Automated Computational Design of Complex Concentrated Alloys for 3D Printing

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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)*

A group of researchers from four Universities in the Louisiana Materials Design Alliance (LAMDA) project have demonstrated how computations can be utilized to efficiently engineer new materials that can be 3D printed with friction stir welding (FSW) with significant greater strength than is currently possible.

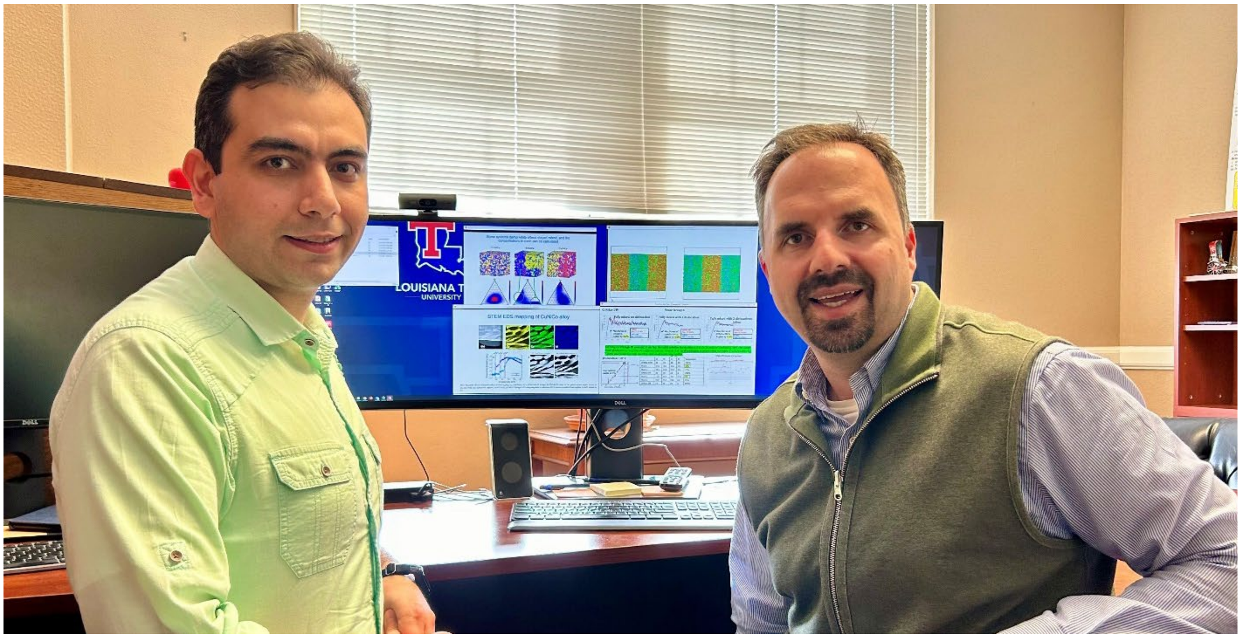
What is the impact? (1-2 simple sentences describing the benefits for science, industry, society, the economy, national security, *etc.*; suggested 50-word maximum)

FSW can make customizable metal parts that can result in significant savings in labor and time. The computational design process developed by LAMDA researchers can optimize the strength of the alloy while malleable enough at higher temperatures to 3D print.

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)

Industrial companies continually seek components with enhanced performance and extended operational lifespans. This demand arises from the necessity to minimize manufacturing costs and component replacement expenses. Achieving this objective requires the adoption of innovative manufacturing techniques like 3D-printing and the development of novel materials such as complex concentrated alloys (CCAs). CCAs contain a large array of elements, which creates a near infinite number of combinations, making experimental testing all of the infeasible. We created a fully automated procedures for creating and testing them computationally, to allow their rapid screening. After the identification of viable CCAs with required properties for FSW 3D-printing purposes, they can be investigated experimentally.

With the development of the automated computational procedures, we identified alloys with unique properties of increased strengths at lower temperatures, yet enhanced malleability at higher temperatures, facilitating their viability for FSW for high strength materials. Furthermore, our simulations provide a deeper understanding of microstructural mechanisms for improving the strength of the alloys, including both precipitate and solid solution strengthening. The methodology will serve as a computational infrastructure for future materials design endeavors that further enhance the development of alloys for FSW and alloy 3D printing.



Hamid Sharifi Torki and Collin Wick in front of recent computational results and experimental comparisons for