Extreme Mechanical Stability at the Nanoscale Through 3D Interfaces

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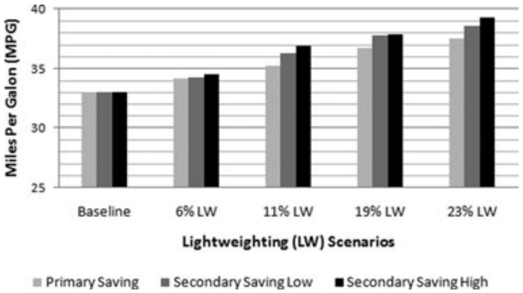
5 – Center for Integrated Nanotechnologies, Los Alamos National Laboratory, Los Alamos, NM
6 – Materials, University of California Santa Barbara, Santa Barbara, CA
7 – Mechanical Engineering, University of California Santa Barbara, Santa Barbara, CA

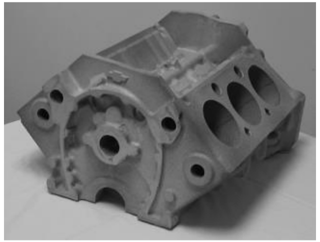
High demand for high strength alloys

Automotive applications

Increase fuel economy…

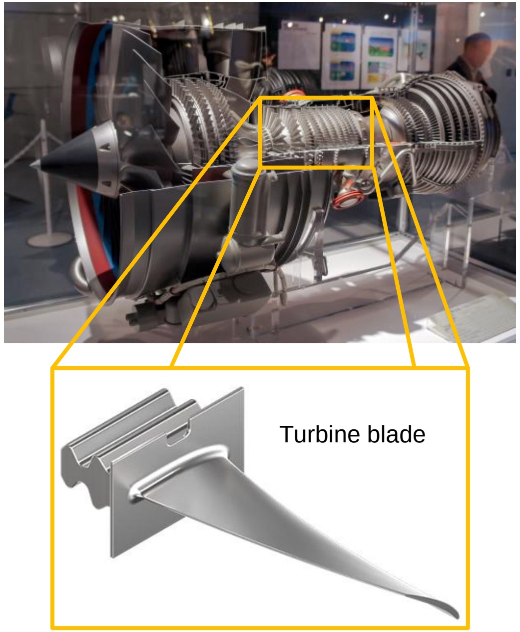


…through higher specific strength materials



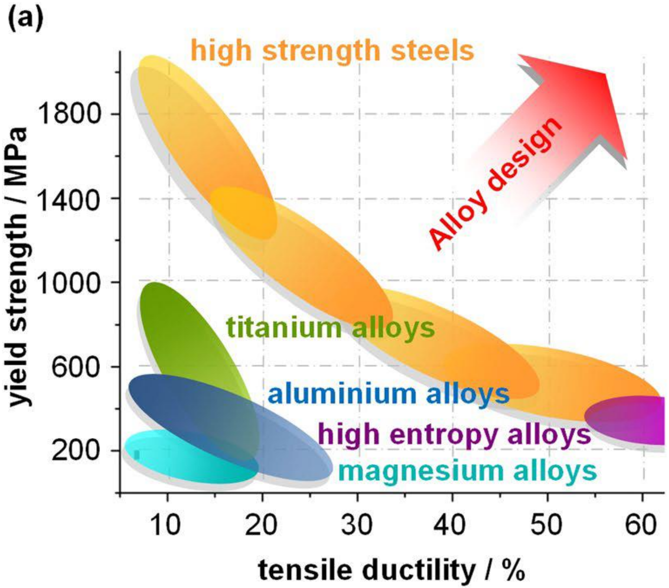
Aerospace engine design

Aircraft turbine



Mechanical stability under extreme temperature (>1500ºC)

Mechanical stability demands high strength and ductility



H.-J. Kim, C. McMillan, G. A. Keoleian, S. J. Skerlos, J. Ind. Ecol. 14, 929–946 (2010).
A. Tharumarajah, P. Koltun, J. Clean. Prod. 15, 1007–1013 (2007).

https://en.wikipedia.org/wiki/IAE_V2500#/media/File:IAE_V2500_engine_cutaway_model_2010_The_Sky_and_Space.jpg
Rolls-Royce plc. (2016) The Jet Engine

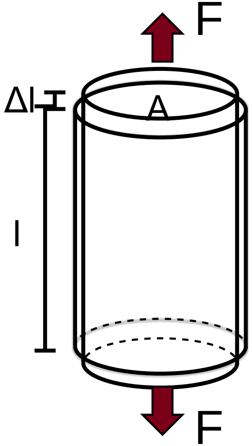
H. Springer, C. Baron, A. Szczepaniak, V. Uhlenwinkel, D. Raabe, Sci. Rep. 7, 2757 (2017).

A (very very) brief introduction to solid mechanics

Gold standard of mechanical testing – tensile testing

Load and displacement are measured continuously during test

Calculation of stress and strain

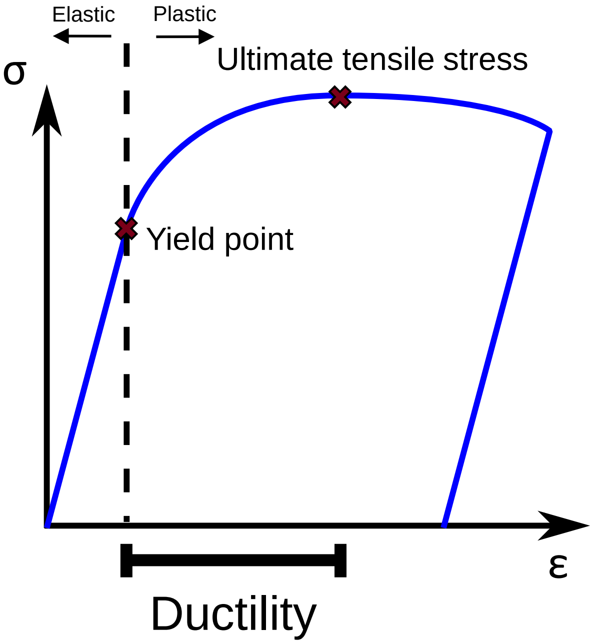


Geometry defined by gage length l and cross-sectional area A

Force F is applied to the specimen

	Stress	Strain
Engineering	$\sigma_e = F/A_o$	$\varepsilon_e = \Delta l/l_o$
True	$\sigma_t = F/A_i$	$\varepsilon_t = \ln\frac{l_i}{l_o}$

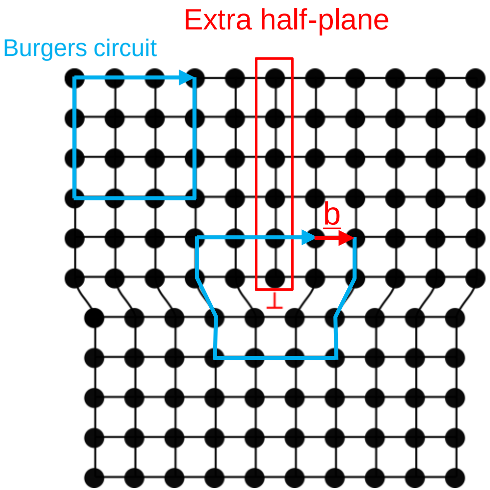
The engineering stress strain curve



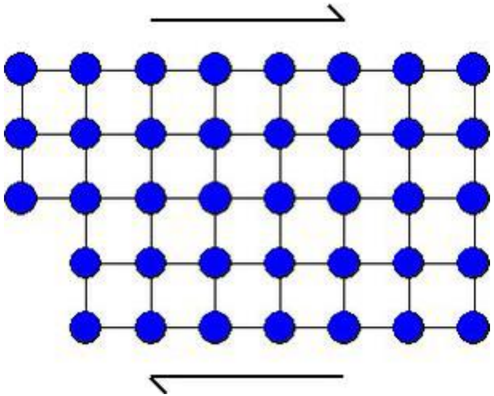
Courtesy of DoITPoMS, The University of Cambridge

