Towards Predicting A Microstructure's Susceptibility to Spall: Non-Equilibirum Molecular Dynamics Simulations of Tantalum

Eric N. Hahn[1,2], Saryu J. Fensin[1], Tim C. Germann[2]
[1]MST-8, Los Alamos National Laboratory; [2]T-1, Los Alamos National Laboratory

Motivation & Introduction

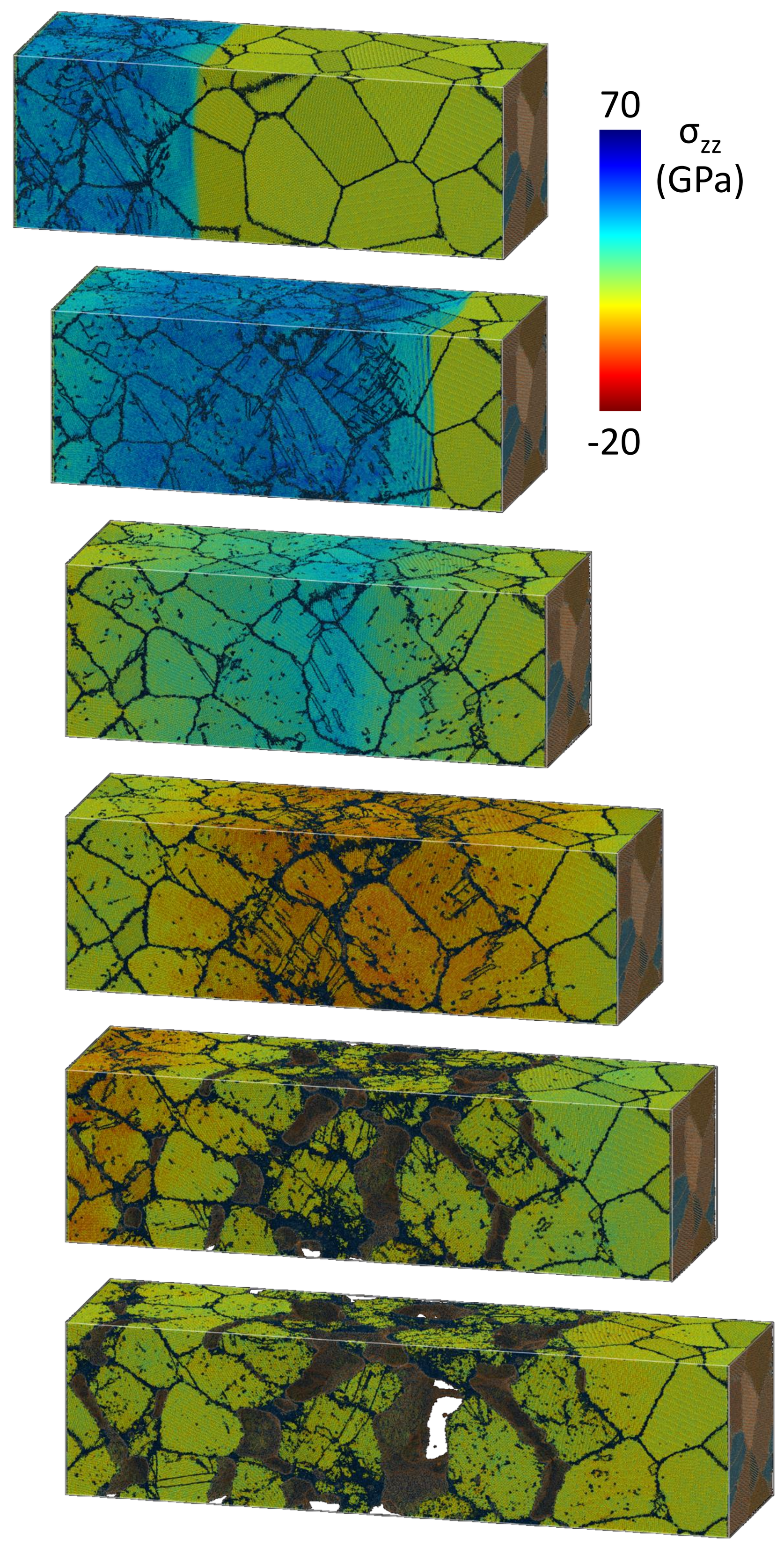
- The capability to accurately predict damage and failure of metals is of critical interest to LANL, DOE, and DoD.
- The current deficiency in predictive modeling capability is tied to a poor understanding of the fundamental correlations between processing, microstructure, properties, and performance under high pressure and high strain-rate loading.
- This has large implications when evaluating the ability of additively manufactured (AM) materials to meet design needs, such as powder bed AM compared to traditionally wrought materials.
- It is critical to make definitive links between the microstructural features, material history, and the stress/strain conditions that lead to damage nucleation; the connections must be mathematically quantifiable such that they can be implanted into a physically-based predictive toolkit.
- Ultimately, we aim to describe the spall strength, σ_{sp}, of tantalum as a function of:

