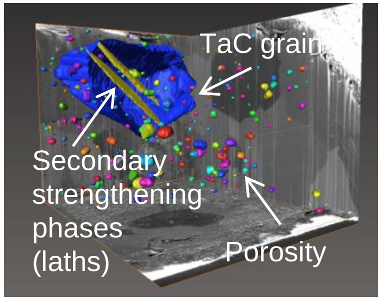
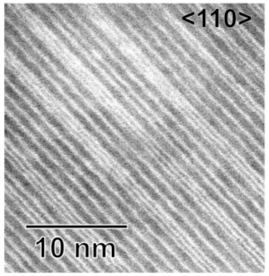
Scientific Objectives, Challenges and Breakthroughs

Scientific Objectives

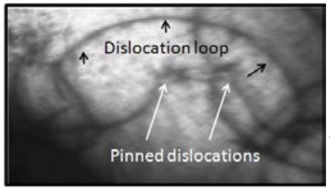
- Elucidate microstructure formation pathways. Microstructure controls properties. Critical to understand phase transformations as a means to engineer a materials properties.
- Combine advanced characterization techniques with state-of-the-art computation simulations to determine deformation mechanisms in tantalum carbide ceramics.



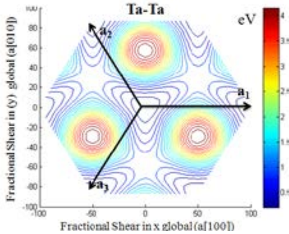
3D representation of microstructure morphology via FIB serial sectioning



Parallel, secondary strengthening phase laths



Frank-Reed dislocation source mechanism for deformation in Ta_2C



First-principle Generalized Stacking Fault Energy curves

Scientific Challenges

- Quantify 2D and 3D lath features in microstructure.
- What is the relationship between the matrix and precipitate phases?
- How and under what circumstances do precipitates control microstructures?
- Determine atomistic conditions for macroscopic deformation.
- Find evidence for dislocations mechanisms.

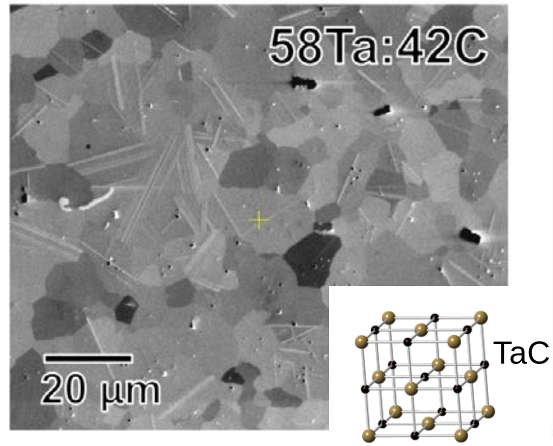
Scientific Breakthrough

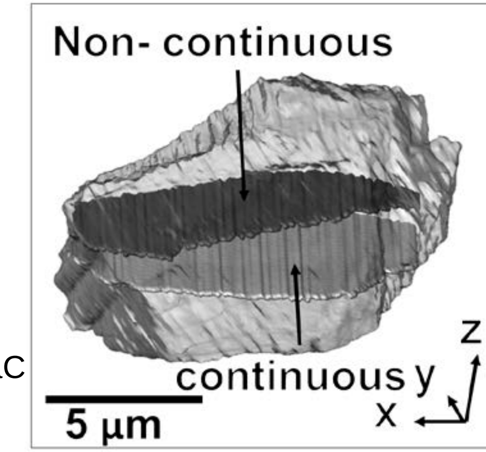
- 3D representation through tomography
  - ➢ Laths are both continuous and discontinuous. Plate-like structures that are tens of nm's thick
- Parent phase symmetry conditions govern morphology
  - ➢ Precipitation from TaC with equivalent {111} variants yields crisscross pattern of phases
  - ➢ Precipitation from Ta_2C with single {0001} plane yields all laths parallel. Also generates acicular grain structure.
- Deformation mechanisms
  - ➢ Basal and non-basal slip in Ta_2C. First principle calculations highlight low barriers for deformation
  - ➢ HRTEM reveals faulting on Ta-Ta not Ta-C bonds

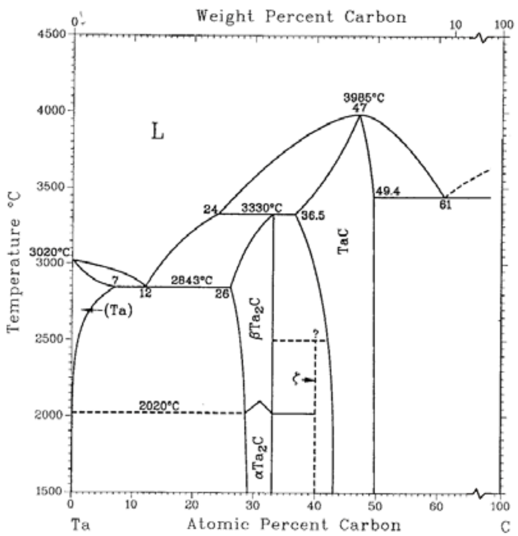
Motivation: Tantalum carbides are a class of ultrahigh melting temperature materials. The precipitation of Ta-rich carbide phases in TaC control microstructure (hence thermo-mechanical properties)

