IMPACTS SUBMISSION

For division/directorate use

Please use the following template to present items that would make persuasive Impacts. Information must be understandable by a lay person.

SUBJECT: Studying manufacturing "fails" providing fundamental scientific knowledge that is vital to the future of the U.S. advanced manufacturing industry.

CATEGORY- Chose U.S./global economy, national security or scientific knowledge:
Scientific knowledge

NSF AWARD(S) - Provide award number hyperlink:
https://nsf.gov/awardsearch/showAward?AWD_ID=1541079

OTHER SUPPORTING INFORMATION:

BRIEF SUMMARY OF OUTCOMES - (Why is this award compelling for use as an Impact?):
High throughput manufacturing of large "macroscale" objects like car doors relies heavily on shaping metals by mechanical means such as stamping, blanking, extruding, etc. These manufacturing technologies do not work well when scaled down to sizes close to or smaller than the diameter of a human hair (about 100 microns). Such small-scale metallic structures are needed in a wide range of applications, including cooling and assembly of high-performance electronics, oil and gas exploration, gas sensing, and medical imaging. Macroscale manufacturing techniques scaled down to micron scales does not perform as well, resulting in flawed parts and damage to the micro manufacturing tools. At the microscale, the physics of the molecules influence each other greatly and these effects are greatly exaggerated compared to manufacturing the macroscale.

Scientists have found that applying a thin ceramic coating onto the tool surfaces can alleviate some of the damage to the tool and the part. However, engineering these tools with ceramic coatings is hampered by a lack of fundamental scientific understanding of the interaction between the metallic tool and the ceramic coating. Poorly designed coatings can lead to premature failure and, consequently, additional tool and part breakage and added costs to the manufacturer.

A team of researchers from Louisiana State University and Louisiana Tech University, assisted by graduate and undergraduate students, are gaining new insights into this fundamental problem of understanding and controlling mechanical integrity of metal/ceramic interfaces. In simplistic terms, they are studying metal/ceramic "fails" at the molecular scale to predict and test new configurations that will work. What is unique about this research is that they have combined microscale mechanical testing with simultaneous microscopic observations with extensive supercomputer simulations and modeling.

The research team came up with new microscale mechanical testing protocols in the lab, and their findings have revealed for the first time that, when metal/ceramic interfaces fail under stress, they are doing so in the metal layer, and very close to where the ceramic layer makes contact with the metal. Computational experiments showed that nanoscale defects, known as "misfit dislocation networks" (a mismatch between the ordering of atoms in the metal and the ceramic across the interface), determine how easily the materials across the interface will slide over one another when force is applied, leading to the failure.

To gain additional insights, computer simulations were carried out to the nanometer (one billionth of a meter) scale and at the atomic scale. The nanoscale computer simulations included the effects of molecular dynamics (the physics of how each atom affect each other), which provided insights into the physical mechanism through which sliding across the interface can occur. The molecular dynamics simulations were validated using first-principles density functional theory (DFT) calculations, which confirmed that the interaction model was accurate. This work opens the way to effective engineering of coating/substrate interfacial regions, which can lead to improved design of strong interfaces.

The research team is part of the Louisiana Consortium for Innovation in Manufacturing and Materials (CIMM), and the primary investigators are: Dr. Wen Jin Meng and Dr. Shuai Shao at Louisiana State University, and Dr. Collin Wick and Dr. Ramu Ramachandran at Louisiana Tech University.