Metallic deformation at the atomic scale

Metallic deformation mediated by dislocation movement in most cases

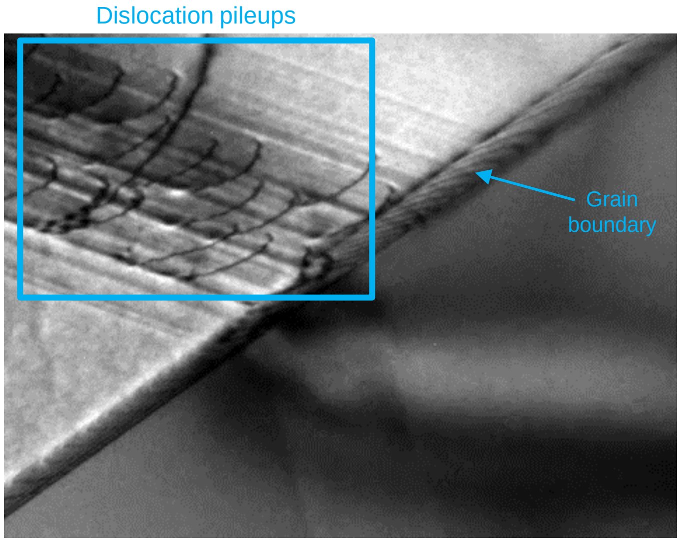


Edge dislocations defined by extra half-plane inserted into crystal lattice



Application of stress generates force on dislocation, causing it to move (slip/glide)

Interaction with other dislocations and microstructure determines strength



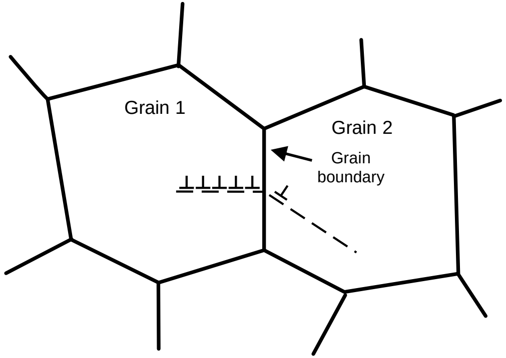
Defect stress fields and atomic structures generate forces on each other that influence mechanical properties

https://www.doitpoms.ac.uk/tlplib/dislocations/dislocation_glide.php

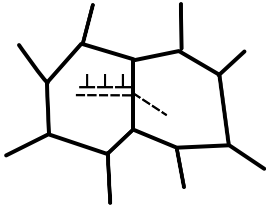
Kacher, J. & Robertson, I. M. Quasi-four-dimensional analysis of dislocation interactions with grain boundaries in 304 stainless steel. *Acta Mater.* **60**, 6657–6672 (2012).

Strengthening of metals at the nanoscale

Grain size affects strength due to dislocation interaction with grain boundaries

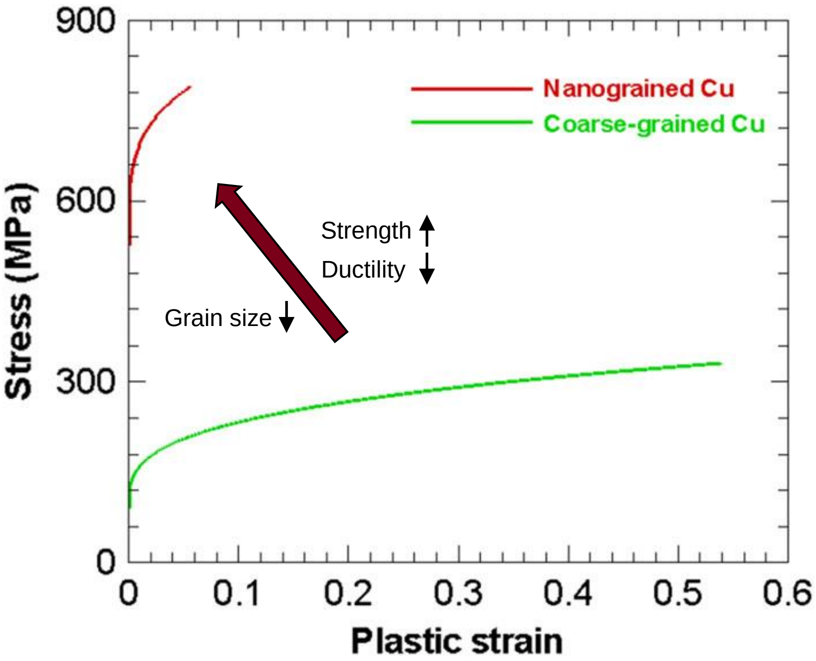


Large dislocation pileups encourage slip transfer across grain boundary



Small grain size limits pileup size, discouraging slip transfer

Decreasing grain size can enhance strength, but at cost of ductility

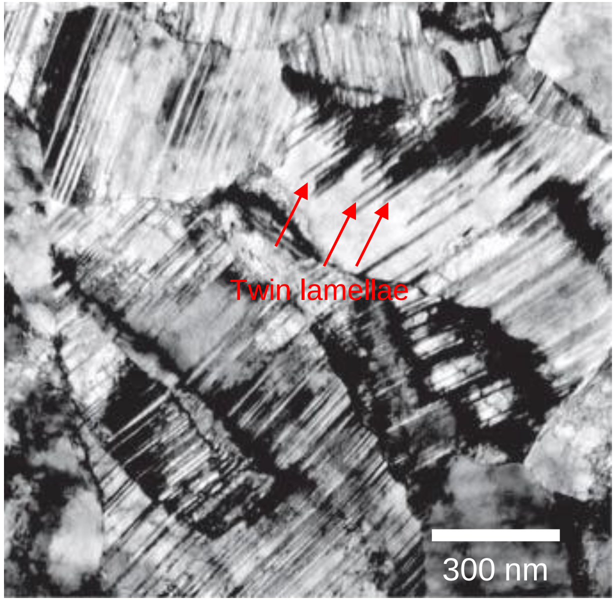


However, high interface content at nanoscale provides opportunity to tailor mechanical response

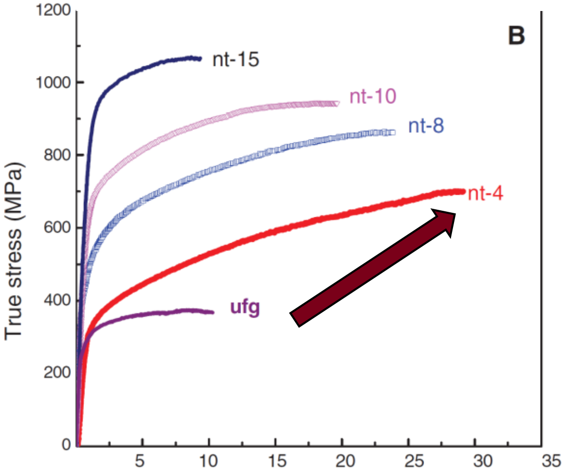
Guo, X., Liu, Y., Weng, G. J. & Zhu, L. L. Tensile Failure Modes in Nanograined Metals with Nanotwinned Regions. Metall. Mater. Trans. A Phys. Metall. Mater. Sci. 49, 5001–5014 (2018).