$$\sigma_{sp} = f(Z, \dot{\varepsilon}, T, h, s) < \sigma_{\max}(Z, s)$$

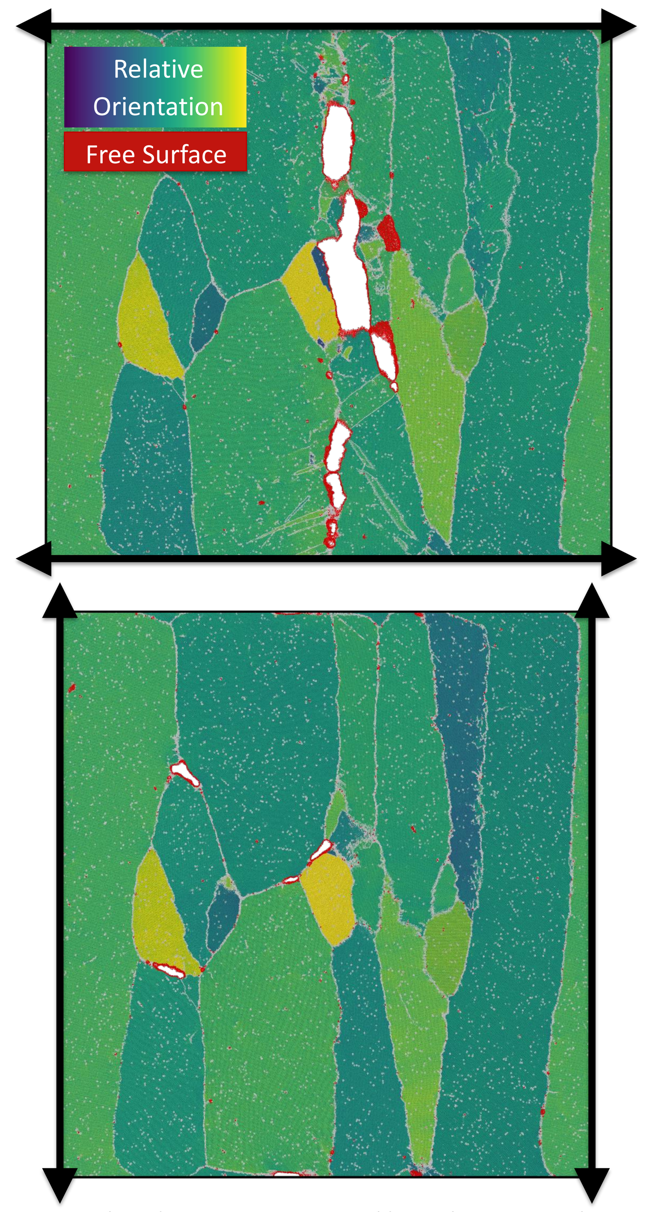
  - Material composition (Z)
  - Strain rate (dε/dt)
  - Temperature (T)
  - Loading history (h)
  - Local microstructure (s)
- The set of microstructure descriptors includes grain size statistics (mean size, distributions of size and/or shape), texture, grain boundary and triple junction character, etc.

