Helium in metal nanocomposites

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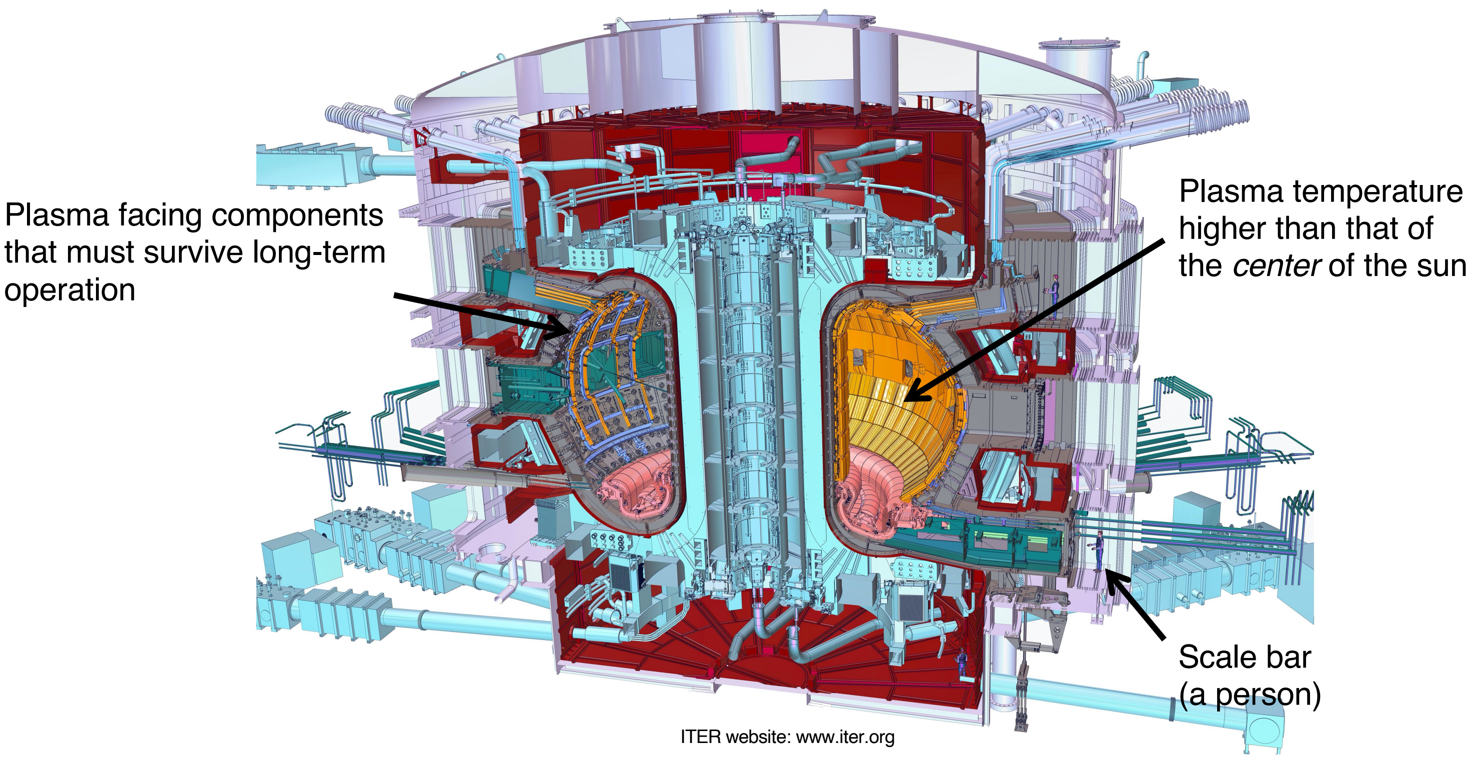
I. D. McCue, S. S. Xiang, K. Xie

Magnetic confinement fusion

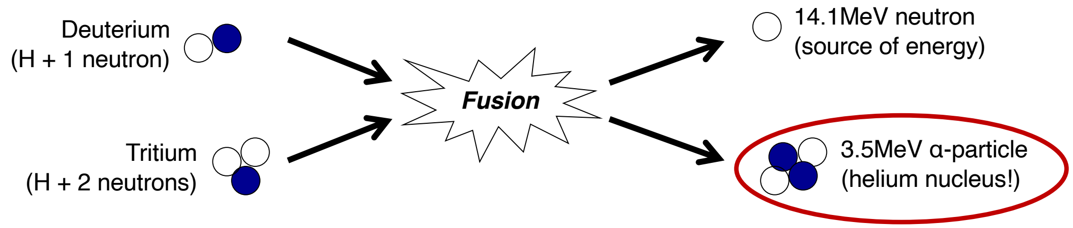
➔clean, ➔safe, ➔plentiful, ➔extremely challenging to realize



ITER website: www.iter.org

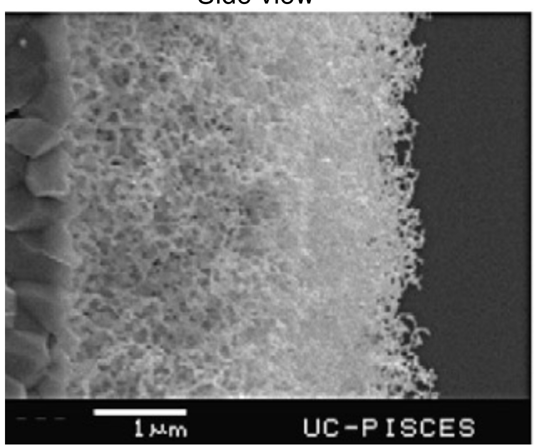
We know how to control the plasma. Now we need the right materials to build a reactor!

He-induced damage



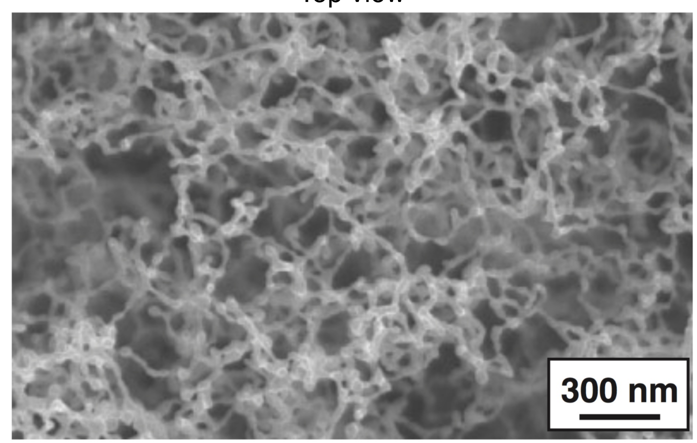
α-particles get implanted into the plasma-facing W wall and turn it into “fuzz"

Side view



M. J. Baldwin and R. P. Doerner, JNM **404**, 165 (2010)

Top view

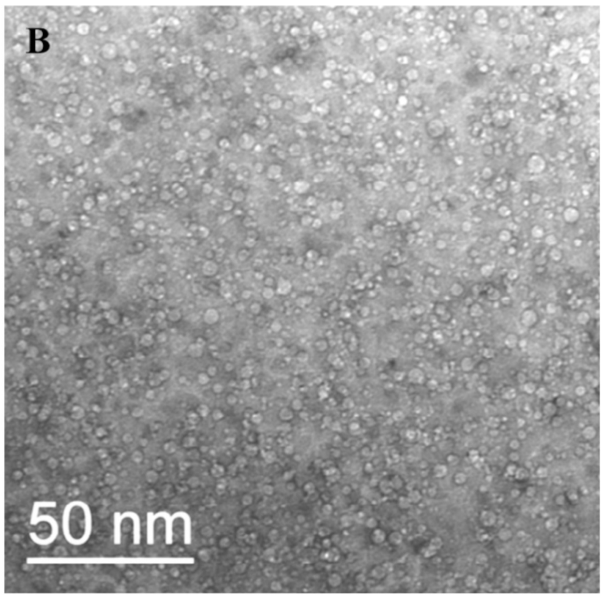


S. Kajita *et al.*, JJAP **50**, 01AH02 (2011)

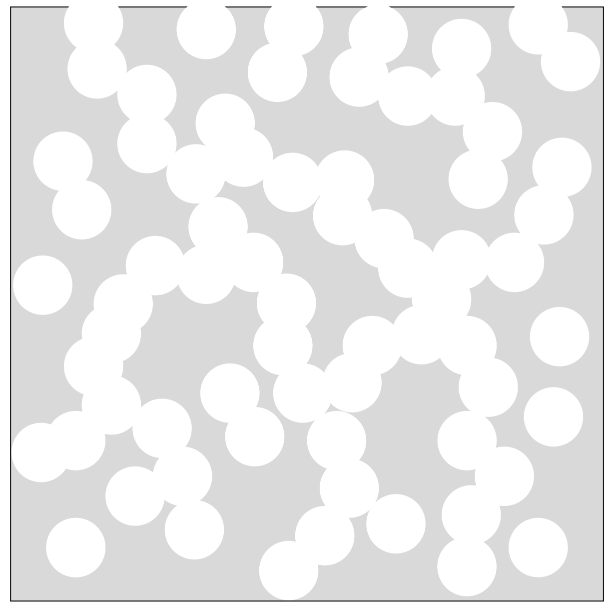
- If W fuzz is deleterious if it leads to greater plasma contamination, reduction in W thermal conductivity, or embrittlement of the first wall
- It can be beneficial if it helps to remove implanted impurities (He and tritium)

