Growing metal/ceramic bi-crystals to better understand interfacial mechanical integrity

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

Researchers in Louisiana have developed a way to synthesize crystals containing both metal and ceramic components with the layers of atoms arranged in differing orientations. These crystals will help with the research on metal and ceramic interfaces, which are critical to developing better advanced manufacturing technologies.

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

Synthesizing these special crystals will help to understand the material response at the interface between the metal and ceramic layers when stressed by advanced manufacturing tools. This fundamental science will develop an understanding of how the orientation of atoms in the crystals determine whether the layers will break, deform or stay intact.

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)

A team of scientists from Louisiana State University and Louisiana Tech University as part of the statewide NSF EPSCoR-funded Consortium for Innovation in Manufacturing and Materials (CIMM), have designed and implemented ultra-high-vacuum (UHV) vapor phase thin film growth capabilities, and used this capability to synthesize copper-titanium nitride (Cu-TiN) thin film bi-crystals.

The research team created crystals with a new Cu/TiN orientation relationship with a different habit plane (Figs. 1 and 2). New molecular dynamics potentials have been developed by the team specifically for performing simulations, to study the fundamental science of Cu/TiN interfaces and their relationship to interfacial structure.

This work continues the research team's ongoing effort on understanding the mechanical response of metal/ceramic interfaces, and an opportunity to better correlate experimental testing results with physics-based simulations. The results are expected to advance the frontier of our knowledge on the mechanical integrity of solid/solid interfaces, and enable a true materials-based design of high performance interfaces in wide ranging engineering applications, such as engine components that are much more durable, lighter and less expensive.

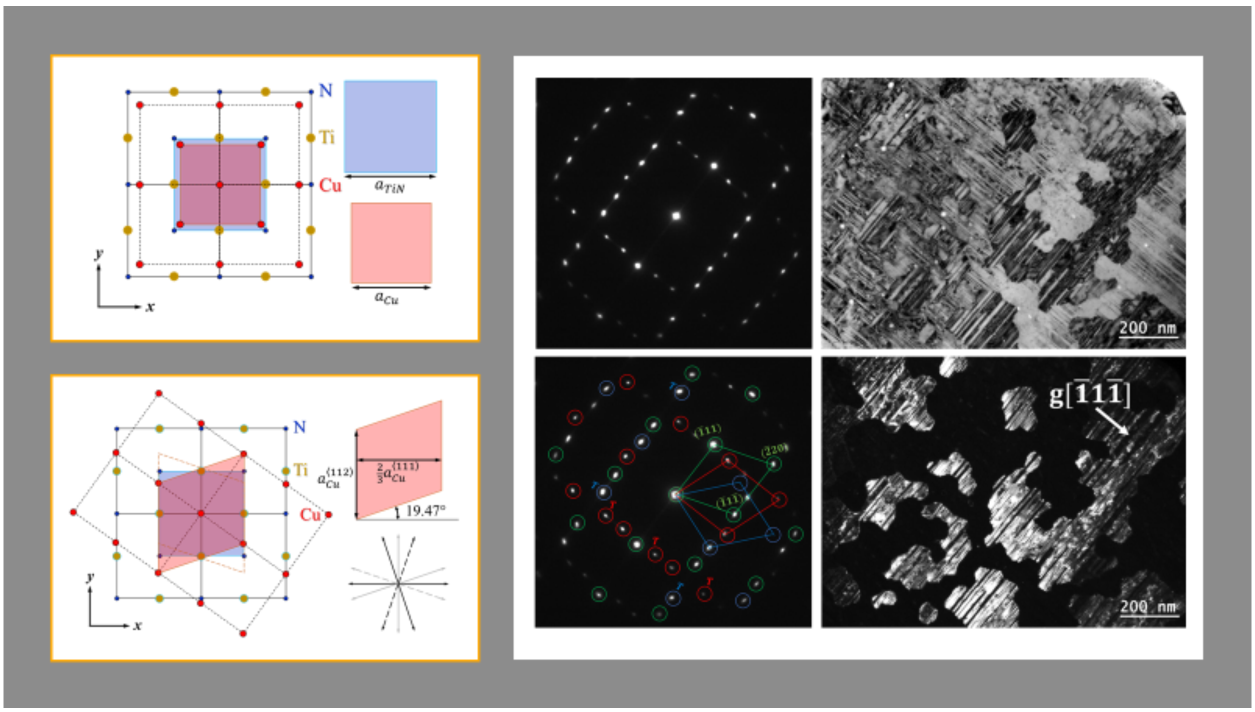

Fig. 1. (left) Illustrations of the cube-on-cube and the new Cu/TiN bi-crystal orientation relationship; (right) electron diffraction pattern and bright/dark field images of a Cu crystal on a TiN(001) template, with a new habit plane of Cu(110)//TiN(001).