Interface-dominated deformation at the nanoscale

Controlled introduction of specific interface types can enhance mechanical properties

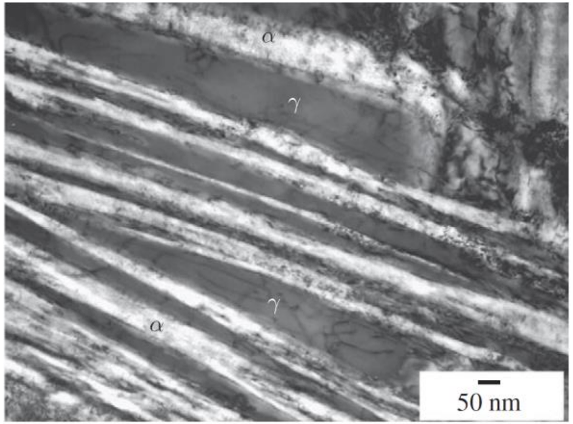


Lamellae thickness avg. 4 nm



Strength and ductility simultaneously improve

Multiphase materials contain heterophase interfaces that can be similarly tailored

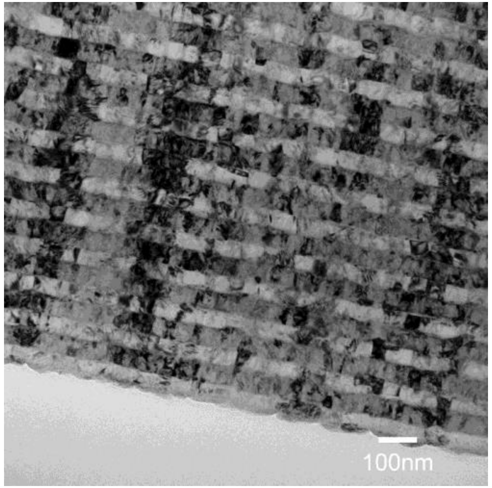


Nanostructured bainitic steel can achieve breakthrough mechanical performance

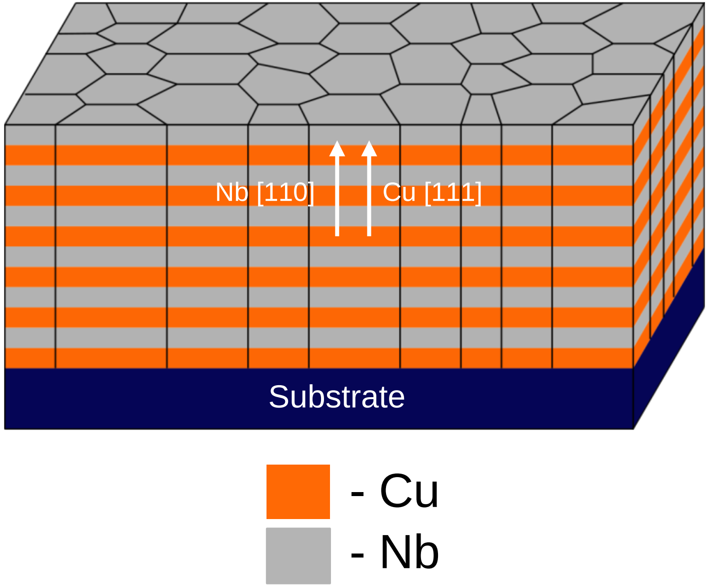
Lu, L., Chen, X., Huang, X. & Lu, K. Revealing the Maximum Strength in Nanotwinned Copper. *Science* **323**, 607–610 (2009).

Nanolaminates used to controllably study heterophase interface-defect interactions

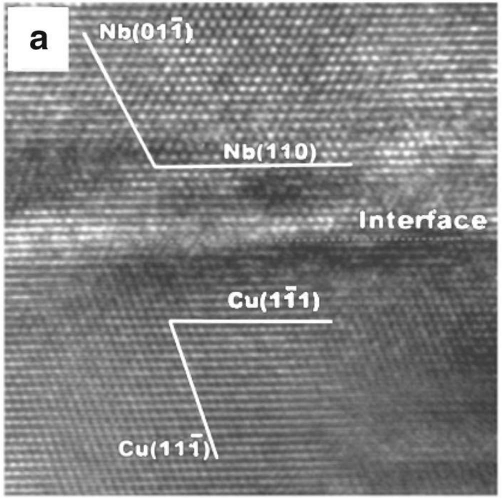
Nanostructured, layered materials have high heterophase interfacial content



Nanolaminates, e.g. Cu/Nb, are textured strongly in the out-of-layer direction



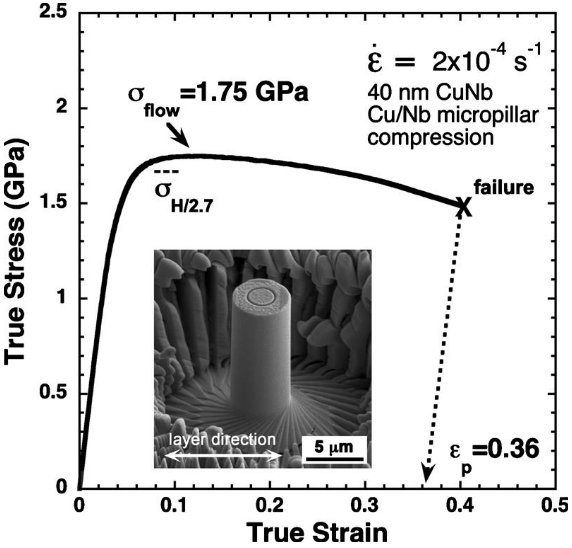
PVD Cu/Nb contains a high proportion of Kurdjumov-Sachs interfaces when deposited with chemically abrupt interfaces



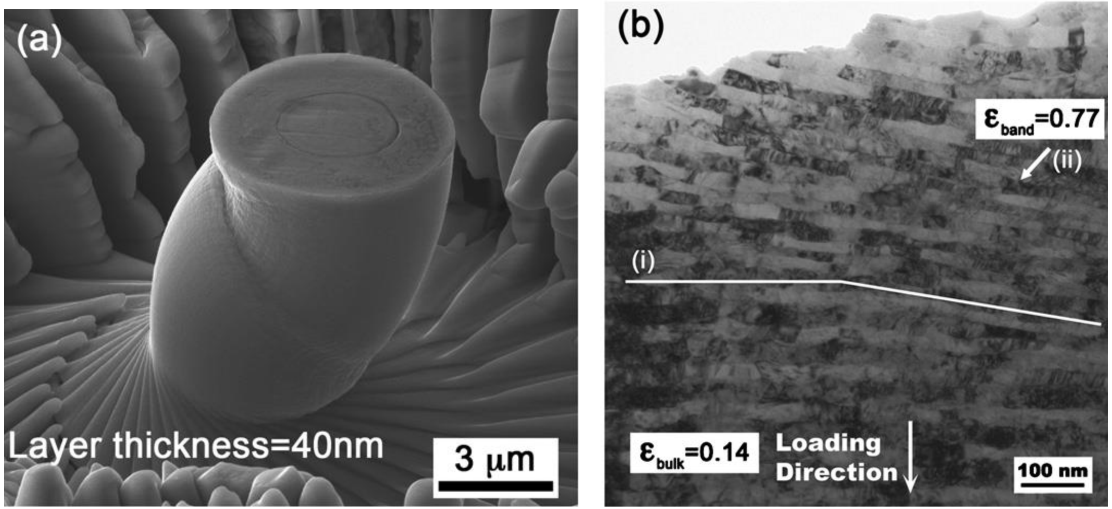
Beyerlein, I. J., Mara, N. A., Wang, J., Carpenter, J. S., Zheng, S. J., Han, W. Z., Zhang, R. F., Kang, K., Nizolek, T. & Pollock, T. M. Structure–Property–Functionality of Bimetal Interfaces. *JOM* **64**, 1192–1207 (2012).

