Ceramic coating research speeds up the design of stronger and longer lasting machine parts

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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)*

First principles computer simulations have revealed that doping metal/ceramic interfaces can significantly increase their tensile strength and resistance to shear. This was verified specifically for Ti/TiN interfaces doped with Al. Work is in progress with experimentalists to verify this prediction.

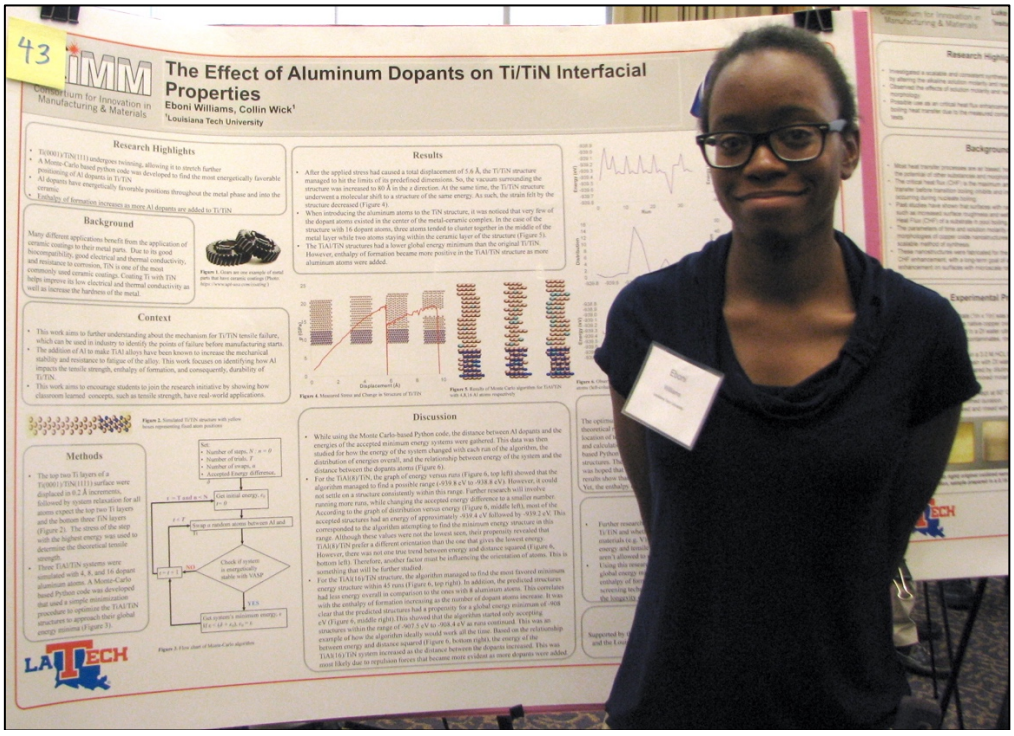
What is the impact? (1-2 simple sentences describing the benefits for science, industry, society, the economy, national security, *etc.*; suggested 50 word maximum)

Metal/ceramic interfaces promote high resistance to deformation and leads to improved design of mechanical components used in gas turbines, aero engines and automobiles. A validated computational model helps to guide the design of new interfaces without expensive trial-and-error in the lab, thus greatly reducing development time and costs.

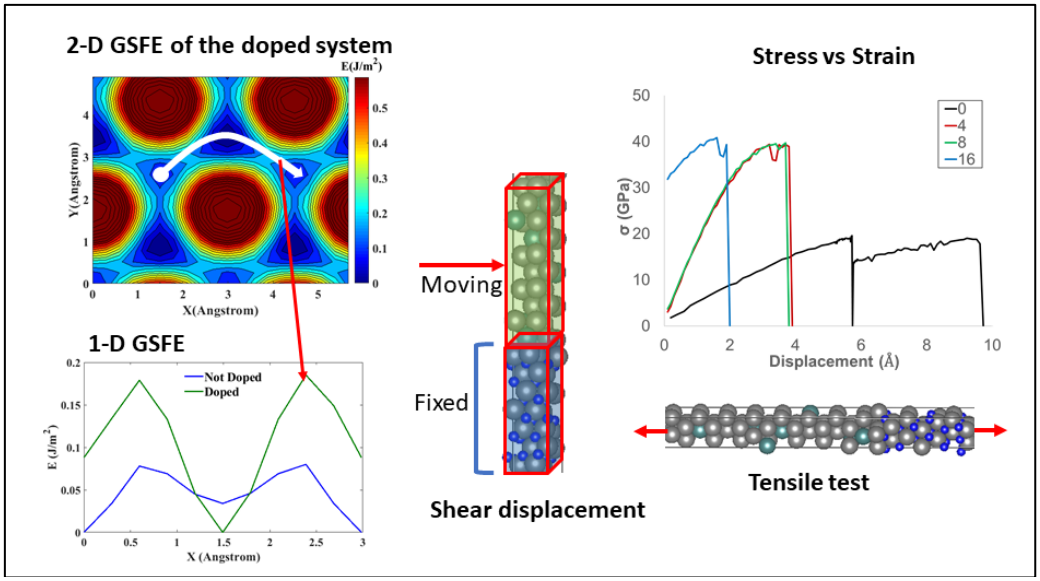
What explanation/background does the lay reader need to understand the significance of this outcome? (1-2 paragraphs that might include, for example, more on who, when, where; NSF's role; support from multiple directorates/offices; what makes this accomplishment unique; additional intellectual merits;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

It was not uncommon for automobile transmissions to wear out while the engine was still in relatively good condition. Then engineers discovered that the strength and durability of machine components operating at high temperature, pressure, and speed can be significantly extended by coating the metal with a thin layer of ceramic. However, the principles involved in choosing the materials for a good interface are unclear, requiring trial-and-error in the lab, which is expensive, time-consuming, and prone to accidents.

Louisiana Tech University researchers have developed a computational simulation tool that helps predict metal/ceramic interface properties. Using this approach, the researchers predicted that "doping" the metal, by adding aluminum to the interface between titanium and titanium nitride will significantly increase its wear resistance, whereas some other dopants had no effect or a negative one. Similar predictions were made for copper/titanium nitride interfaces doped with zinc and nickel. These results were obtained in a matter of hours on powerful computers. The team is now collaborating with experimentalists to validate their results. If experiments validate the computational predictions, the protocol can be used to rapidly screen additives to coatings that optimize wear resistance, and to rule out the less effective ones, thus saving significant time and money for the manufacturing industry.



Eboni Williams, a senior majoring in chemistry and computer science at Louisiana Tech University, presents her research poster titled, "The effect of aluminum dopants on Ti/TiN interfacial properties," at the CIMM annual research symposium in Baton Rouge, LA.



This illustration shows the global stacking fault energy (GSFE) landscape between layers of the metal Ti phase and ceramic TiN. Higher values represent higher barriers for shear displacement in which the metal areas are moved in the directions parallel to the interface, while the ceramic layers are kept fixed. The tensile test also showed a significant increase in the tensile strength of the systems. Addition of Aluminum atoms nearly doubles the barrier for shear displacement indicates that Aluminum has a profound effect on increasing the wear resistance of the Ti/TiN interface. Credit: Collin D. Wick, Abu Mohammad Miraz, Eboni Williams and Bala Ramachandran, Louisiana Tech University.