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Collaborative Research: Revealing the Role of Vacancy Order in Regulating the Dislocation Behavior in Transition Metal Carbides

Christopher Weinberger, Colorado State University

As the carbon-metal (C/Me) ratio is reduced from 1, the transition metal carbides can stabilize a series of vacancy ordered and stacking fault phases. Particular to the vacancy ordered phase formation, it is difficult to process them because of their low temperature stability and limited diffusivity at these temperatures.

Through our research we have discovered a yet to be reported phase that formed in the niobium hemicarbides. Specifically, the niobium carbides have a vacancy formation energy near zero which has facilitated their capacity to stabilize vacancy ordered phases. Nevertheless, we have shown that as carbon is depleted from a rocksalt niobium carbide towards a niobium hemicarbide, the system readily faults, with these faults stabilizing the metastable C6 structure. The C6 structure has a localized metallic bond in the unit cell which is shown to dramatically regulate the deformation mechanisms in carbides.

Through a collaborative experimental and computational approach, our research has unraveled the underlying compositional and structural contributions in how metastable vacancy-ordered and fault forming phases evolve.

Intellectual merit impact: One of the challenges of ceramics is their brittle behavior. By understanding phase stability, and the processing space to facilitated metastable phases with metallic-like bonding, the program offers opportunities to increase their fracture toughness and avoid catastrophic failure.

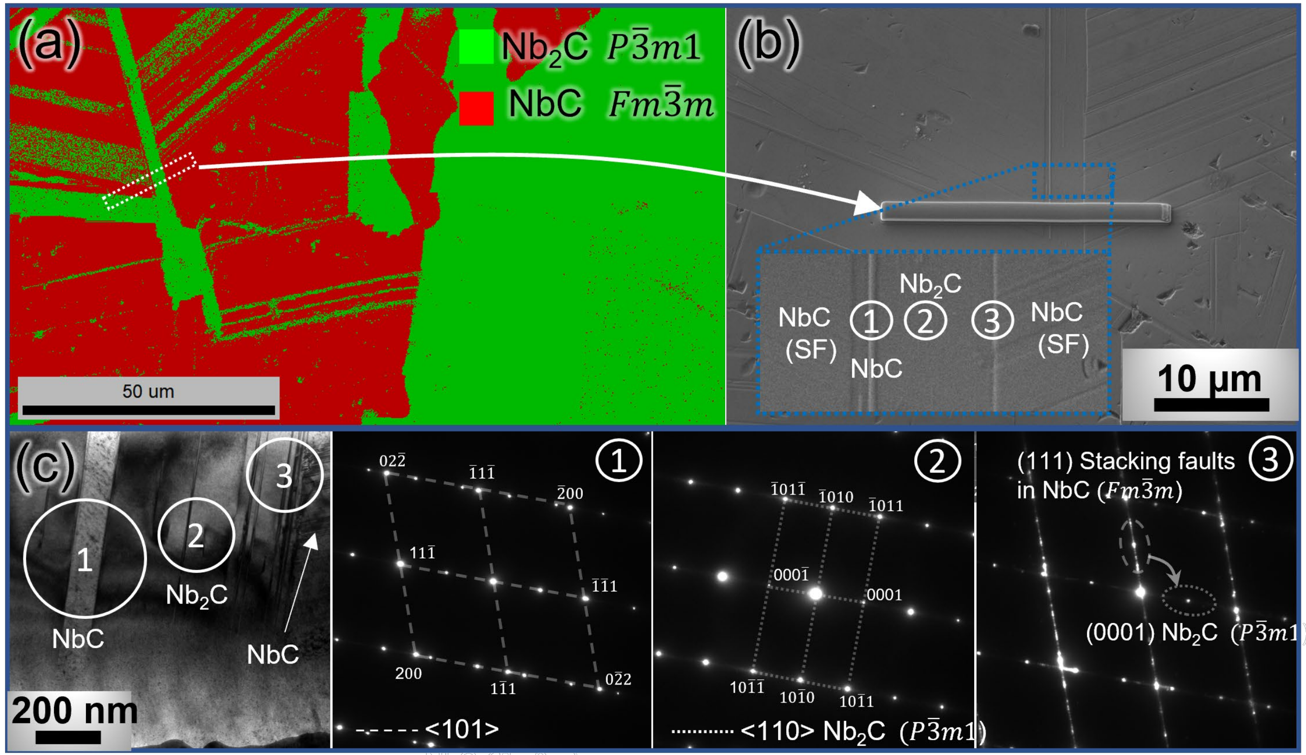

Figure: **(a)** Phase map that reveals laths of Nb_2C (green) forming in NbC (red) **(b)** Site specific sample extraction of a lath region **(c)** electron microscopy image revealing nanoscale laths with 1, 2, and 3 being electron scattering patterns confirming the new C6 structure. More details at doi.org/10.1007/s11837-023-06084-y

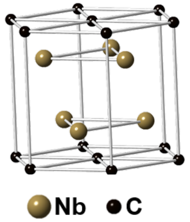

Figure: C6 unit cell. Note the metal-metal bonding in the interior of the cell.

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Dissemination and Development of the Raising Generation of Ceramic Scientists and Engineers

Christopher Weinberger, Colorado State University

Thompson and Weinberger developed a new teaching module that was introduced to secondary school teachers at the University of Alabama's ASM Materials Camp held June 16-23, 2023.

This camp provides a one week on-campus experience for teachers to learn how to incorporate materials into their physics, chemistry, and physical science classrooms. Through this grant, teachers are supported with on-campus dormitories that allows them to be part of the program. By doing so, we reach well beyond the near city locations. In 2023, teachers from Virginia and Arkansas were able to come and participate.

This module, initially tested with students in Colorado State University's Upward Bound program, was translated to the UA camp. Using various chocolate bars, balanced between two surfaces, and mechanically loaded with a cup that holds ever increasing coins, a three-point beam test is achieved. The module teaches principles of mechanical testing, composite design (nuts in chocolate), measurement error, fracture behavior, and temperature dependance on fracture (by placing the chocolate in a freezer prior to testing). At the end, it also offers a tasty treat too!

Through the support of NSF, this program enables the investigators in developing instructional tools that are translated to teachers who then disseminate it the concepts to a larger number of students. By doing so, a rising generation of students are excited into the STEM fields.

Thompson (red shirt) instructing the teachers at the University of Alabama Materials camp in the use of a teaching module on mechanical behavior that was developed and tested at Colorado State University.