Sharp interface Cu/Nb is strong but prone to shear localization

Strengths achieved in excess of 1.5 GPa at layer thickness of 40 nm



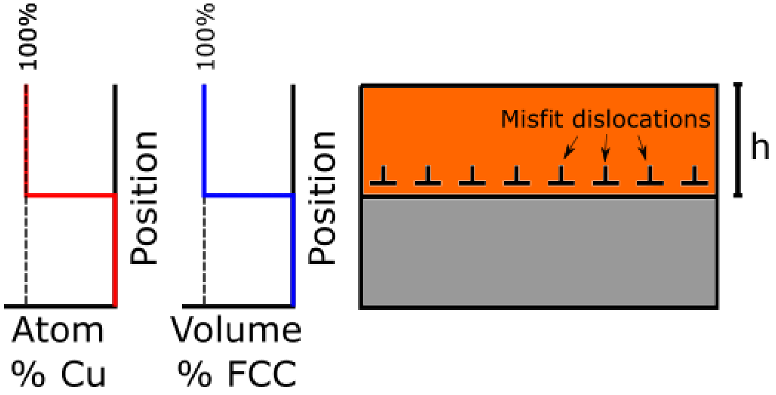
Shear localization causes strain softening and limits deformability



Mara, N. A., Bhattacharyya, D., Hirth, J. P., Dickerson, P., & Misra, A. (2010). Mechanism for shear banding in nanolayered composites. *Applied Physics Letters*, *97*(2). https://doi.org/10.1063/1.3458000

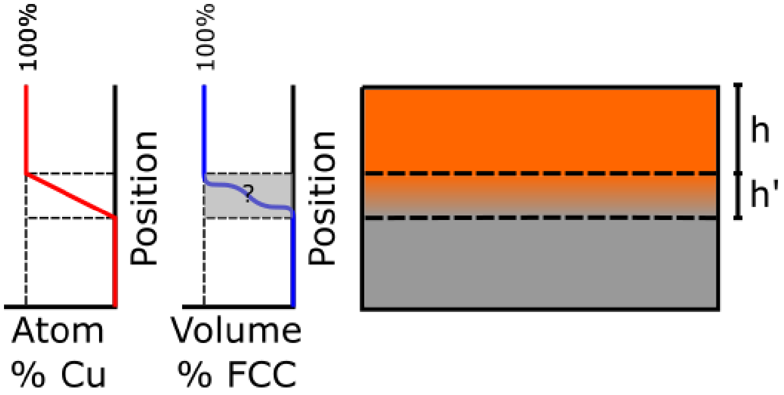
Avoiding shear localization with thick interfaces

2D interfaces display discontinuity in phase properties (e.g. lattice parameter, crystal structure), giving characteristic interface structure



2D Cu/Nb

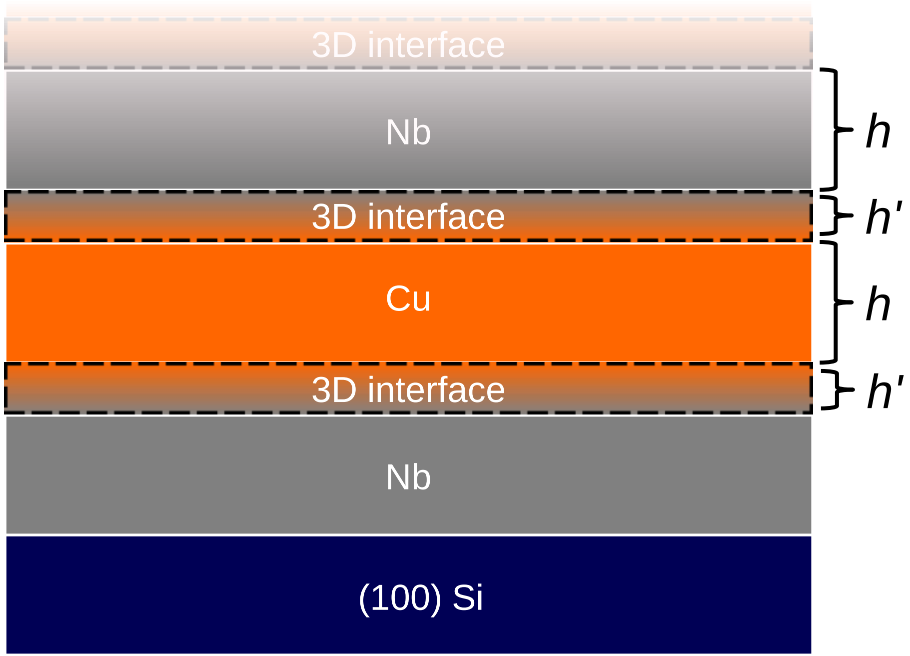
3D interfaces accommodate misfit through a finite thickness – total misfit remains the same as 2D



3D Cu/Nb

M. J. Demkowicz, R. G. Hoagland, J. P. Hirth, Interface Structure and Radiation Damage Resistance in Cu-Nb Multilayer Nanocomposites. *Phys. Rev. Lett.* **100**, 136102 (2008).

Synthesizing interfaces with 3D character



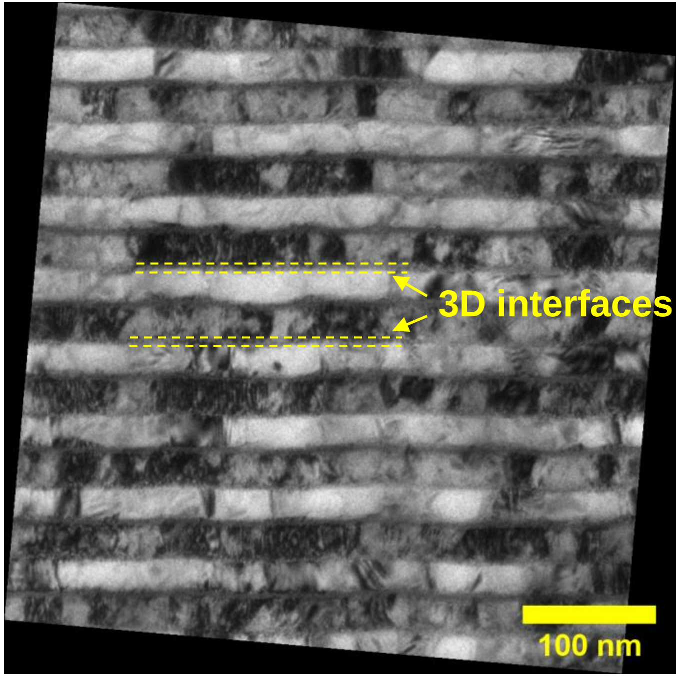
Conditions: Cu deposited at 150 W, Nb deposited at 400W at room temperature under 3mTorr Ar.
Substrate: (100) Si with native oxide

1. Deposit pure metal 1 (e.g. Nb)
2. Perform linear ramp from 100% power to 0% power for metal 1, while ramping from 0 to 100% power for metal 2 (e.g. Cu)
3. Deposit pure metal 2 (e.g. Cu)
4. Perform step 2 in reverse
5. Repeat steps 1-4

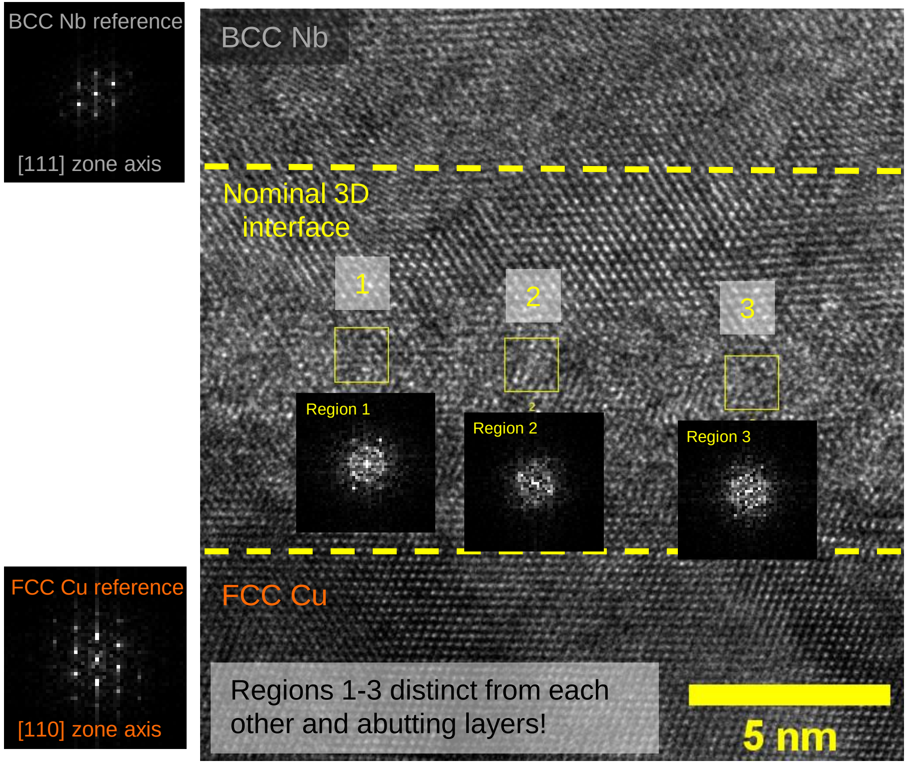
Samples referred to as *h-h'*, e.g. 10-10 has h = 10 nm and h' = 10 nm