He bubbles

Agglomeration of He bubbles into continuous networks the cause of W fuzz formation?



C. D. Judge *et al.*, JNM **457**, 165 (2015)

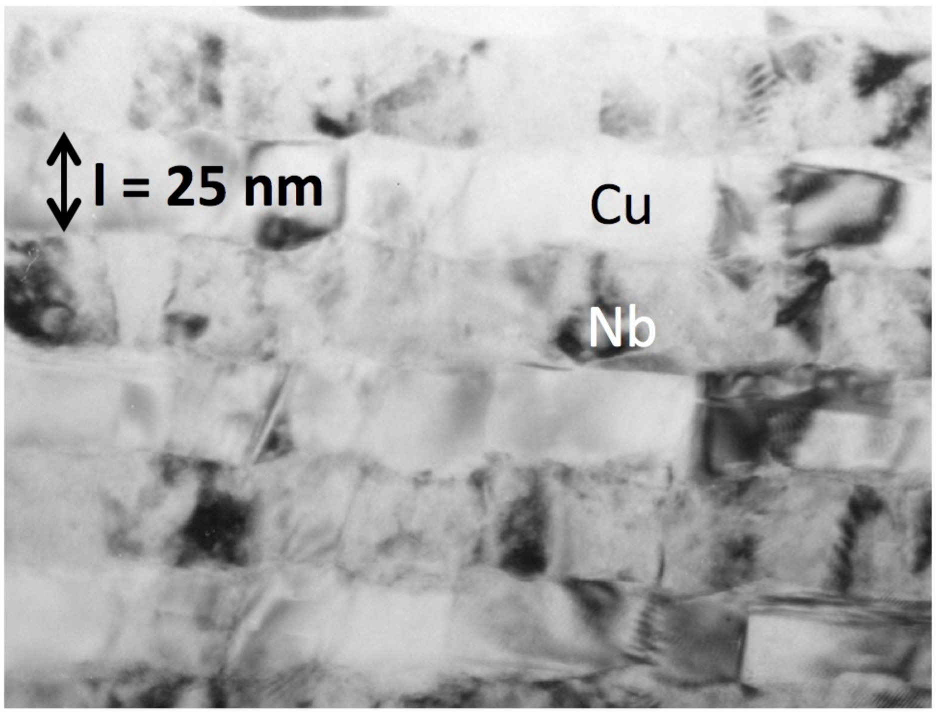


Can we guide the agglomeration of He bubbles into networks that enable impurity outgassing while maintaining mechanical cohesion and thermal conductivity?

Outline

- ***A primer on He research in metal multilayers***
- Self-organization of He bubbles into nano-channels
- Outlook for future applications

Physical vapor deposited metal multilayers



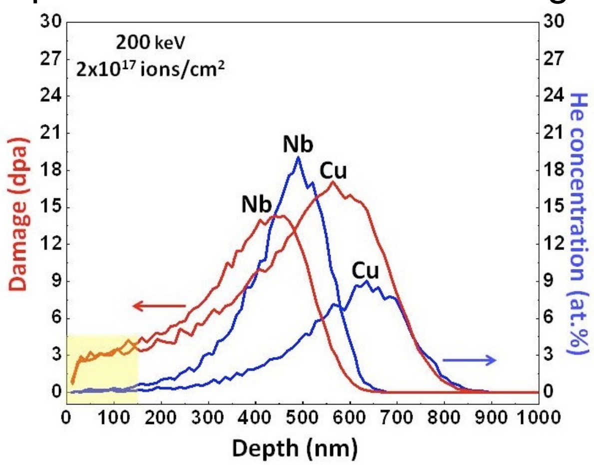
M. J. Demkowicz *et al.*, PRB **84**, 104102 (2014)

- An extremely useful model material for conducting basic research
- Easily synthesized from a wide range of constituents
- Layer thicknesses may be ”dialed in” with nm-level precision
- Highly perfect microstructure: continuous layers with atomically-sharp interfaces

Ion beams

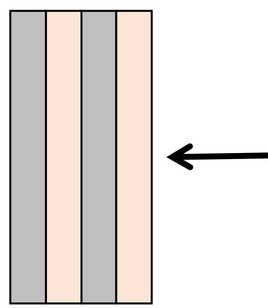
Testing radiation effects without a reactor

Depth profiles of implanted species and ion-induced damage



- Calculate using the SRIM Monte Carlo code
- Measure using techniques such as ERD, NRA, neutron or x-ray reflectometry, etc.

