Ceramic coating research speeding 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)*

Louisiana Tech University researchers have developed a computational tool to predict the changes in wear resistance of ceramic coatings on metal when small amounts of impurities (i.e. dopants) are introduced.

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

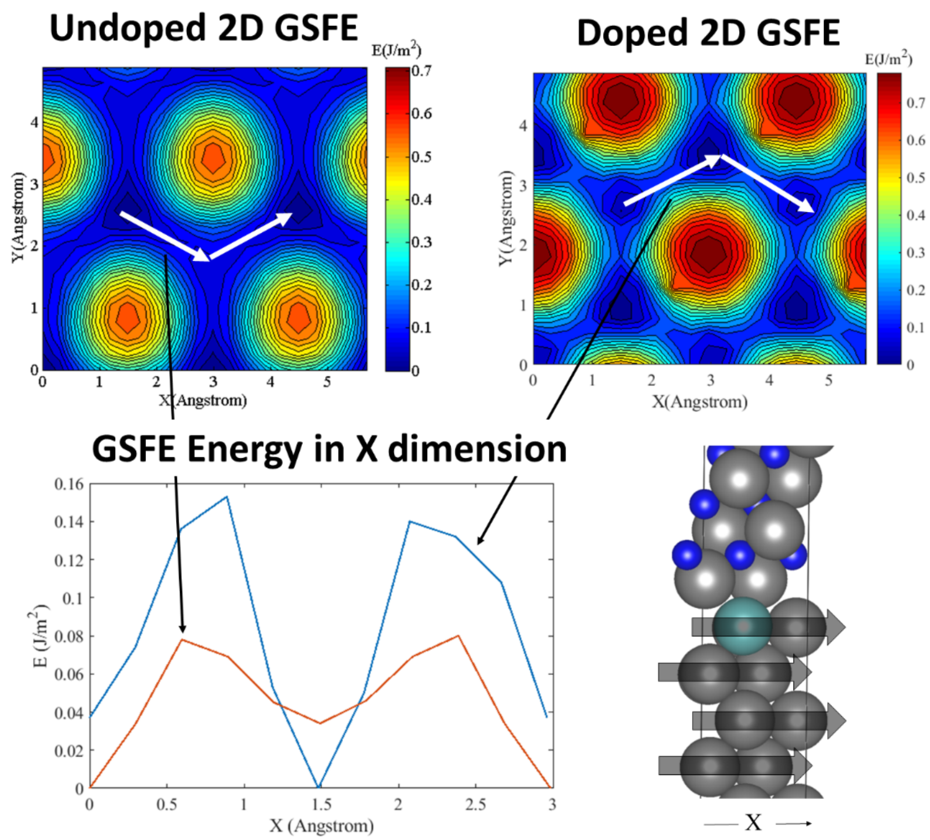
Strong metal-ceramic interfaces will lead to the design of coatings for gears and other machine parts with greatly improved wear resistance. Utilizing a computational approach allows interface properties to be studied and predicted without fabricating the material, thus greatly reducing the research 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)

Ceramic coatings protect metal gears and machine parts from wear and heat, significantly increasing their lifetimes. Computer calculations can be carried out without any input from experiment, and thus serve as a powerful tool for not just understanding how different metals and ceramics interact, but as a predictive tool for screening which metal/ceramic combinations will resist wear.

For example, in this Louisiana Tech University computational research, it was predicted that adding aluminum to the interface between titanium and titanium nitride will significantly increase its wear resistance. Computations also predicted that some other dopants had no effect or had a negative effect on the shear resistance of the interface. These results were obtained in a matter of hours on powerful computers, without the need for costly, slow, and sometimes excessive trial and error laboratory work. The team will now test these predictions in the lab for experimental confirmation of these results. Once validated, a long-term computational screening can be implemented to rapidly identify additives to ceramic coatings that optimize wear resistance, and to rule out the less effective ones, thus saving significant time and money.

Illustration:



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 itnerface, while the ceramic layers are kept fixed. The fact that adding a single 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, and Bala Ramachandran, Louisiana Tech University.