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New nanoscale toughening mechanisms mitigate embrittlement in binary nanocrystalline alloys

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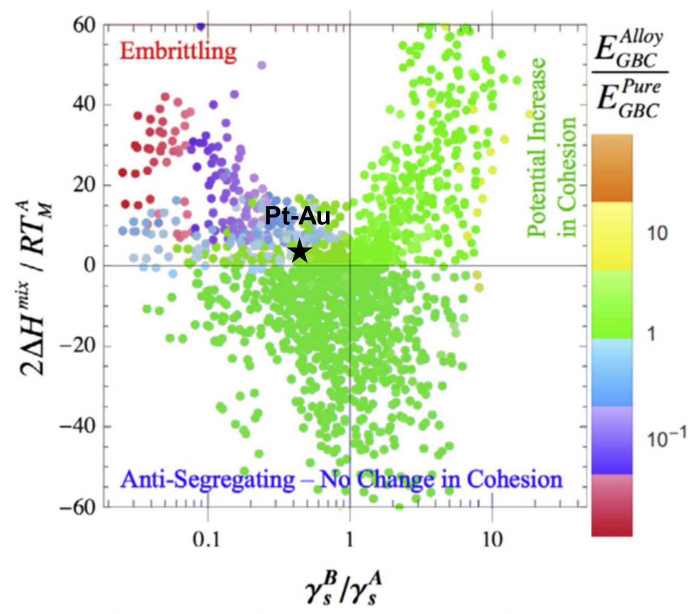
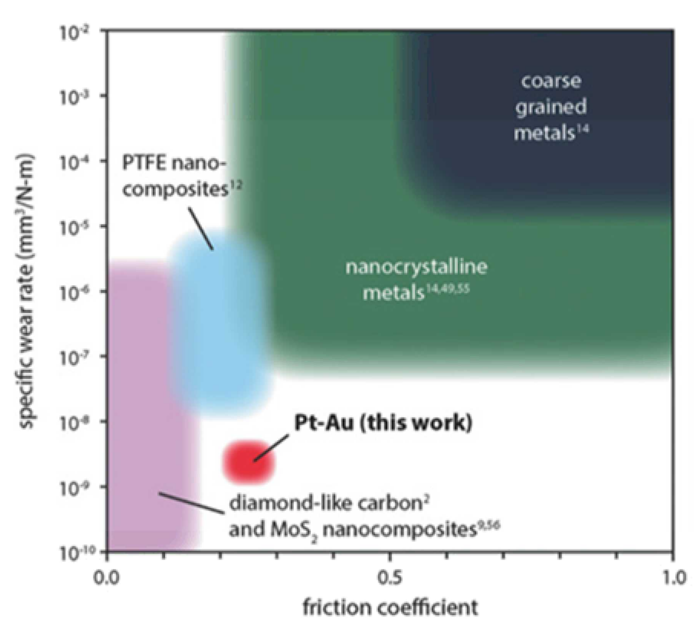
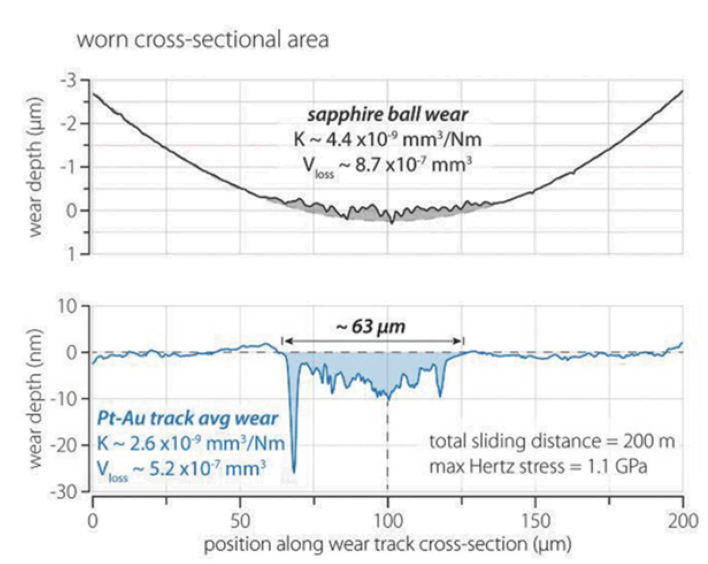
Motivation: Nanocrystalline Pt-Au

- Grain boundary segregated binary nanocrystalline metals offer potential for thermodynamic stability
- Solute atoms can potentially embrittle grain boundaries
- Embrittling behavior not explicitly demonstrated in any nanocrystalline alloys