Microstructure

Poly-crystal



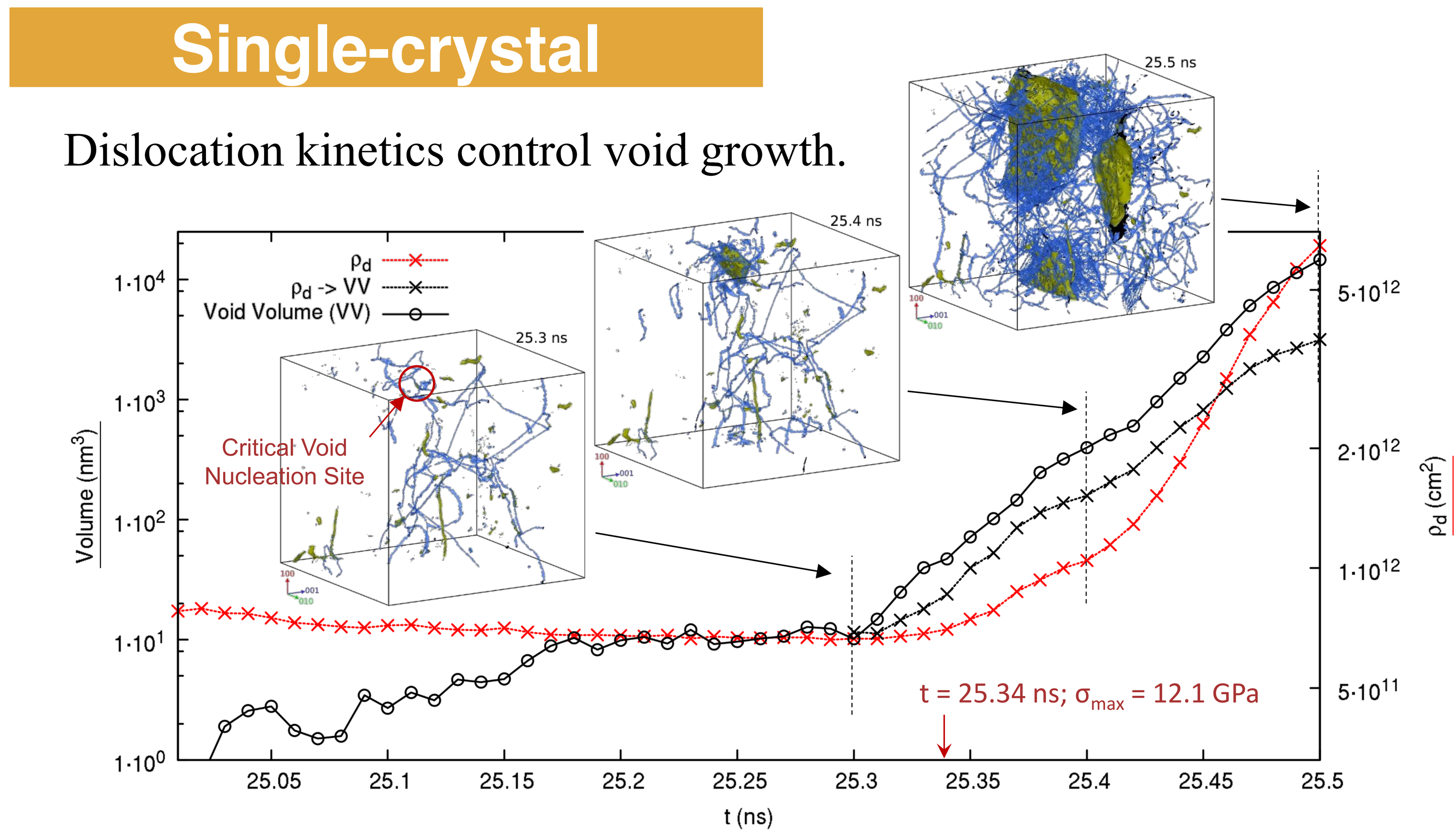
Void nucleation occurs principally at grain boundaries, when they are present, due to local stress concentrations.



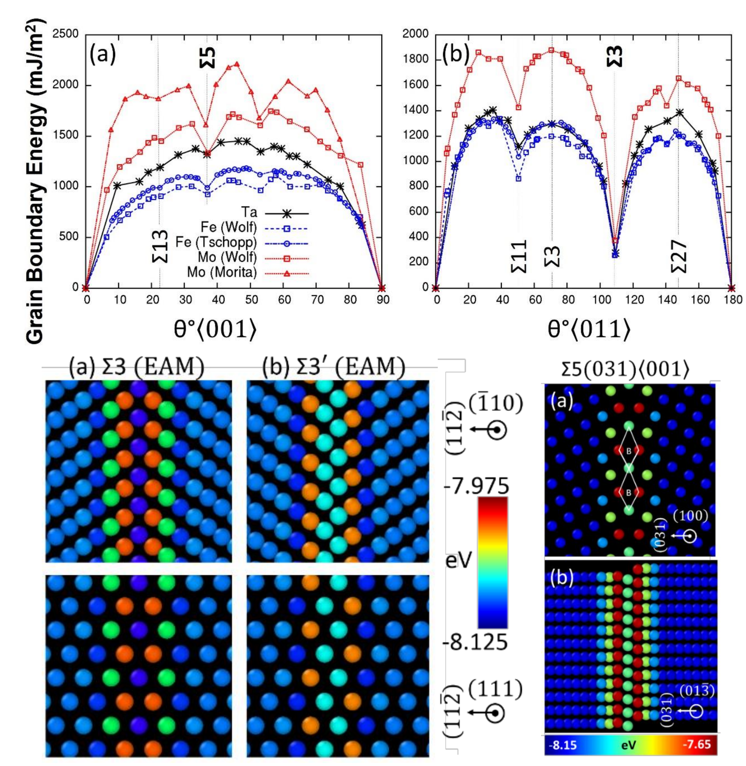
Boundaries perpendicular to the loading direction fail preferentially. This has important ramifications for AM materials with highly textured microstructure.