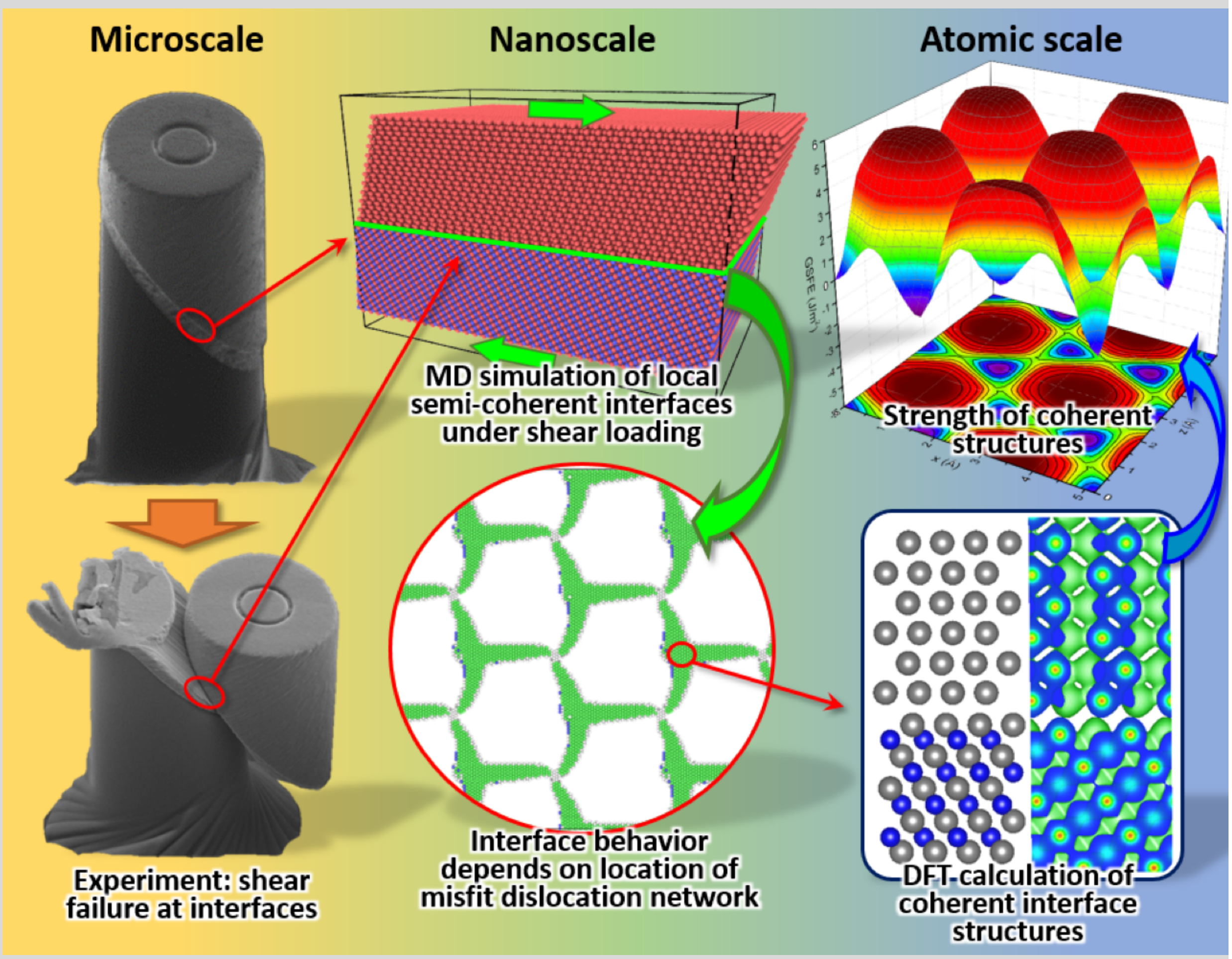

Image: To understand how metal/ceramic interfaces fail under stress, researchers custom-fabricated pillars approximately the thickness of human hair (~100 microns) containing the interfaces studied,

and subjected them to compression until they failed (left top and bottom). To gain insights into the failure mechanism, the effect of shear loading (force applied in the lateral direction) on the interface was studied using molecular dynamics. This showed that nanometer-scale defects known as "misfit dislocation networks," which exist because of the mismatch between the ordering of atoms in the metal and the ceramic across the interface, determine how easily the materials across the interface will slide over one another when force is applied, leading to interfacial failure (middle top and bottom). The molecular dynamic (MD) simulations were validated using a more sophisticated method based on density functional theory (DFT) at the atomic scale, which confirmed that the atomic interaction model used for MD simulations provided qualitatively correct behavior (right top and bottom). This synergistic combination of experiments at the micron scale and computational simulations at the nanometer and atomic scales have yielded new insights into the failure mechanisms of metal/ceramic interfaces. These investigations and those currently in progress will help make high throughput micromanufacturing technologies more competitive. Metal and alloy products with micron-scale features are needed in a wide range of applications, including cooling and assembly of high-performance electronics, oil and gas exploration, gas sensing, and medical imaging.
Credit: Wen J. Meng, Louisiana State University, wmeng1@lsu.edu

THREE REASONS this award outcome impacts U.S./global economy, national security or scientific knowledge:
Understanding the factors controlling mechanical integrity of metal/ceramic interfaces has been a long-standing scientific problem, and is not well understood at present. This fundamental problem has also significant practical implications, especially to manufacturing of metal- and alloy-based parts at the micron scales. The present research team conceptualized and utilized new microscale mechanical testing protocols, combined experimentation with atomistic calculations/simulations, and achieved a significant advance in scientific knowledge regarding this problem.

Developing experimentally validated computational approaches allows a wide variety of metal/ceramic interfaces to be studied and understood faster than through laboratory-based testing alone. The physical insights gained from such simulations establish the foundation for true materials-based engineering of metal/ceramic interfaces and help accelerate application-specific metal/ceramic interface design and implementation.

High throughput manufacturing of metal- and alloy- based parts at the micron scales will help meet a critical need in many industrial sectors. By contributing to making high throughput micro-manufacturing technologies more competitive, the current research contributes to technology development and potential economic development.

NSF Directorate(s)/Division(s): OIA

State(s): Louisiana