Gibson and Schuh, *Acta Materialia*, 2015



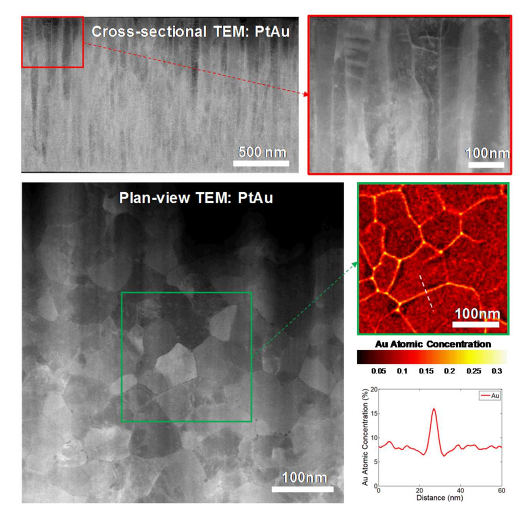


Curry et al., *Advanced Materials*, 2018

- Extraordinary wear properties of nanocrystalline Pt-10at.%Au, demonstrated by Curry et al.
- Outperforms other nanocrystalline metals in wear by orders of magnitude
- More wear to sapphire tip (H>20 GPa) than the actual material

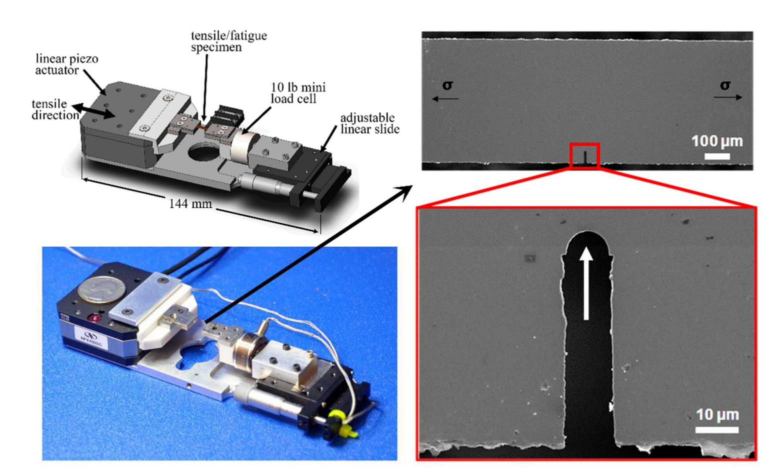
- Expanding on this, this study seeks to explore the tensile behavior of binary nanocrystalline Pt-Au
- Explore deformation mechanisms and how these influence mechanical properties.

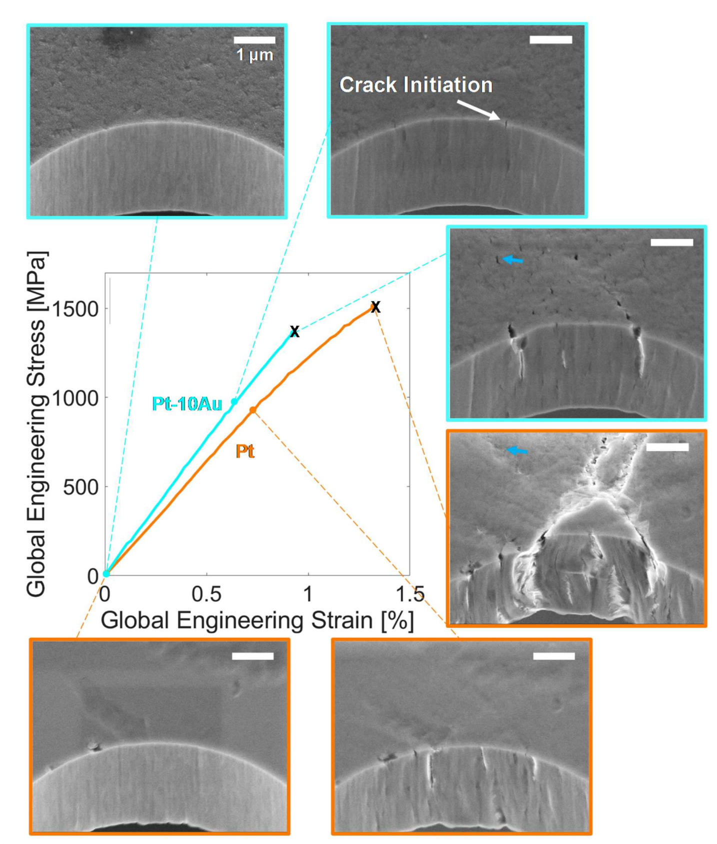
Experimental: In-situ SEM Tensile Test



- 5 µm thick Pt and Pt-10at.%Au films synthesized by magnetron sputtering
- Both samples contained [111] textured columnar grains
- Mean columnar grain width of 50 nm in each film