Single-crystal

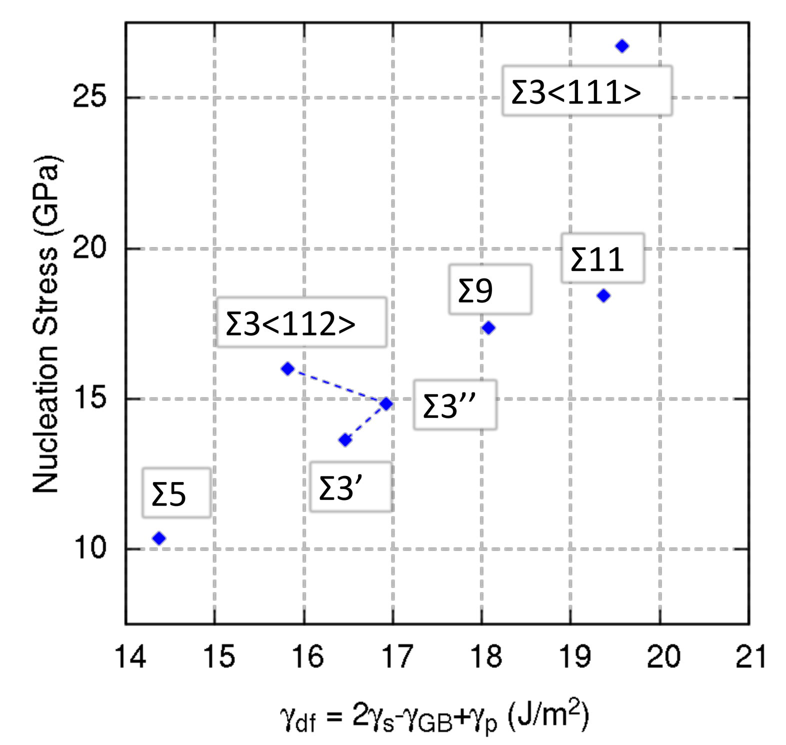
Dislocation kinetics control void growth.