- **How do these phase form?**
- **How do they control microstructure?**

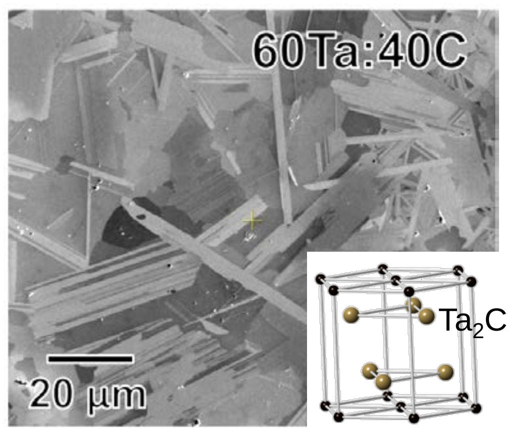
Apply 2D and 3D Microscopy

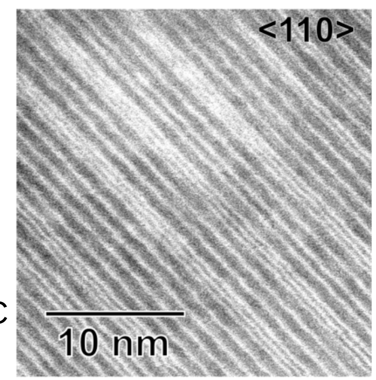


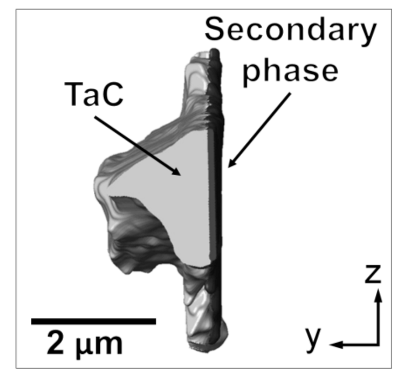




Ta_2C/Ta_4C_3 precipitates out of equiaxed TaC grains maintaining close packed planes and directions. TaC is a rock-salt structure with four varients of {111} planes yielding crisscross pattern of laths within the grains, which are and are not continuous in the grain.

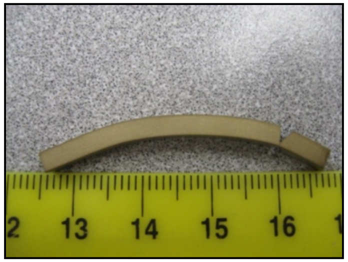




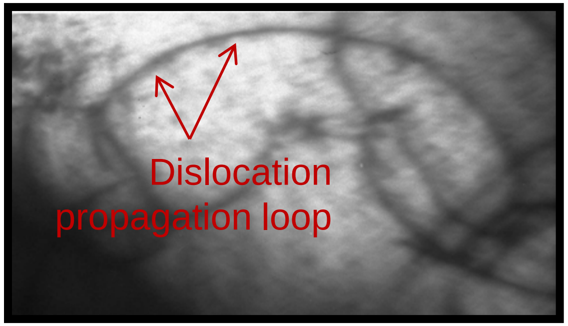


Phase diagram taken from O. M. Barabash and Y. N. Koval, *A Handbook on the Structure and Properties of Metals and Alloys*.1986

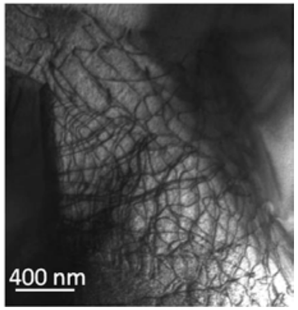
Secondary strengthening phase laths span the entire acicular Ta_2C grains. These laths are along major axis of the acicular grains. These TaC/Ta_4C_3 secondary phases precipitate from Ta_2C, which has only one close packed plane, (0001), controlling orientation and grain shape



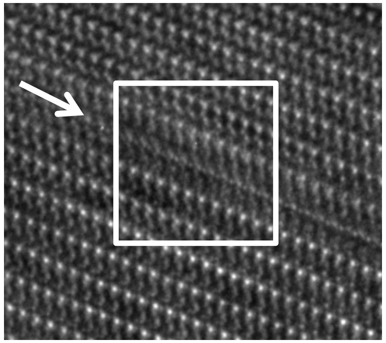
Ta_2C four-point bend test at ~2000°C shows significant plasticity. Deformation mechanisms include basal and non-basal slip (dislocations) and stacking faults. Collaboration with Dr. Chris Weinberger, Sandia National Laboratories, provided first principle calculations of Generalized Stacking Fault Energies.

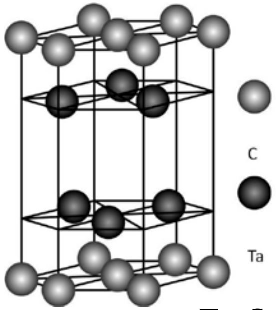


Frank-Reed Dislocation source



Dislocation forest





Ta_2C

HRTEM confirms faults on Ta-Ta layers, consistent with modeling predictions for easily slip directions

Ta-Ta bonds << Ta-C bonds