- Samples notched in FIB to create stress and strain concentration
- In-situ tests performed at oblique angle in JEOL IT300HR SEM

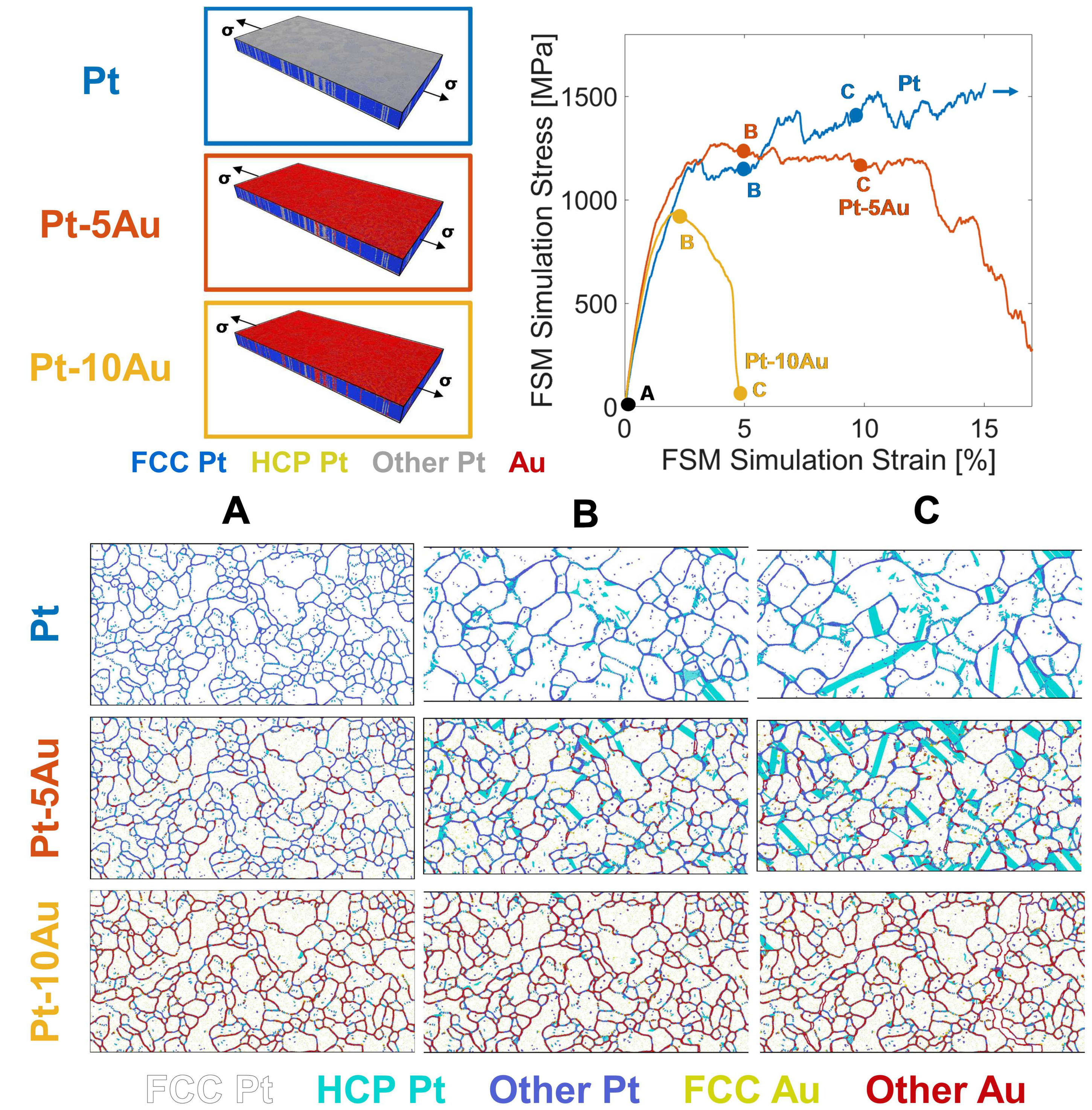




- Pt-10Au formed crack network ahead of notch
- SEM and TEM analysis (not shown) revealed the formation of intergranular cracks along Au-rich grain boundaries