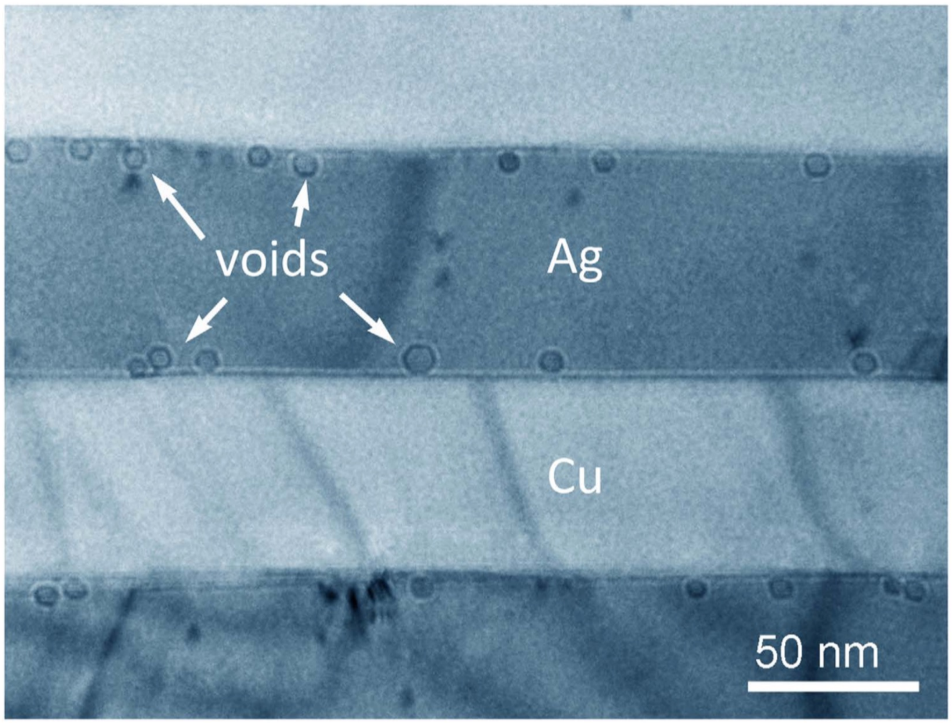
Target



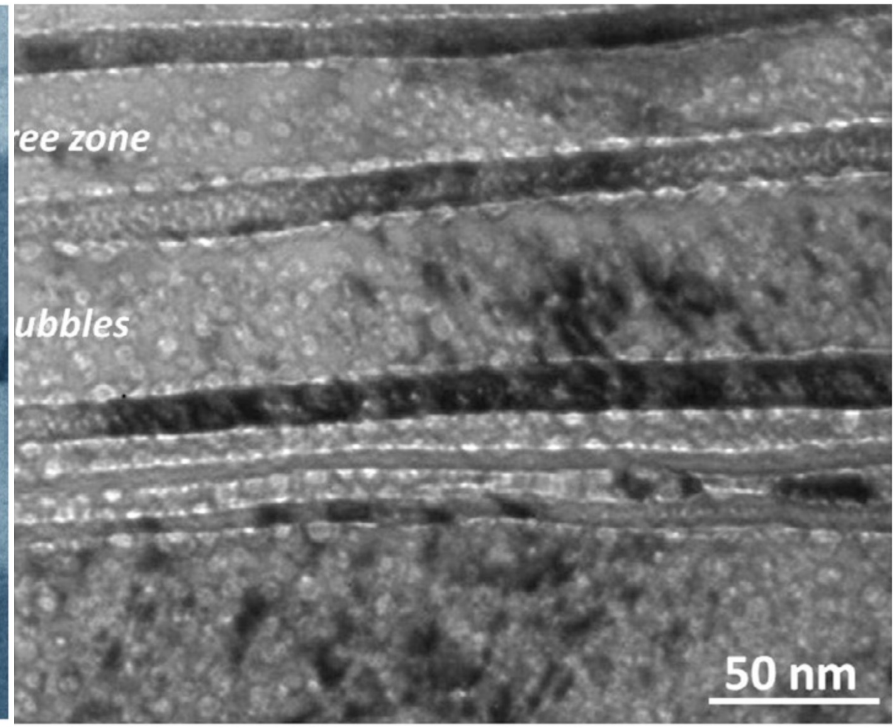
Danfysik ion implanter

- Fast: hundreds of DPA and 10s of % implanted species may be obtained within ~1 day
- A wide range of accessible ion types, charge states, energies, and fluences
- Low penetration depth (not a problem for multilayers!)

He bubble distributions are non-uniform



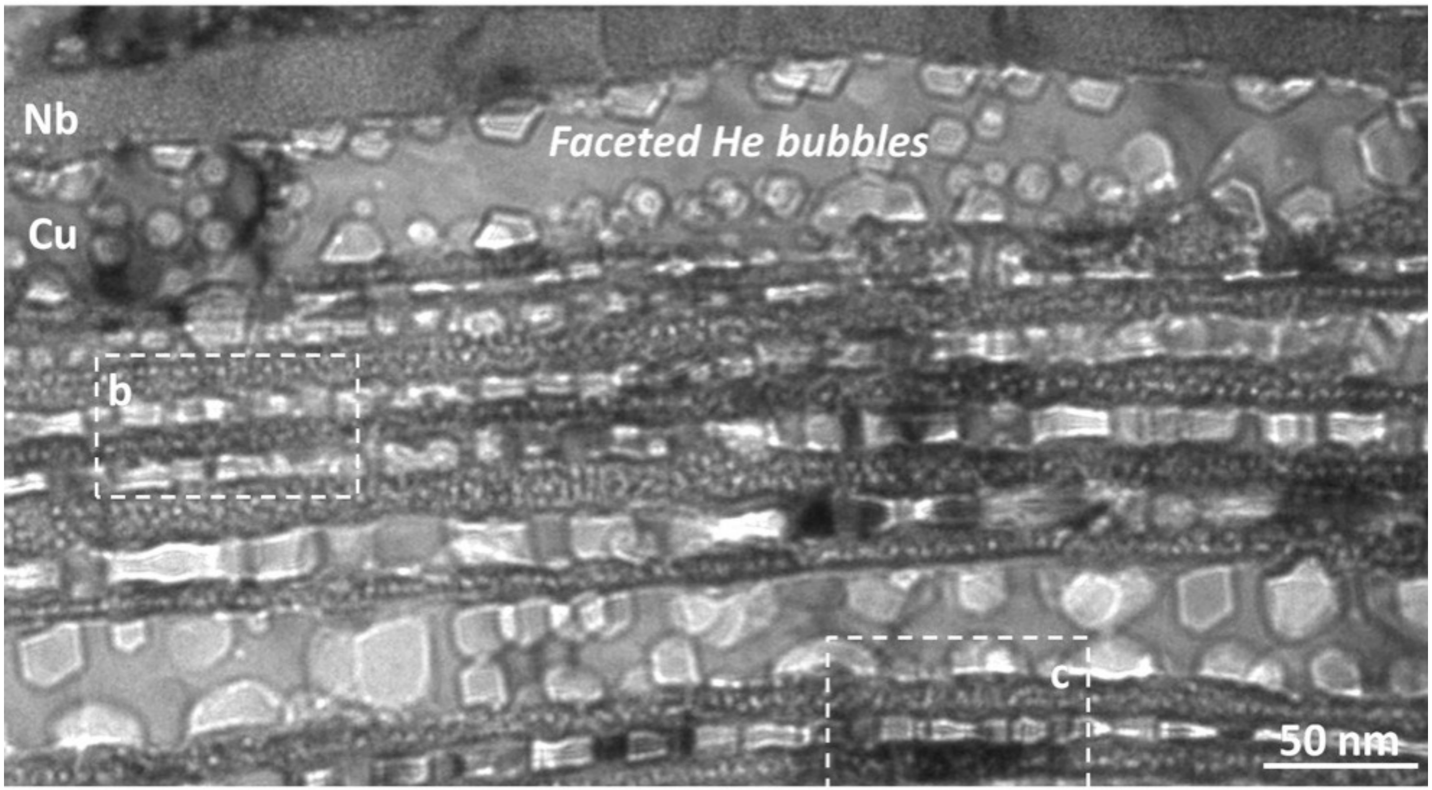
S. Zhang *et al.*, Sci. Rept. **5**, 15428 (2015)



W. Z. Han *et al.*, J. Nucl. Mater. **452**, 57 (2014)

Bubbles (and voids) preferentially grow a) along interfaces and b) into metals with lower vacancy and surface formation energies

Confinement of He precipitates



W. Z. Han *et al.*, J. Nucl. Mater. **452**, 57 (2014)

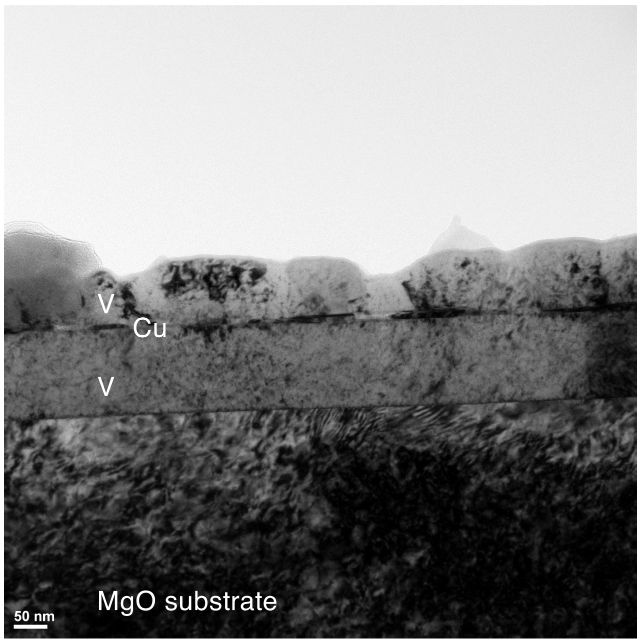
BCC layers confine He precipitates to remain within FCC layers

Outline

- A primer on He research in metal multilayers
- ***Self-organization of He bubbles into nano-channels***
- Outlook for future applications

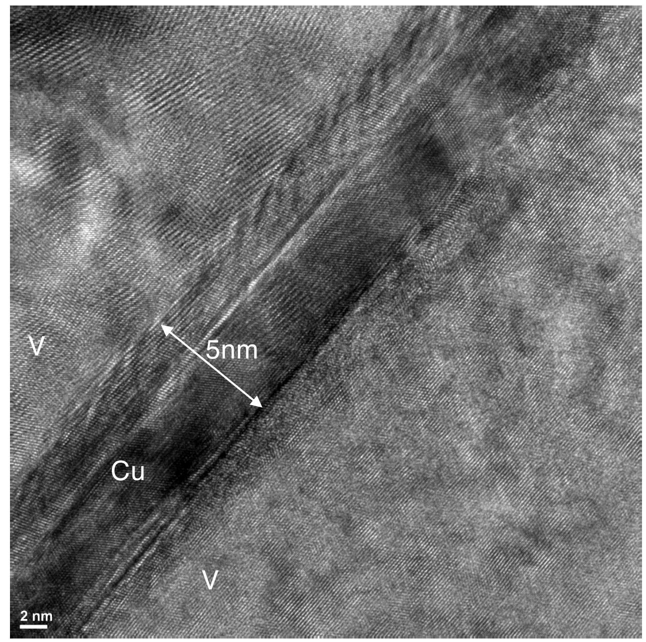
Model material: 5nm Cu layer confined by two adjacent V layers