Bi-crystal

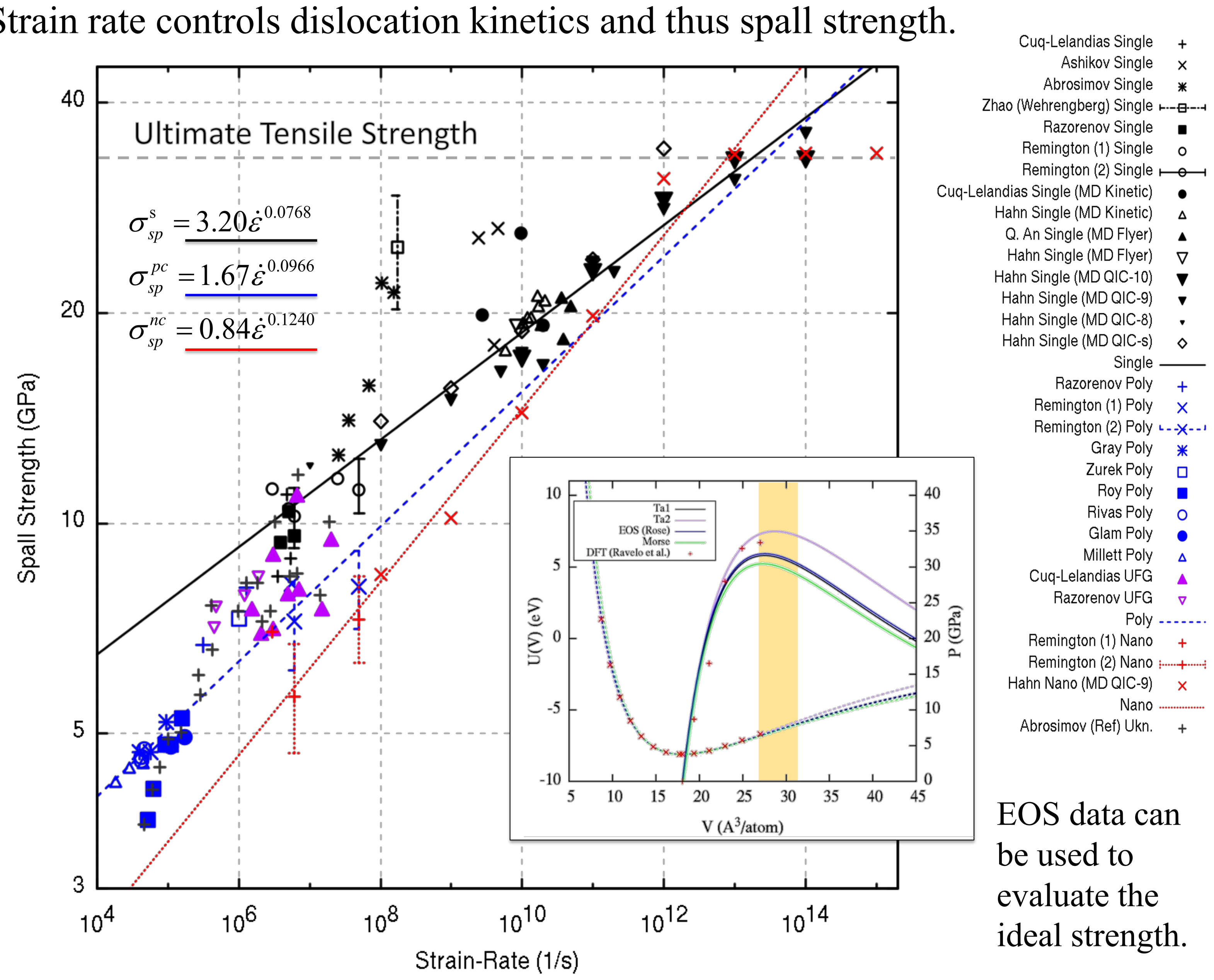


Ductile work has a strong influence on grain boundary failure.