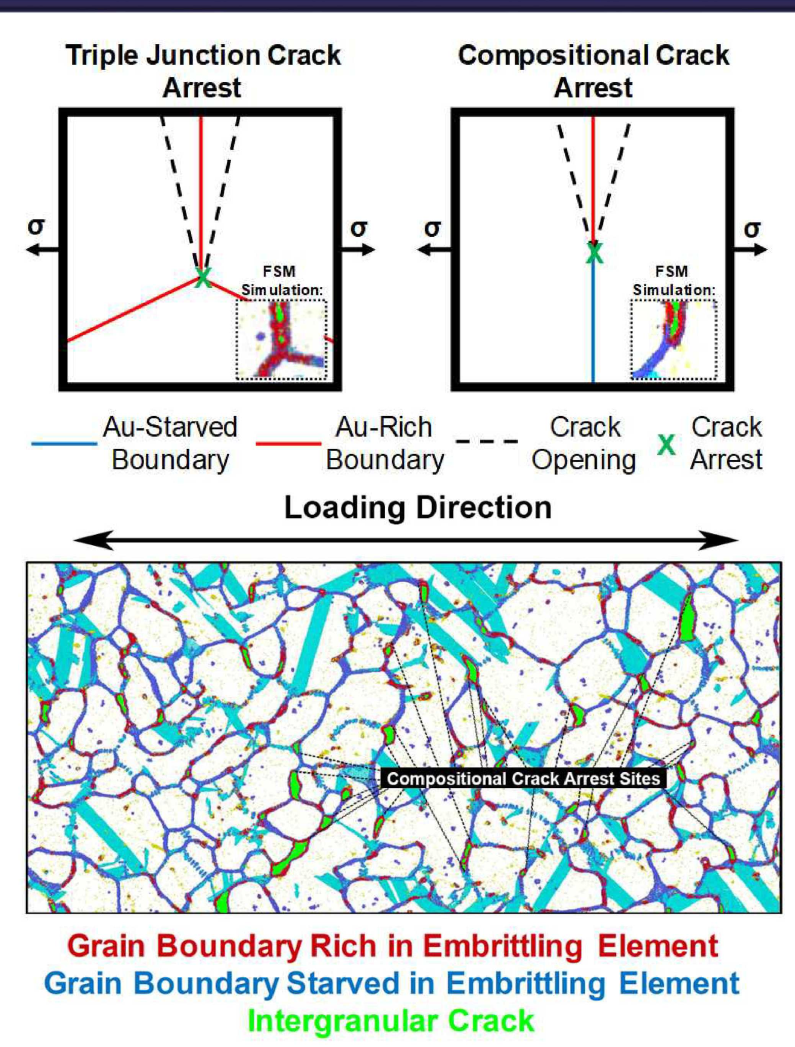
- Pt showed primarily plastic deformation
- SEM and TEM analysis (not shown) revealed microstructural transformation and grain growth

Simulations: Tensile tests of films with Free Surface constraint



- Pure Pt showed highest ductility and deformed largely through grain boundary migration driven grain growth
- Pt-5Au showed substantial ductility and distributed nanocrack networks were observed to form
- Pt-10Au showed poor ductility and distributed nanocrack networks formed, but coalesced into a critical crack

Nanocrack Networks and Crack Arrest



- Nanocrack crack network formation depends on competition between crack formation and crack arrest
- Simulations reveal two potential methods for cracks to arrest, both of which allow for the formation of nanocrack networks
- Triple junction crack arrest, observed primarily in Pt-10Au sample, doesn't allow for significant ductility
- Compositional crack arrest (newly observed mechanism), observed primarily in Pt-5Au, allows for more overall toughening

Conclusions and Future Work

Nanoscale toughening through the formation of distributed nanocracks was observed in nanocrystalline Pt-Au alloys. The crack networks form due to competing grain boundary embrittlement and crack arrest. Two modes of crack arrest were observed: triple junction crack arrest and compositional crack arrest, a newly observed mechanism. Compositional crack arrest, which depends on the heterogeneous segregation of an embrittling element to grain boundaries, allows for more overall toughening compared to triple junction crack arrest. By varying the composition of nanocrystalline alloys, the role of each of these mechanisms can be adjusted in order to tune toughness of the materials. An understanding of how grain boundary segregated nanocrystalline alloys deform allows for the realization of nanocrystalline metals with a unique combination of high strength, thermal stability, and damage tolerance.*

Future work seeks to explore the influence that other alloying elements have on the deformation behavior. Specifically, other solutes are expected to *enhance* the boundary cohesion. Through similar tests, we seek to understand the mechanisms by which these materials deform.

*Note this work was recently accepted for publication and will soon be available in *Nanoscale Journal*

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