Edge-on view



As deposited

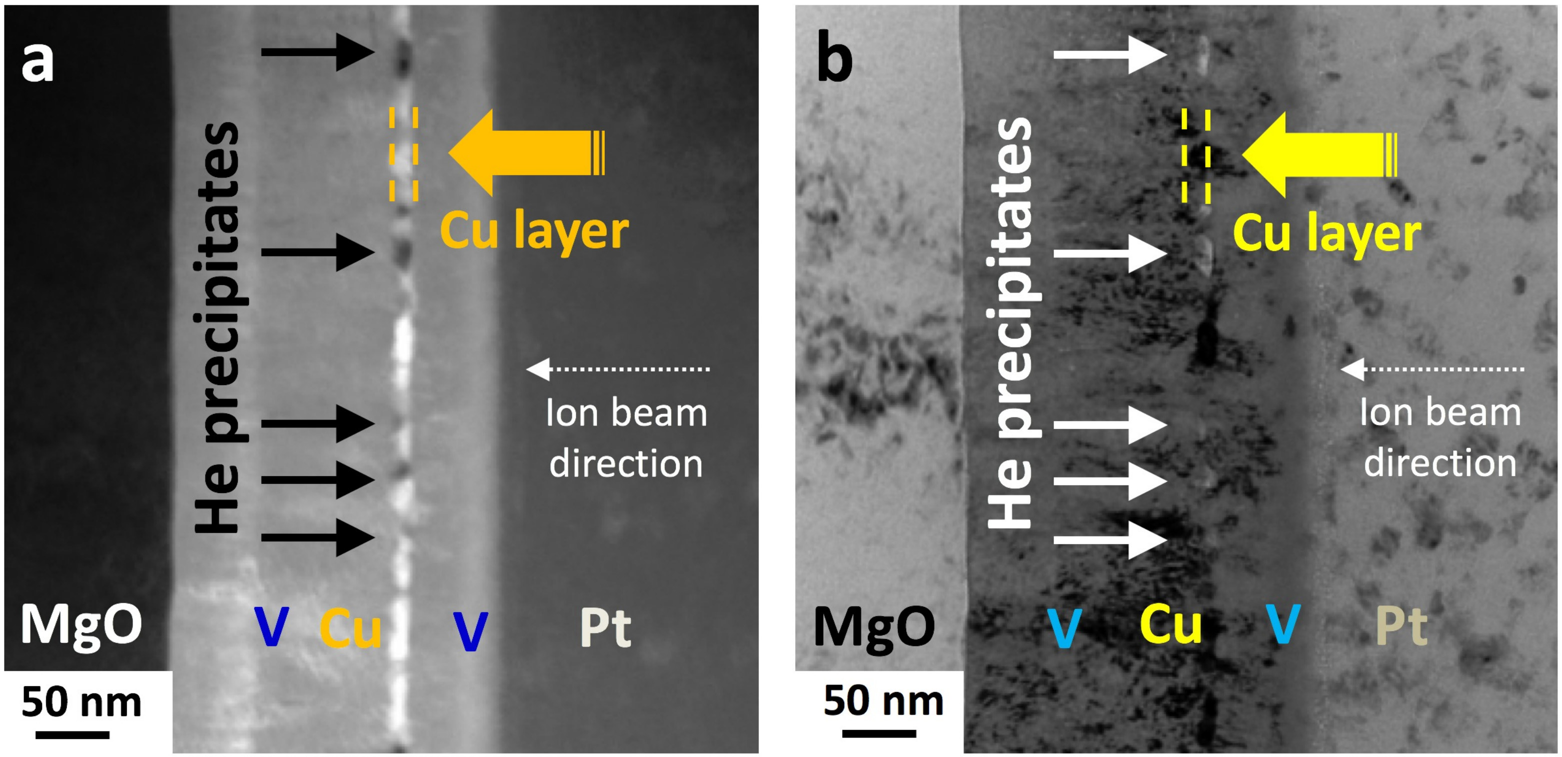
Edge-on view, high resolution



As deposited

Sample is designed to enable plan-view imaging of He precipitates

Preferential He bubble growth in the Cu layer



Dark field STEM

20 keV He^+,10^{16} ions/cm^2
Edge-on view

Bright field TEM

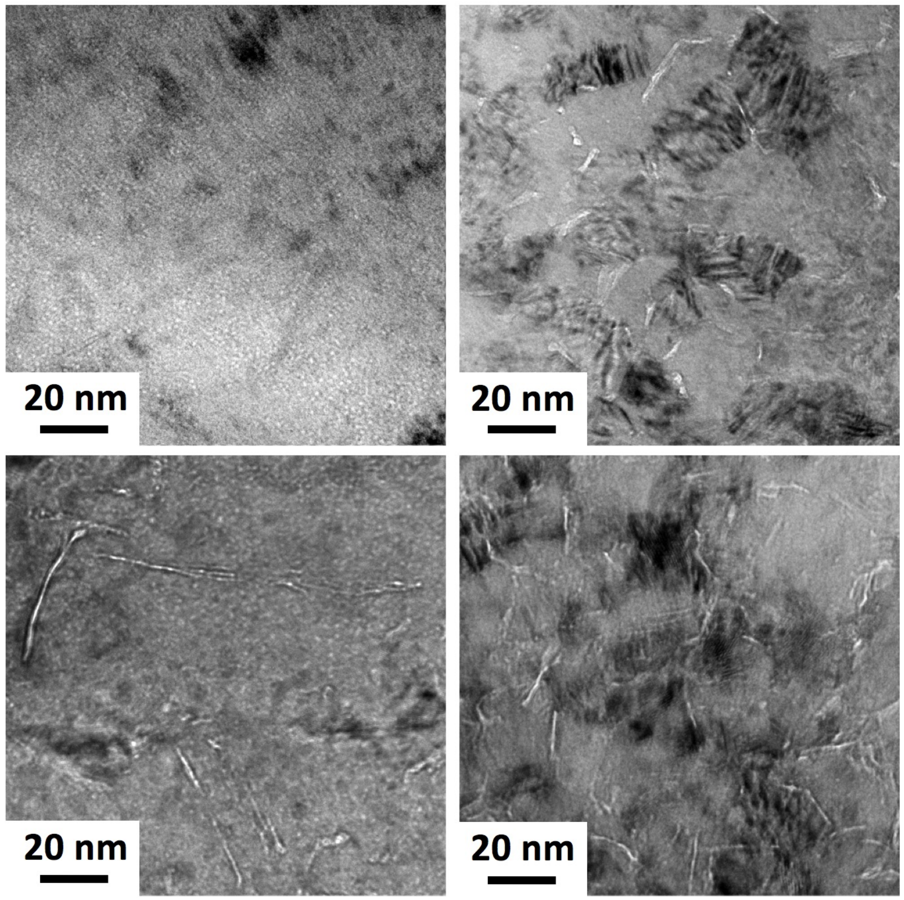
Formation of elongated He "channels"