3D interfaces phase segregated at fine length scales

3D interfaces exhibit diffraction contrast under TEM (20-10 Cu/Nb)



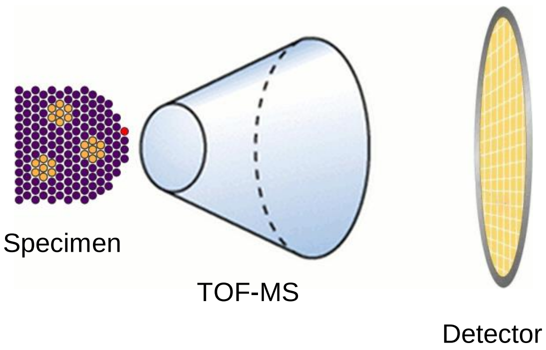
3D interfaces have lateral and through thickness structural heterogeneities



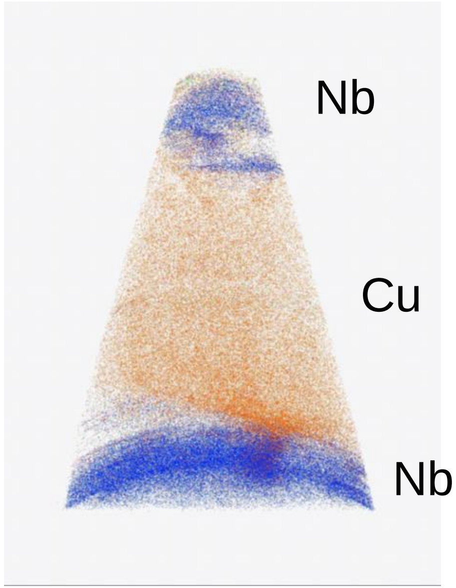
Regions 1-3 distinct from each other and abutting layers!

Atom probe tomography reveals chemical segregation

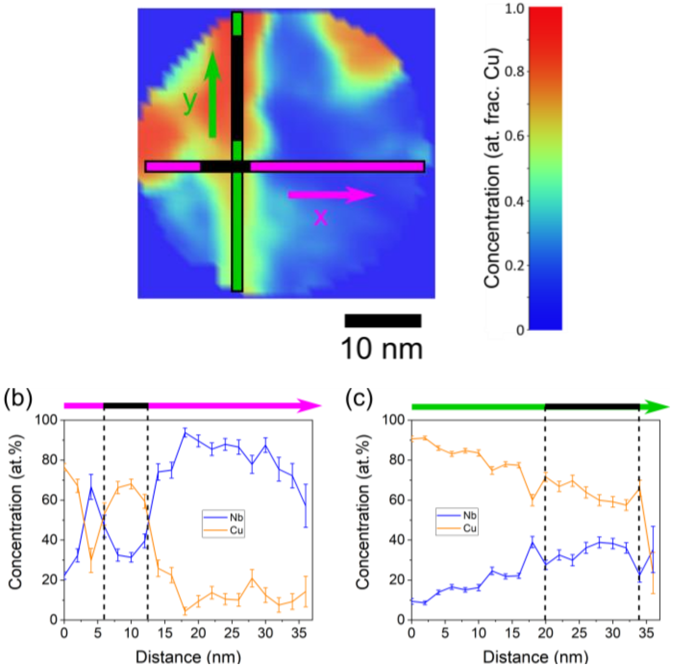
Atom probe tomography vaporizes a needle specimen to provide a 3D chemical map



3D maps of Cu/Nb reveal lateral chemical homogeneities



X-Y section at bottom 3D interface reveals chemical heterogeneities a few nm wide

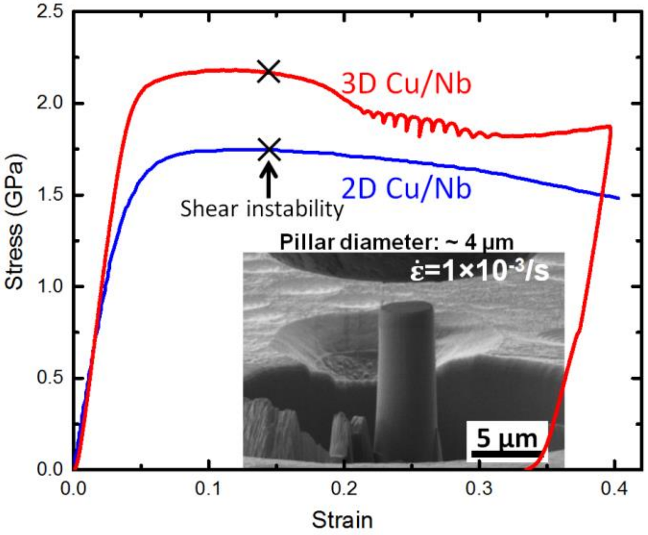


http://www.arc.nucapt.northwestern.edu/index.php?title=File:LEAP.gif&limit=20

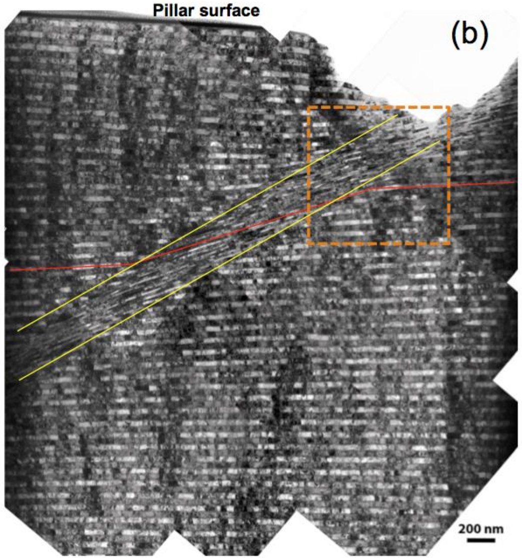
Li, Z., Cheng, J. Y., Poplawsky, J. D., Xu, S., Baldwin, J. K., Beyerlein, I. J. & Mara, N. A. Critical length scales for chemical heterogeneity at Cu/Nb 3D interfaces by atom probe tomography. *Scr. Mater.* **223**, 115078 (2023).

Introduction of 3D character at interfaces enhances mechanical properties in uniaxial compression

3D interfaces strengthen Cu/Nb without sacrificing plasticity at h = 40 nm



Codeformation occurs by reorientation of lattice towards easy slip, then shearing of pure phases and interface

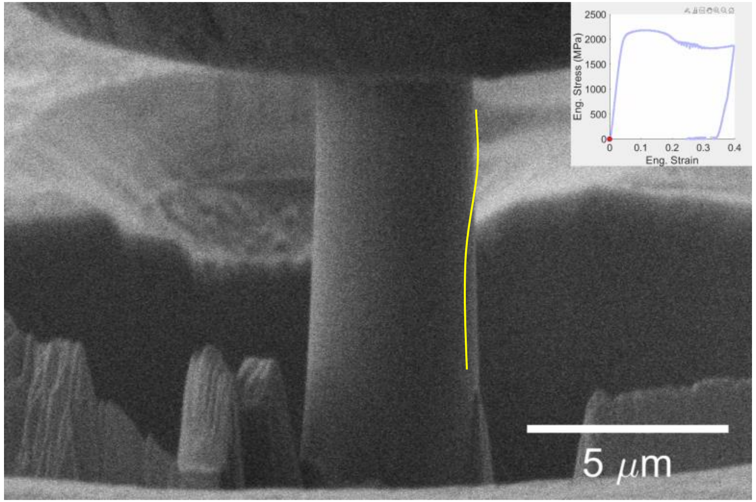


What happens as *h* is reduced with constant *h'*?