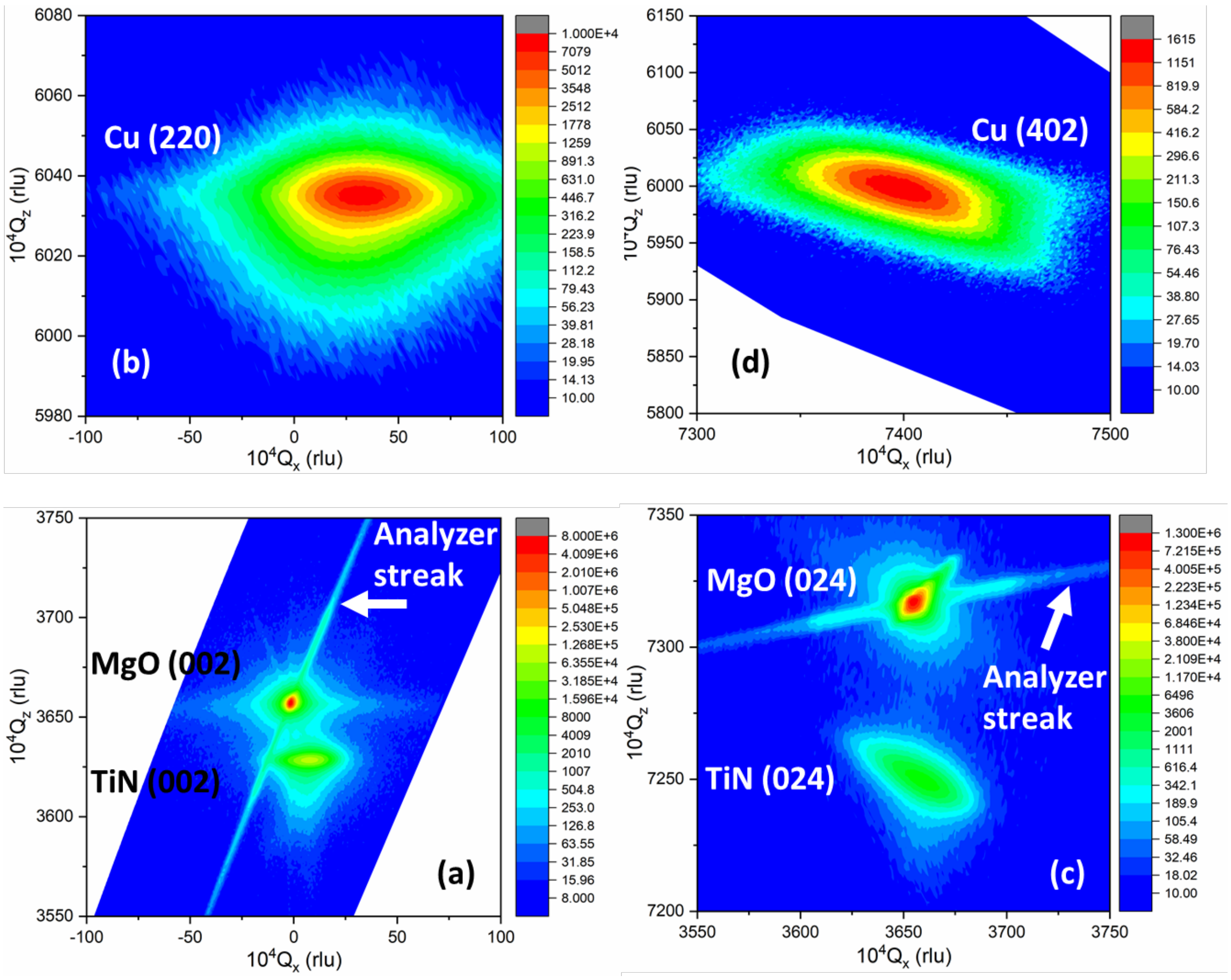

Fig. 2. X-ray reciprocal space mapping of a Cu/TiN bi-crystal thin film specimen, in which the Cu-TiN orientation relationship is Cu(110)//TiN(001) in the growth direction and Cu<111>//TiN<100> in-plane.