10^{15} ions/cm^2

$3 \cdot 10^{15}$ ions/cm^2

$5 \cdot 10^{15}$ ions/cm^2

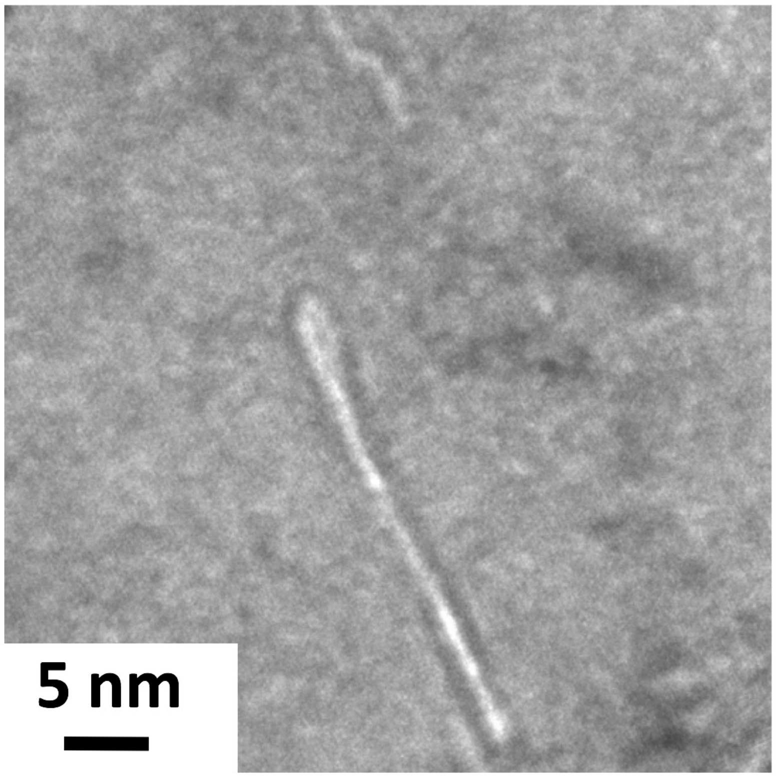
10^{16} ions/cm^2



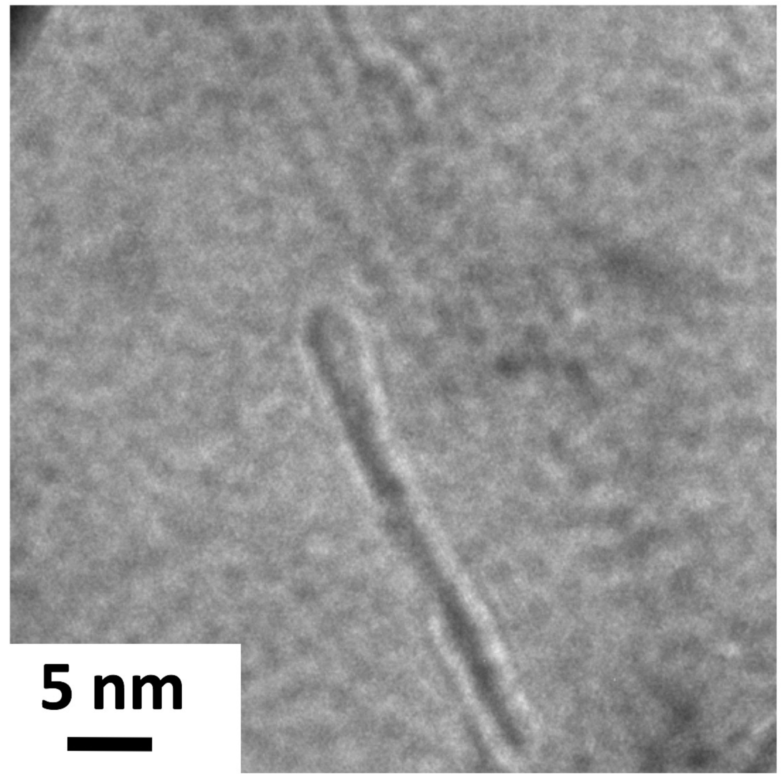
All images are taken in "plan" view, i.e. looking perpendicular to the Cu layer

D. Chen *et al.*, Science Advances **3**, eaao2710 (2017)

The channels really are He precipitates

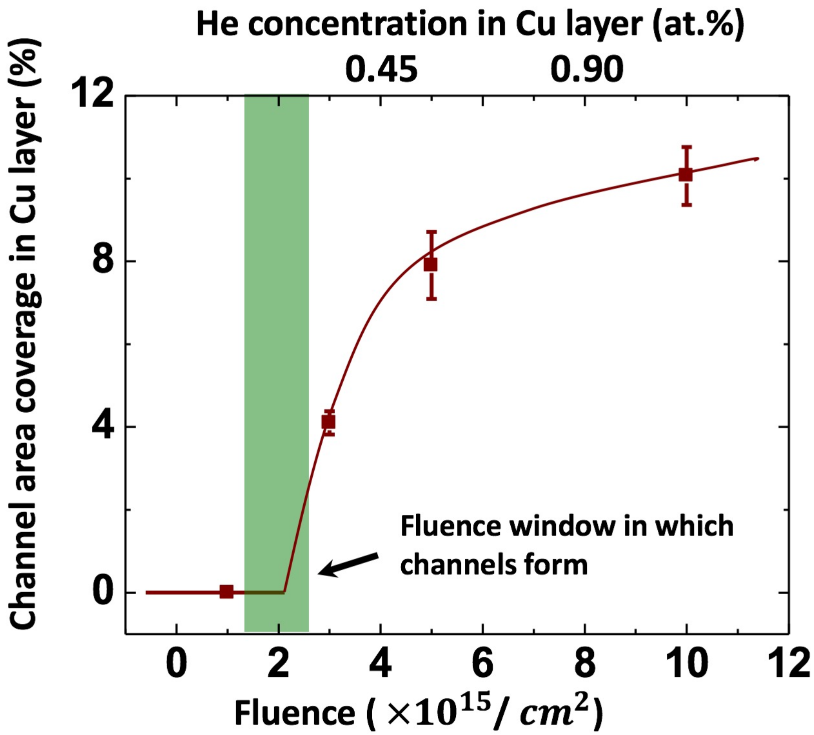


400 nm under-focus

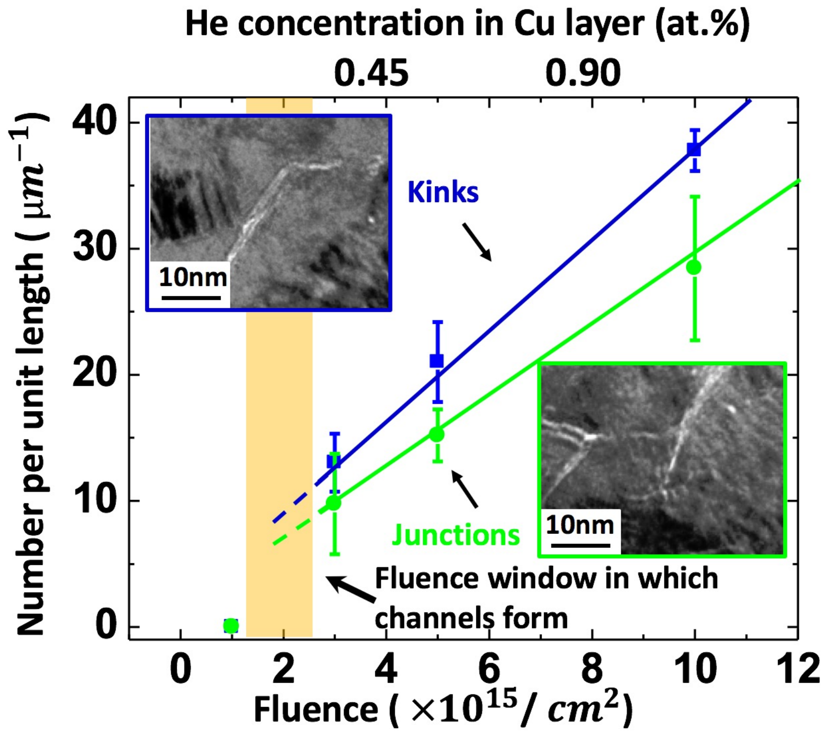


400 nm over-focus

The connectivity of He channels increases with fluence



Asymptotic convergence with increasing fluence to ~12%: bond percolation threshold in 2-D?

