models led to the first predictive multiscale models for covetics [1].

WHY BLUE WATERS

The Blue Waters supercomputer and NCSA researchers were essential for this research project. Blue Waters is necessary because such multiscale modeling requires very high computational resources due to the hierarchical structure of covetics.