New Computational Model to Accurately Simulate Mechanical Behavior of Metal/Ceramic Systems

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What is the outcome or accomplishment? (1-2 short sentences describing it and why it is transformative; 50 word max. suggested)*

Louisiana Tech University researchers have developed a new interatomic potential computer model for simulating Cu-Ti-N ternary systems at length scales of several nanometers. Shear loading simulations using the new model for Cu/TiN interfacial systems compare favorably with those obtained from laboratory experimentations.

What is the impact? (1-2 simple sentences describing the benefits for science, industry, society, the economy, national security, *etc.*; suggested 50 word maximum)

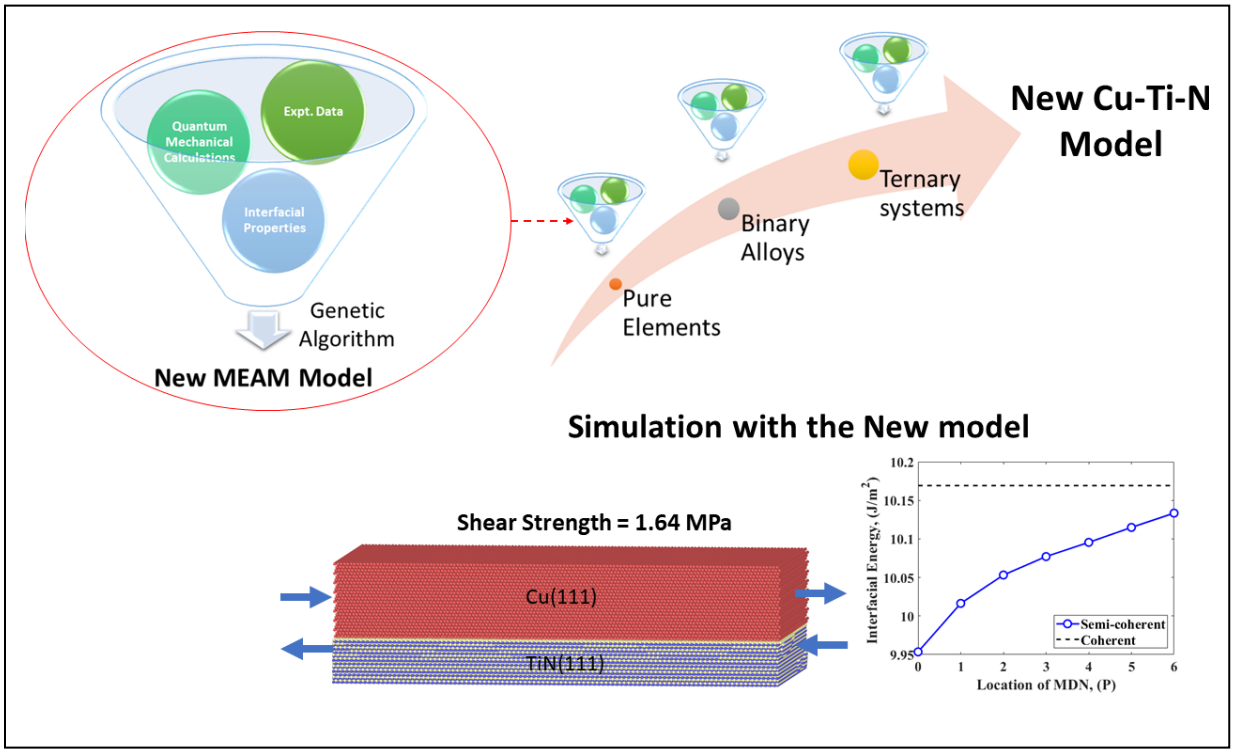
An experimentally verified simulation tool for predicting the interatomic potential of materials involving Cu, Ti and N and their binary/ternary combinations such as metal/ceramic interfaces greatly reduces expensive laboratory trial-and-error, reduces development time, and efficiently guides the development of models for other metal/ceramic systems.

What explanation/background does the lay reader need to understand the significance of this outcome? (1-2 paragraphs that might include, for example, more on who, when, where; NSF's role; support from multiple directorates/offices; what makes this accomplishment unique; additional intellectual merits; or broader impacts such as education, outreach, or infrastructure improvement that are integral to this outcome; suggested 150 word maximum)

Systems with binary and ternary combinations of Cu, Ti and N are found in many technological applications such as protective coatings in electronic circuits and automobile components. While the phase diagrams for these systems are known, the mechanical behavior of metal/ceramic interfacial systems involving these elements (such as Ti/TiN and Cu/TiN) is not well-understood. First-principles quantum mechanical (QM) calculations provide insights into highly localized interfacial behavior. However, to make comparisons with complementary experiments, larger scale simulations that incorporate misfit dislocations and different interfacial coherency

scenarios are required. To achieve this, mathematical functions that describe the interactions between atoms (interatomic potentials) are required. Louisiana Tech researchers have developed a potential that enables computational simulation of systems consisting of all three elements. The inherent challenge is accurately transferring the information obtained from QM calculations at the smaller scales to larger scales.

To create the new model, physical properties at the atomic-level were obtained from a combination of experimental results and QM calculations. The model was then parameterized to reproduce these properties. A genetic algorithm was used to efficiently screen parameters and arrive at optimum values. The resulting shear response of Cu/TiN systems predicted by this model is found to closely follow experimental observation, providing novel insights into the atomic mechanism for shear failure. Using this model, the application-specific characteristics of Cu-Ti-N systems can be investigated under different process conditions, thus saving significant time and money for the manufacturing industry.



This illustration shows the procedure for developing Cu-Ti-N interatomic potential model. First, the pure elements are fit, followed by their binary, and then the Cu-Ti-N ternary system. In each stage, a newly developed genetic algorithm was used to optimize the parameterization of the model to experimental and quantum mechanically derived properties. The new model is used to calculate interfacial properties, interfacial energies, and shear strength, with experimental validation.
Credit: Abu Shama Mohammad Miraz, Bala Ramachandran, and Collin D. Wick, Louisiana Tech University.