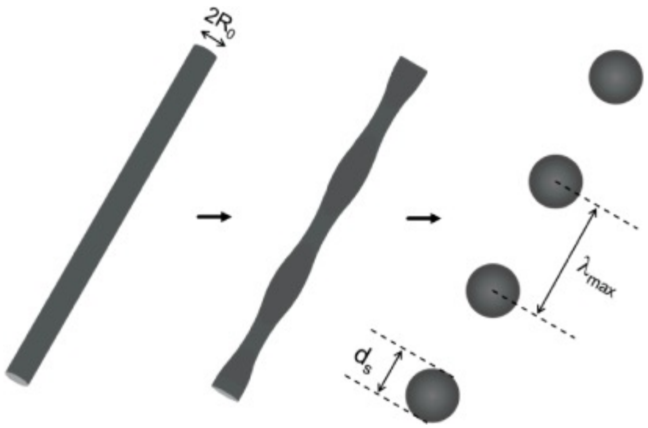


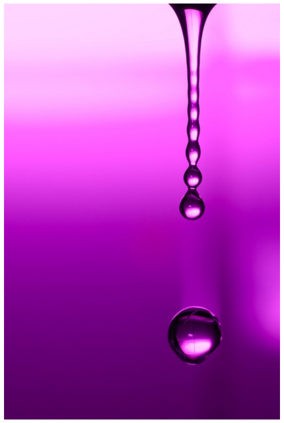
Increasing interconnectivity of ligaments leads to the formation of a "vascular network"?

Does He outgassing in multilayers occur through a vascular network of nanochannels?

Confinement by adjacent V layers stabilizes He nanochannels

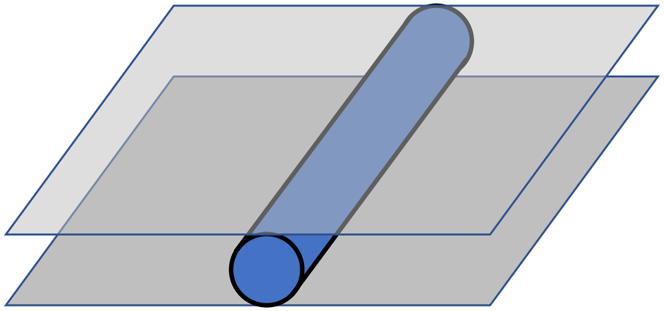
Unconfined cylinders decompose into spheres by the Plateau-Rayleigh (P-R) instability





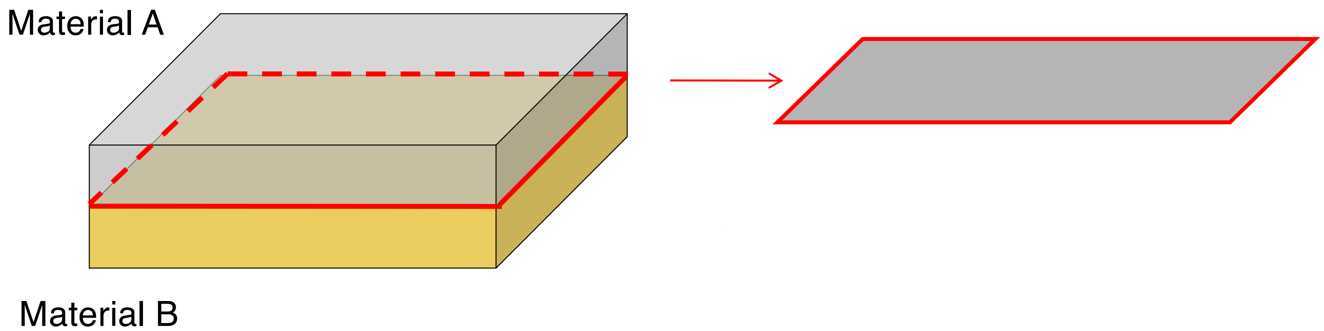
Decomposition is spontaneous because it has no energy barrier

Cylinders pinched between two layers do not undergo the P-R instability



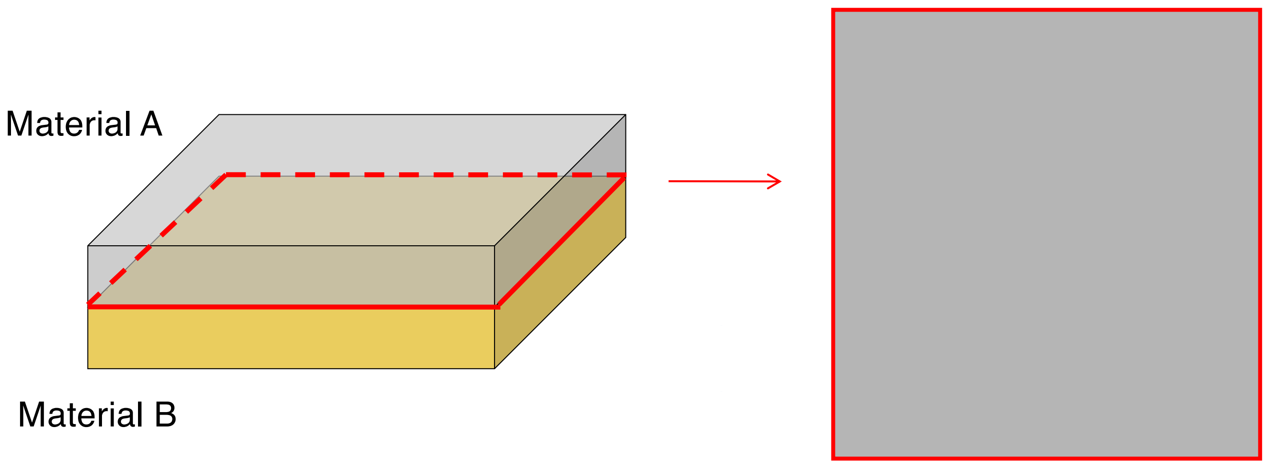
Even through there are lower energy shapes, decomposition is prevented by an energy barrier

Preferential precipitation at specific locations within interfaces



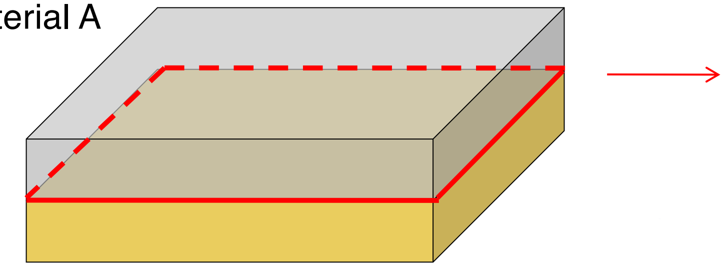
A solid state interface forms
between layers of Material A
and Material B

Preferential precipitation at specific locations within interfaces

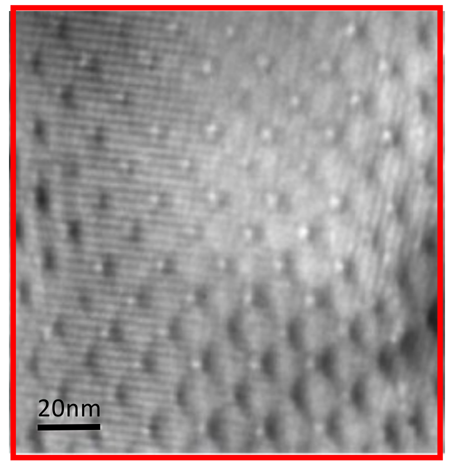


A solid state interface forms between layers of Material A and Material B

Preferential precipitation at specific locations within interfaces



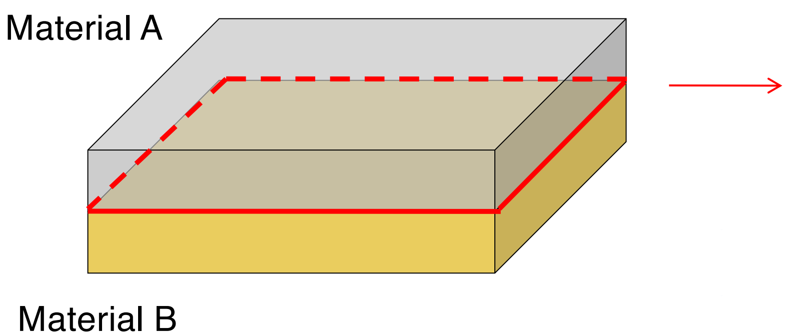
A solid state interface forms between layers of Material A and Material B



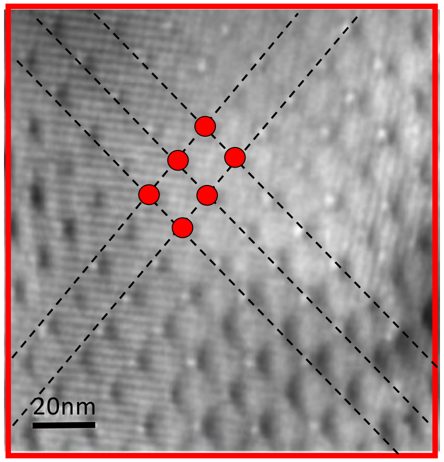
Z. F. Di *et al.*, PRB **84**, 052101 (2011)