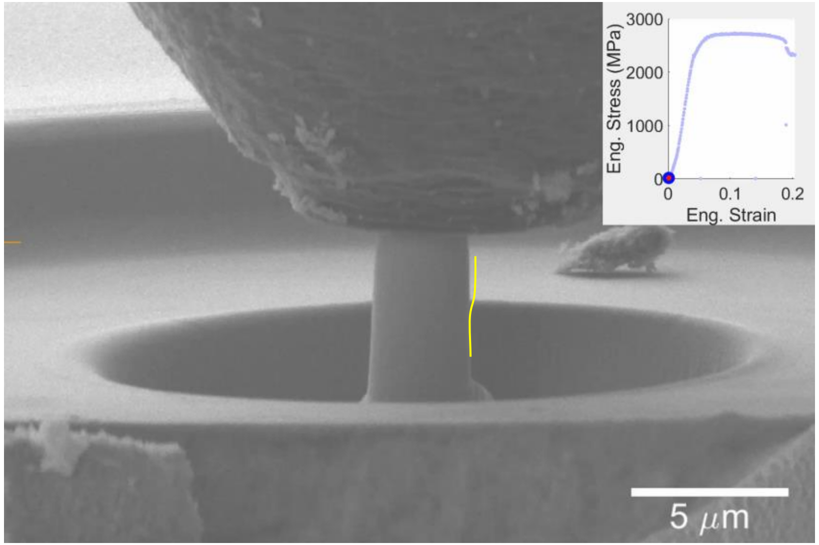
Y. Chen, N. Li, R. Hoagland, X.-Y. Liu, J. K. Baldwin, I. Beyerlein, J. Y. Cheng, N. Mara, Effects of three-dimensional Cu/Nb interfaces on strengthening and shear banding in nanoscale metallic multilayers. *Acta Mater.*

Decrease in *h* with constant *h’* delays onset of shear banding

40-10 Cu/Nb



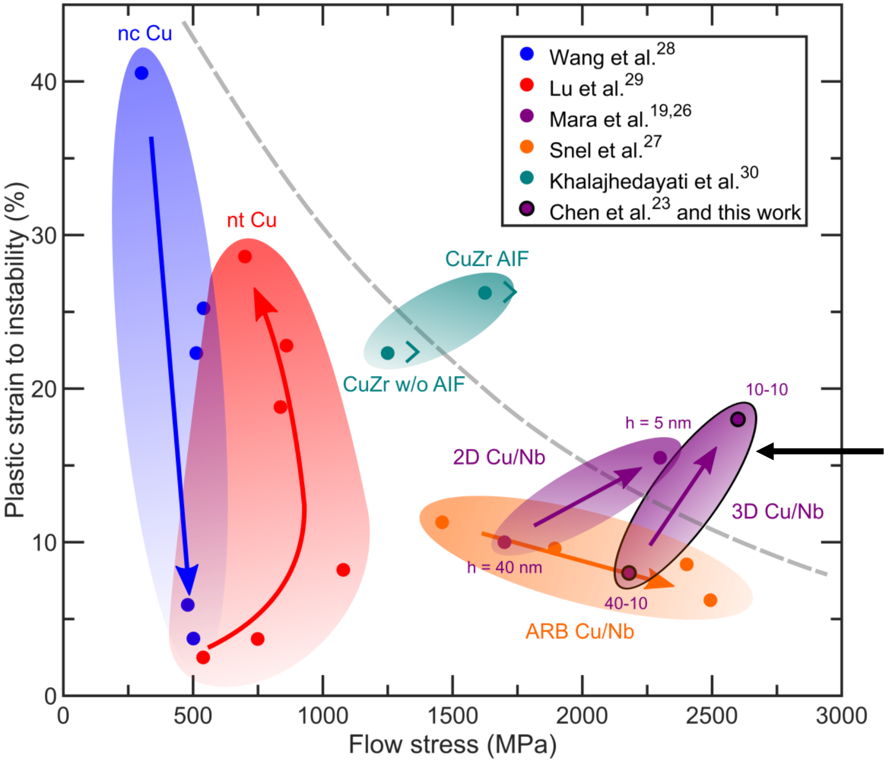
10-10 Cu/Nb



Cheng, J. Y., Xu, S., Chen, Y., Li, Z., Baldwin, J. K., Beyerlein, I. J., & Mara, N. A. (2022). Simultaneous High Strength and Deformable Nanocomposites with Thick Biphase Interfaces (In Press). *Nano Letters*. https://doi.org/10.1021/acs.nanolett.1c04144

Y. Chen, N. Li, R. Hoagland, X.-Y. Liu, J. K. Baldwin, I. Beyerlein, J. Y. Cheng, N. Mara, Effects of three-dimensional Cu/Nb interfaces on strengthening and shear banding in nanoscale metallic multilayers. *Acta Mater.*

Decrease in *h* with constant *h’* simultaneously improves strength and deformability



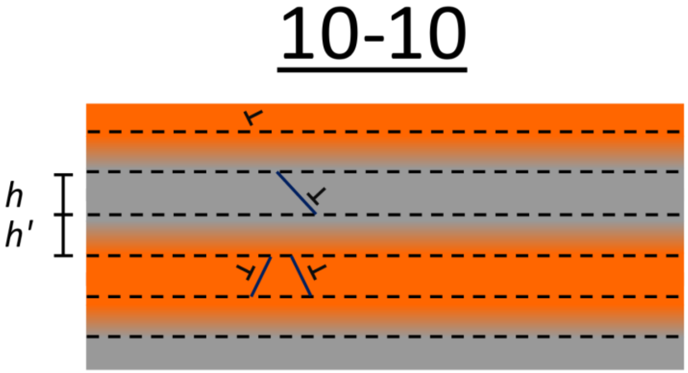
Material	Flow stress (MPa)	Plastic strain to failure (%)
40-10 3D Cu/Nb	2200	8.3
10-10 3D Cu/Nb	2500±70	16±2

10-10 Cu/Nb shows no tradeoff between strength and deformability

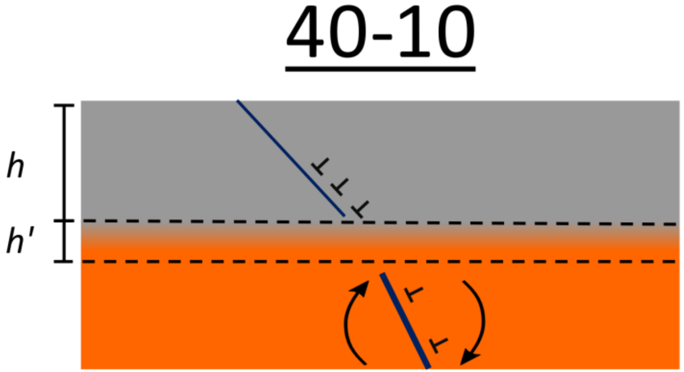
Cheng, J. Y., Xu, S., Chen, Y., Li, Z., Baldwin, J. K., Beyerlein, I. J., & Mara, N. A. (2022). Simultaneous High Strength and Deformable Nanocomposites with Thick Biphase Interfaces (In Press). *Nano Letters*. https://doi.org/10.1021/acs.nanolett.1c04144

Hypothesis: 3D interfaces enhance mechanical properties by discouraging shear banding at low *h’* relative to *h*

Dislocations must overcome 3D interface slip barrier to induce slip transfer and subsequent shear banding



Pileups of limited size relative to 3D interface can’t effectively produce shear banding



Larger pileups can drive slip along common systems across layers to cause shear banding

Test hypothesis with phase field dislocation dislocation dynamics (PFDD)

Y. Chen, N. Li, R. Hoagland, X.-Y. Liu, J. K. Baldwin, I. Beyerlein, J. Y. Cheng, N. Mara, Effects of three-dimensional Cu/Nb interfaces on strengthening and shear banding in nanoscale metallic multilayers. *Acta Mater*

Cheng, J. Y., Xu, S., Chen, Y., Li, Z., Baldwin, J. K., Beyerlein, I. J., & Mara, N. A. (2022). Simultaneous High Strength and Deformable Nanocomposites with Thick Biphase Interfaces (In Press). *Nano Letters*. https://doi.org/10.1021/acs.nanolett.1c04144