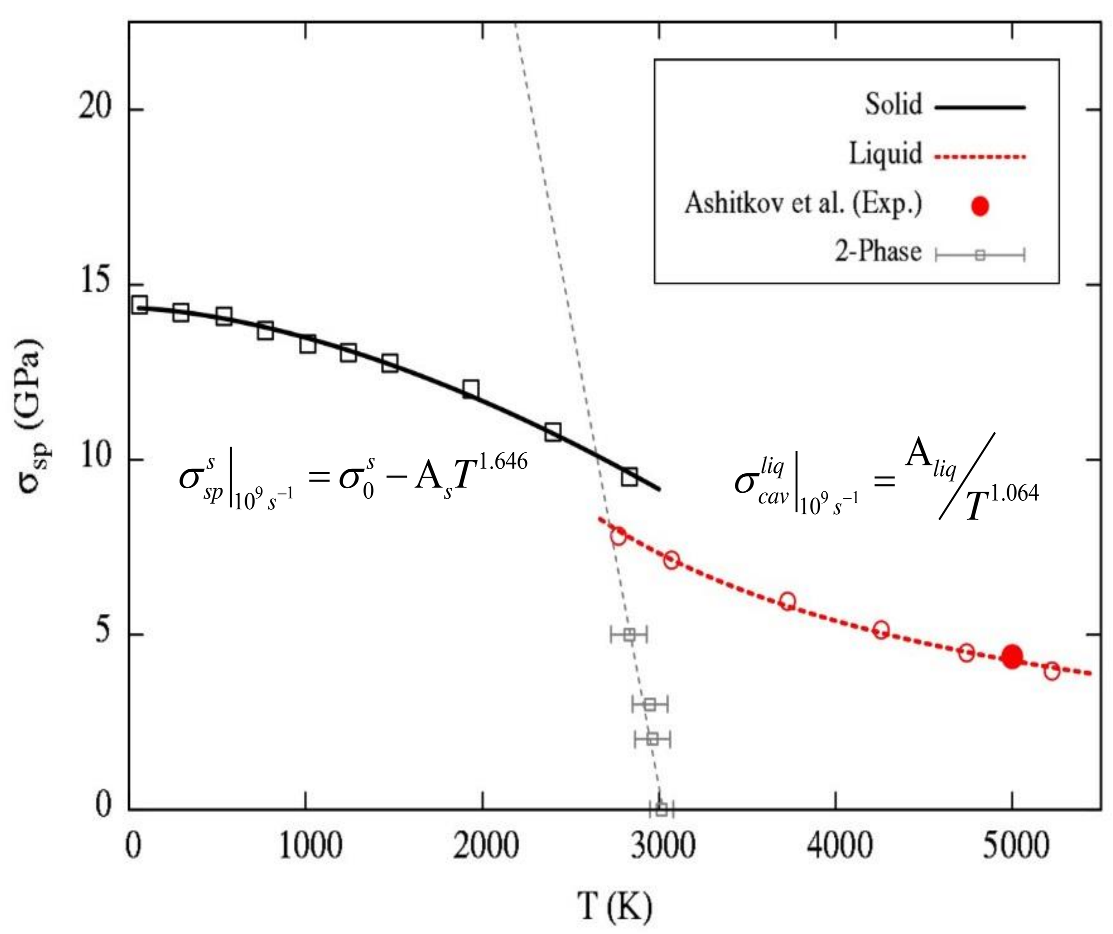
Strain Rate

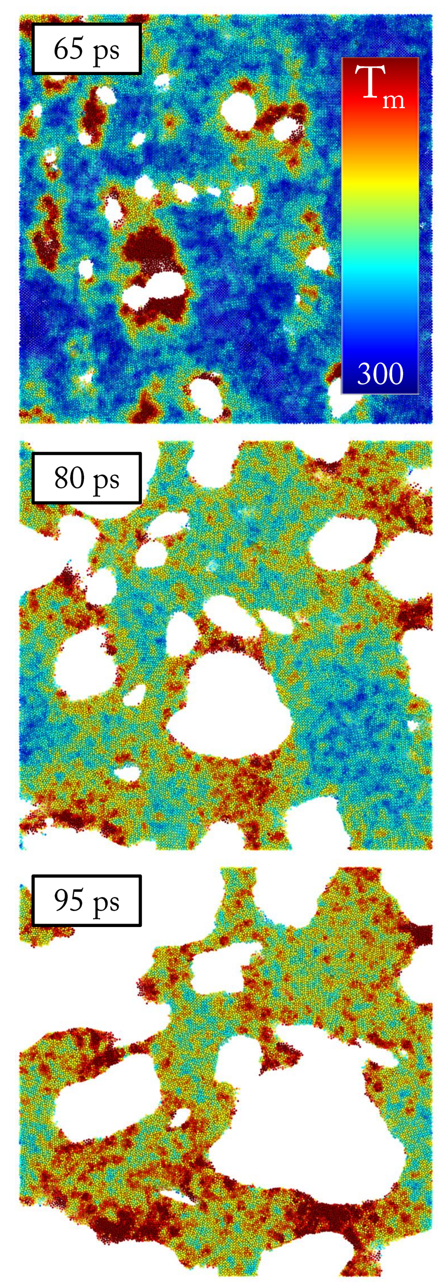
Strain rate controls dislocation kinetics and thus spall strength.



EOS data can be used to evaluate the ideal strength.

Temperature





(Above) Increasing the temperature softens the lattice resistance to deformation. There is a clear jump in spall strength of solid and liquid tantalum. (Right) Spall below the melting temperature still shows evidence of localized melting and viscous ligament flow.

Conclusions

- Strain rate plays a governing role in the motion of defects which are intimately tied to void nucleation and growth.
- Temperature can not be ignored in the determination of an effective spall strength and thus shock induced temperature rise and local heat generation due to plastic work must be taken into account.
- The amount of ductile work a material undergoes influences a grain boundaries' ability to release stress by alternate modes in lieu of failure, thus suppressing void nucleation.
- Grain boundaries operate as stress concentrators due to local compatibility requirements and serve as preferential void nucleation sites.
- The loading orientation and grain boundary orientation dictate that higher stresses occur at perpendicular boundaries which fail preferentially.

References

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