Plane view of Au bicrystral

Preferential precipitation at specific locations within interfaces



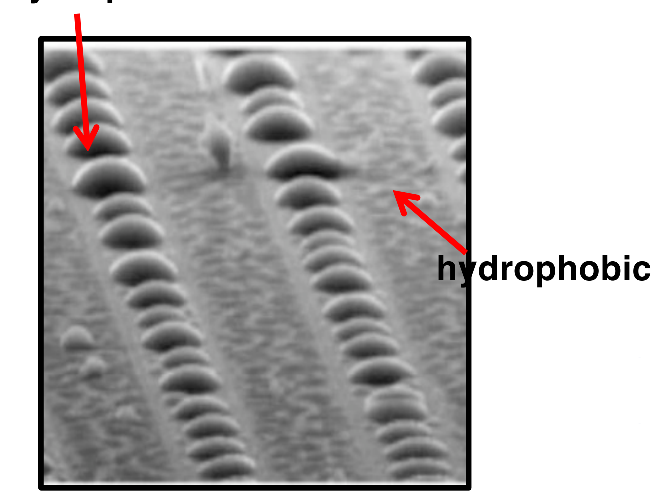
A solid state interface forms between layers of Material A and Material B



Z. F. Di *et al.*, PRB **84**, 052101 (2011)

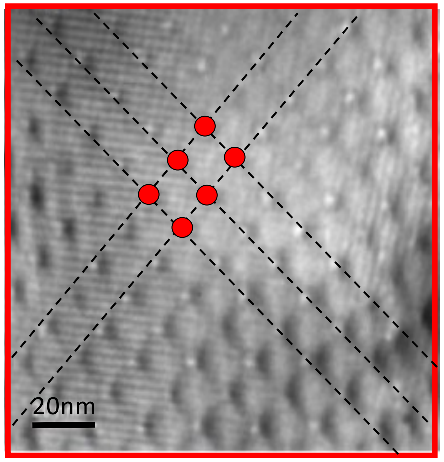
Plane view of Au bicrystral: He precipitates at MDIs

Preferential precipitation at specific locations within interfaces



K. K. Varanasi *et al.*, APL **95**, 094101 (2009)

Precipitation of water on surface



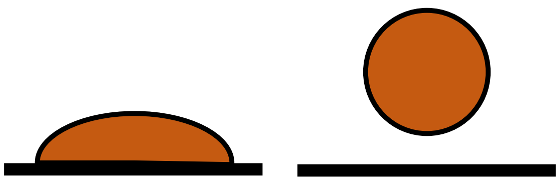
Z. F. Di *et al.*, PRB **84**, 052101 (2011)

Plane view of Au bicrystral: He precipitates at MDIs

Wetting at misfit dislocation intersections in Cu-Nb interfaces

Wetting Coefficient:

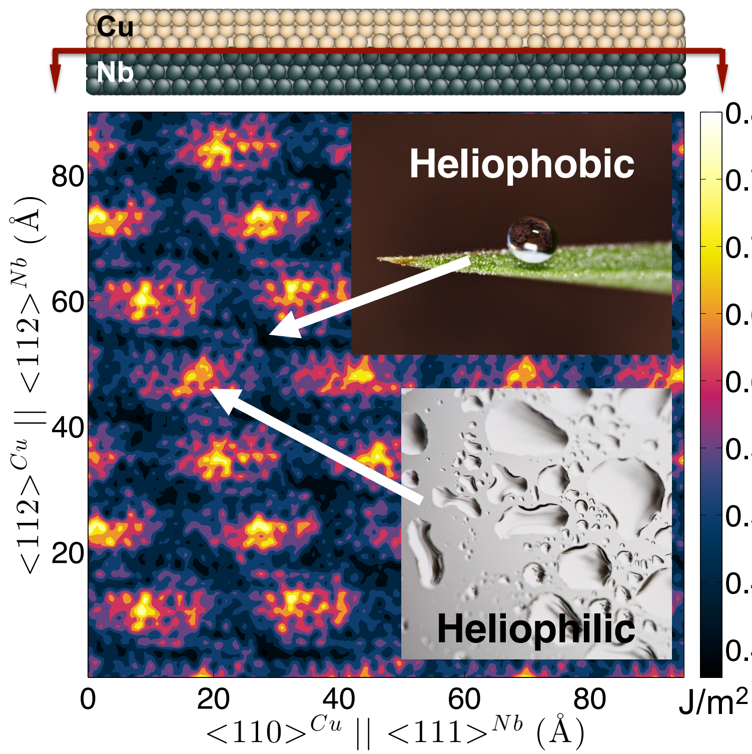
$$W = \gamma_{Cu\text{-}Nb} + \gamma_{He\text{-}Cu} - \gamma_{He\text{-}Nb}$$