PFDD can simulate collective motion of multiple dislocations under quasistatic loading with atomic fidelity

Homogeneous material

Minimize energy function parameterized by applied strain ϵ and order parameter ϕ (indicating degree of slip)

$$\psi(\boldsymbol{\epsilon}, \boldsymbol{\phi}) = \psi_{\text{ela}}(\boldsymbol{\epsilon}, \boldsymbol{\phi}) + \psi_{\text{lat}}(\boldsymbol{\phi}) - \psi_{\text{ext}}(\boldsymbol{\phi})$$

$$\psi_{\text{ela}}(\boldsymbol{\epsilon}, \boldsymbol{\phi}) = \frac{1}{2}[\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^{\text{p}}(\boldsymbol{\phi})] \cdot \boldsymbol{C}[\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^{\text{p}}(\boldsymbol{\phi})]$$

Elastic strain energy

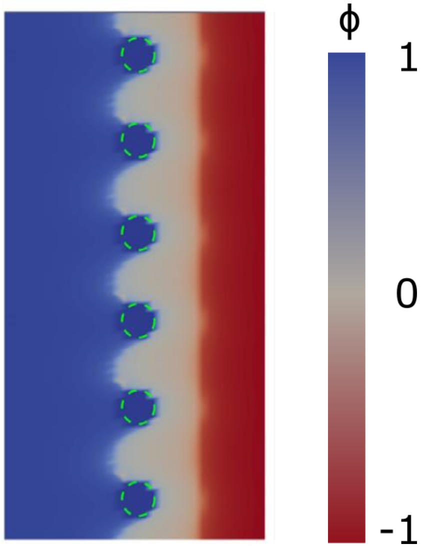
$$\psi_{\text{lat}}(\boldsymbol{\phi}) = \frac{\gamma_{\text{gsf}}(\boldsymbol{\phi})}{l_{\text{gsf}}}$$

Lattice friction, i.e. Peierls barrier given by GSFE curve

$$\psi_{\text{ext}}(\boldsymbol{\phi}) = \boldsymbol{\sigma}_{\text{app}} \cdot \boldsymbol{\epsilon}^{\text{p}}(\boldsymbol{\phi})$$

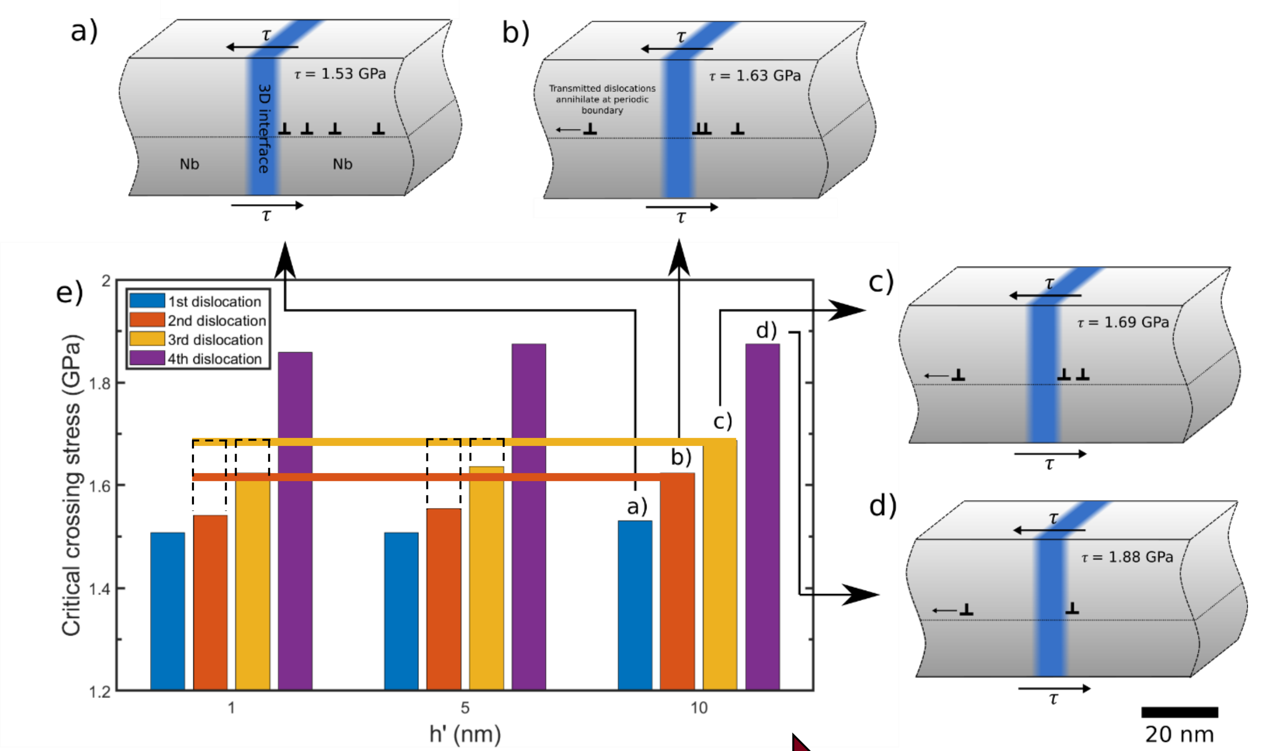
Plastic work expended by material

Extend to include heterogeneities like particles and voids



S. Xu, J.Y. Cheng, Z. Li, N.A. Mara, I.J. Beyerlein, Comput. Methods Appl. Mech. Eng. 389 (2022) 114426.

PFDD simulations show that thick 3D interfaces stifle mechanical advantage dislocation pileups confer to slip transfer

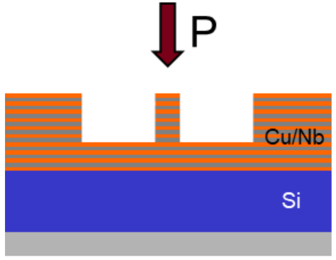


Thicker 3D interface

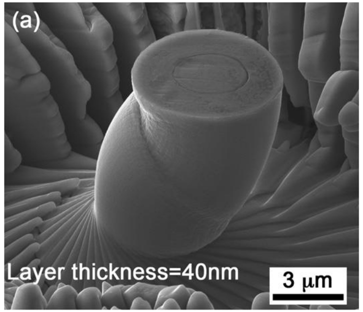
Cheng, J. Y., Xu, S., Chen, Y., Li, Z., Baldwin, J. K., Beyerlein, I. J., & Mara, N. A. (2022). Simultaneous High Strength and Deformable Nanocomposites with Thick Biphase Interfaces (In Press). *Nano Letters*. https://doi.org/10.1021/acs.nanolett.1c04144

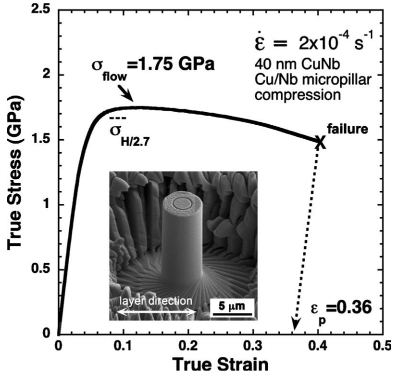
Abrupt interfaces cause early shear localization in multiple loading orientations

Normal compression

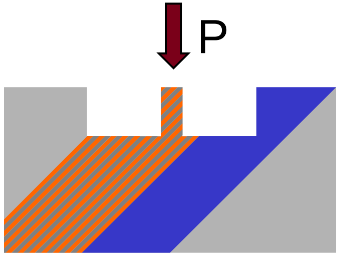


Normal

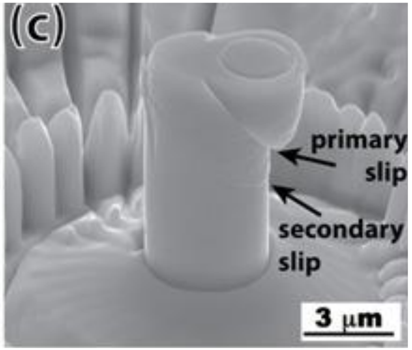


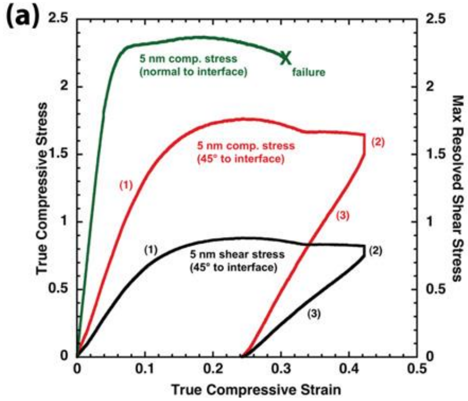


45 degree compression



45 degrees



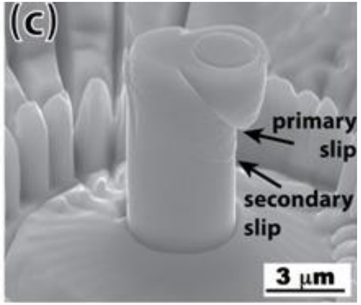


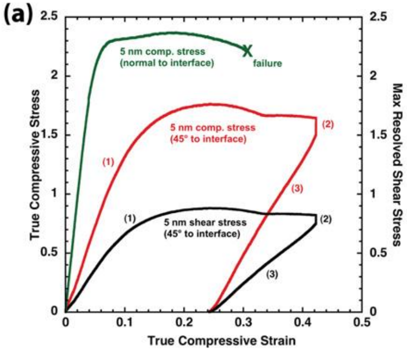
- Interface shear strength measured to be ~0.5 GPa
- Failure precipitated by interface sliding

Mara, N. A., Bhattacharyya, D., Hirth, J. P., Dickerson, P., & Misra, A. (2010). Mechanism for shear banding in nanolayered composites. *Applied Physics Letters*, *97*(2).
Li, N., Mara, N. A., Wang, J., Dickerson, P., Huang, J. Y. & Misra, A. Ex situ and in situ measurements of the shear strength of interfaces in metallic multilayers. *Scr. Mater.* **67**, 479–482 (2012).

3D interfaces enhance deformability in 45º compression

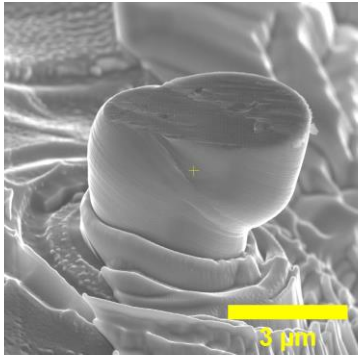
h = 5 nm 2D Cu/Nb

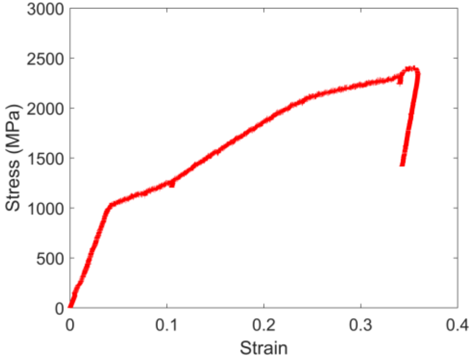




UCS: 1750 MPa
Eng. plastic strain to failure: 11%

10-10 3D Cu/Nb

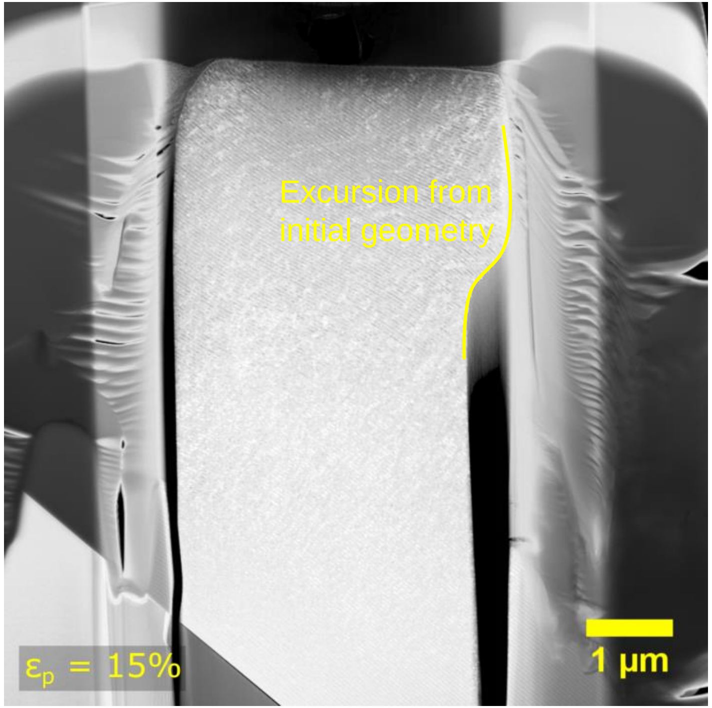


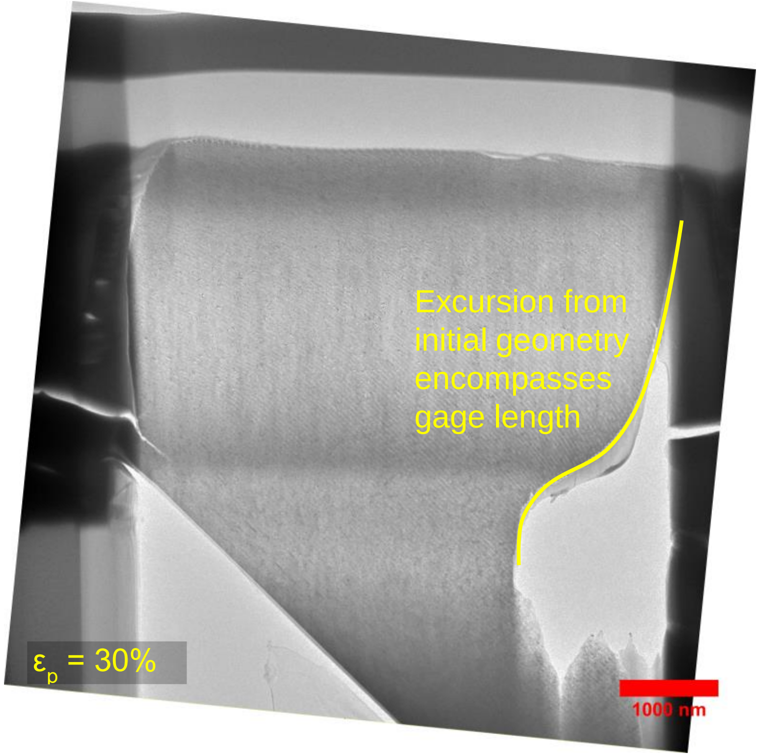


UCS: 2250 MPa
Eng. plastic strain: 30%

Li, N., Mara, N. A., Wang, J., Dickerson, P., Huang, J. Y. & Misra, A. Ex situ and in situ measurements of the shear strength of interfaces in metallic multilayers. *Scr. Mater.* **67**, 479–482 (2012).

No shear instability in 10-10 Cu/Nb 45º compression





Despite gross pillar shape change, no shear instability

Conclusions

1. Thick 3D interfaces produce oustanding mechanical properties in Cu/Nb even at the nanoscale
2. When *h* is low compared to *h’*, shear banding is discouraged
3. 3D interface enhance mechanical behavior in multiple loading orientations

Acknowledgements

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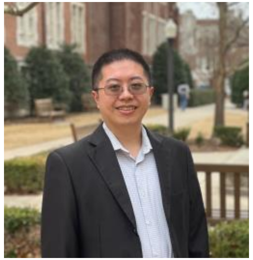
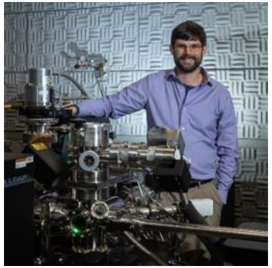


OAK RIDGE
National Laboratory



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