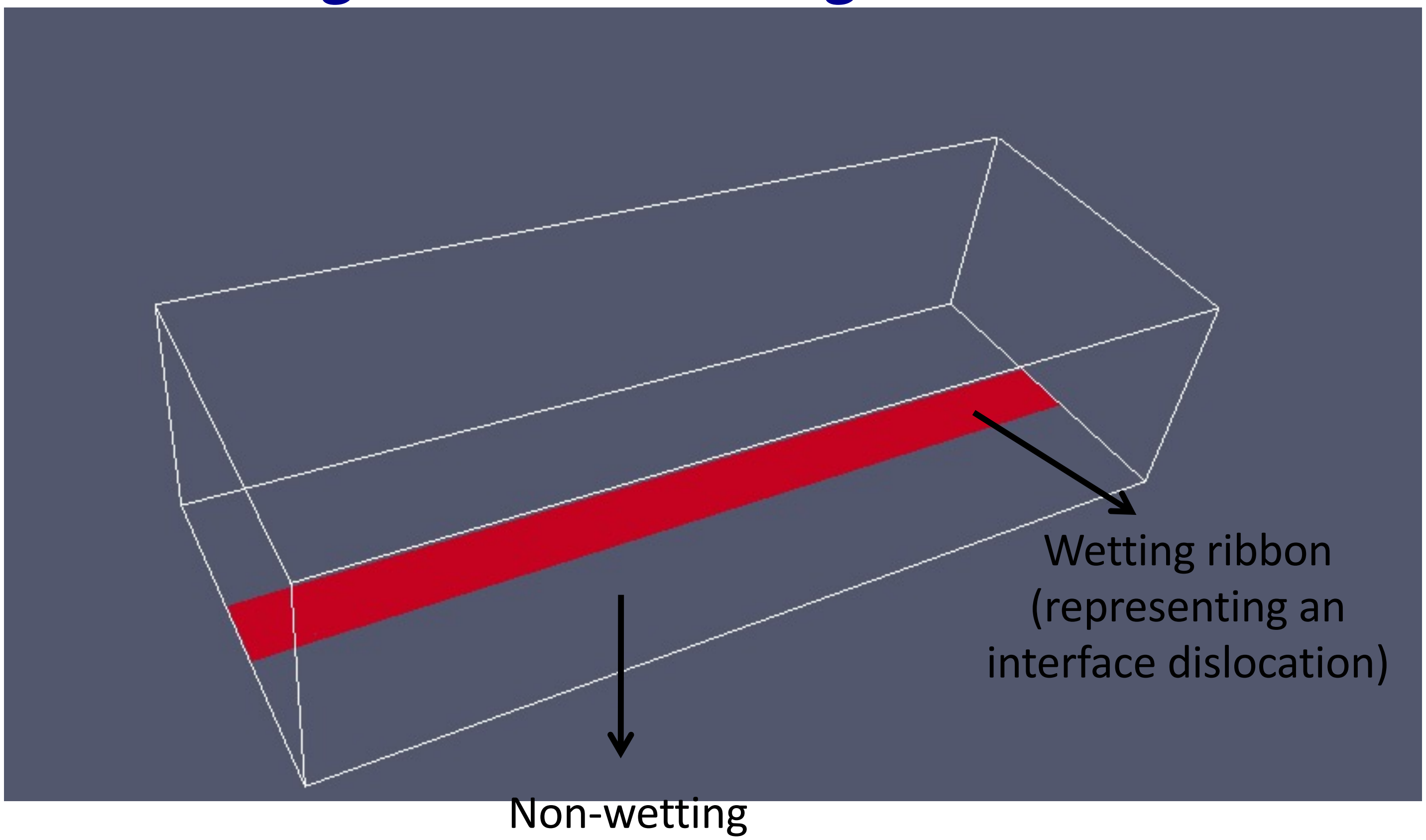
Wetting $W > 0$

Non-wetting $W < 0$

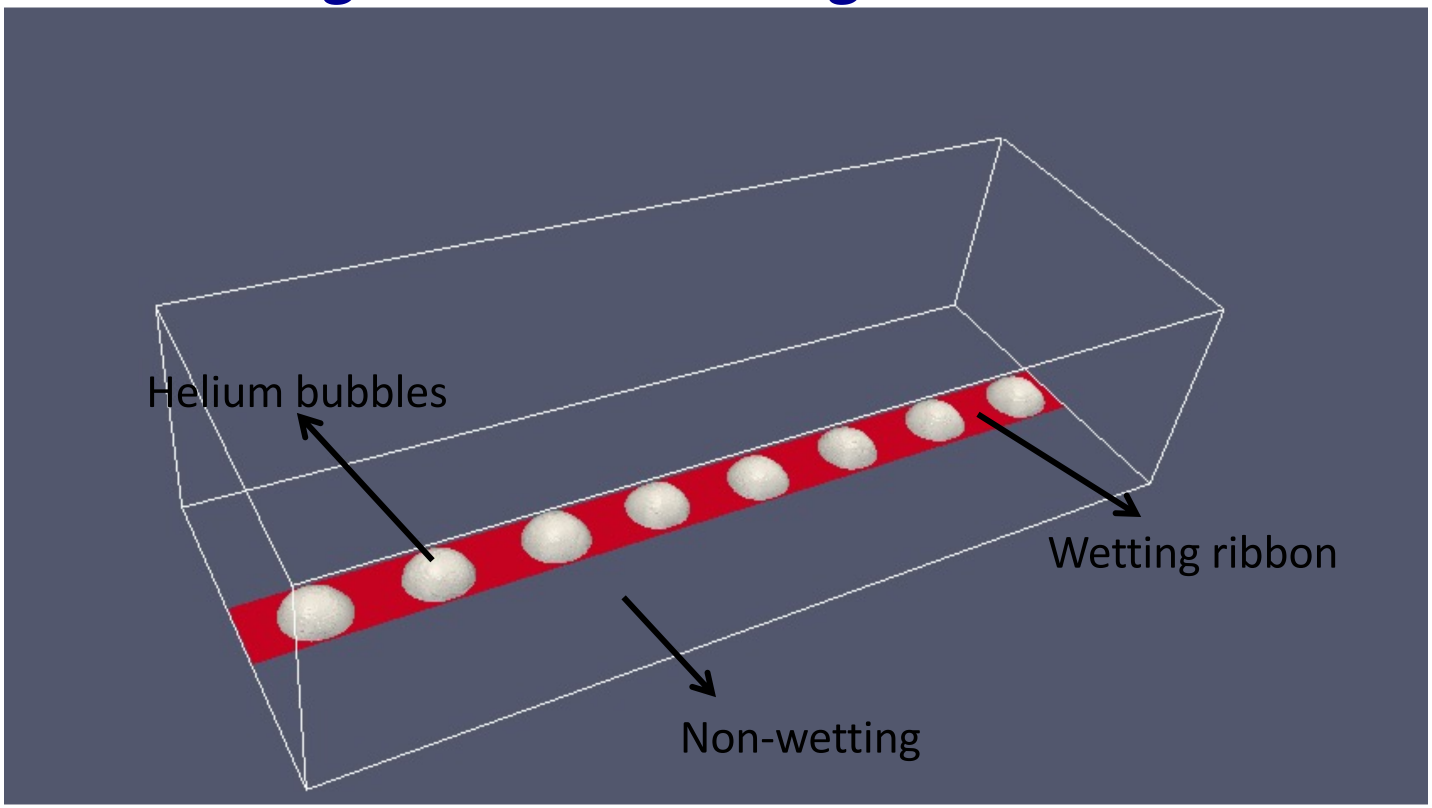
	Interface Energy (J/m²)
$\gamma_{He\text{-}Cu}$	1.93
$\gamma_{He\text{-}Nb}$	2.40
$\gamma_{Cu\text{-}Nb}$	Depends on location in the interface plane



Bubble growth on wetting ribbons

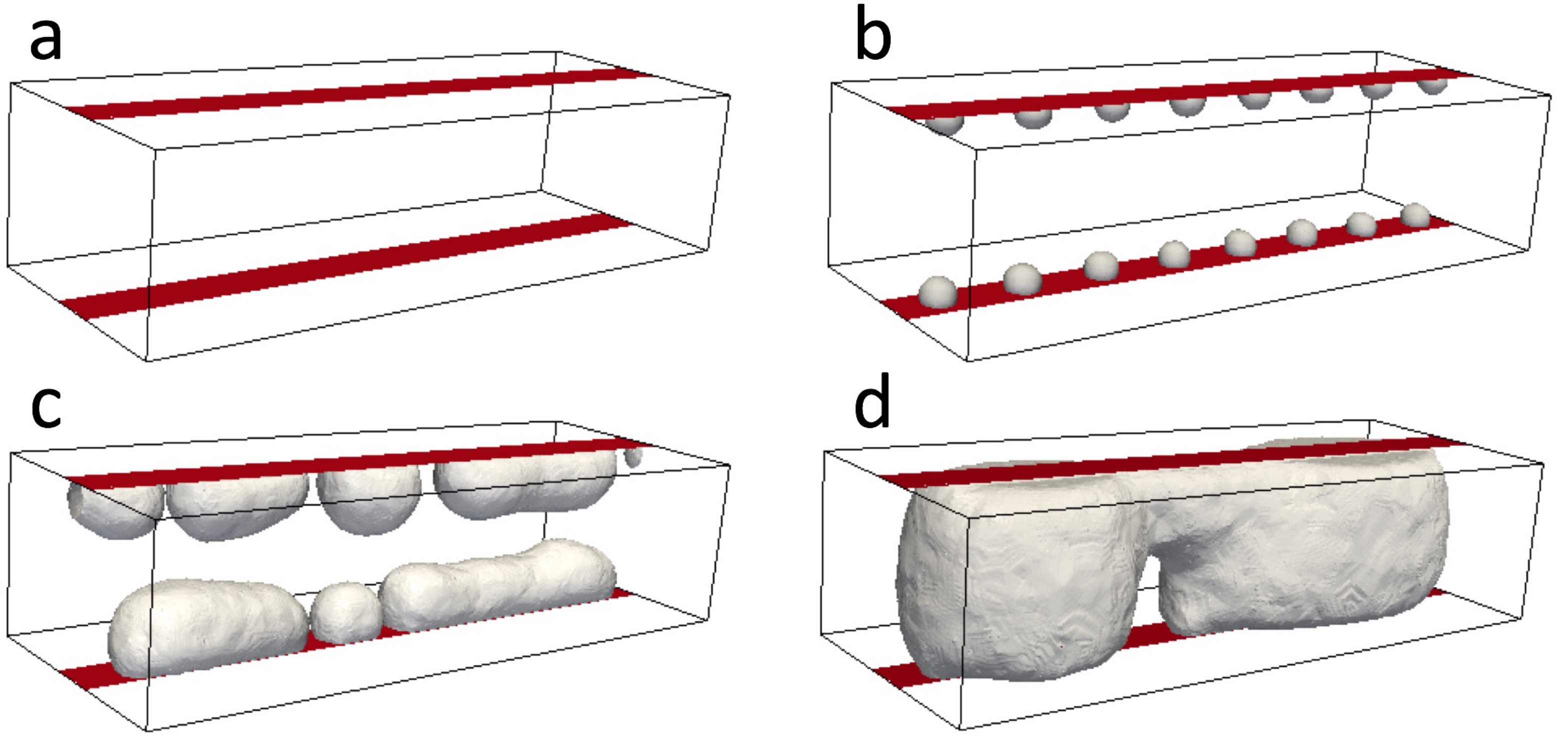


Bubble growth on wetting ribbons



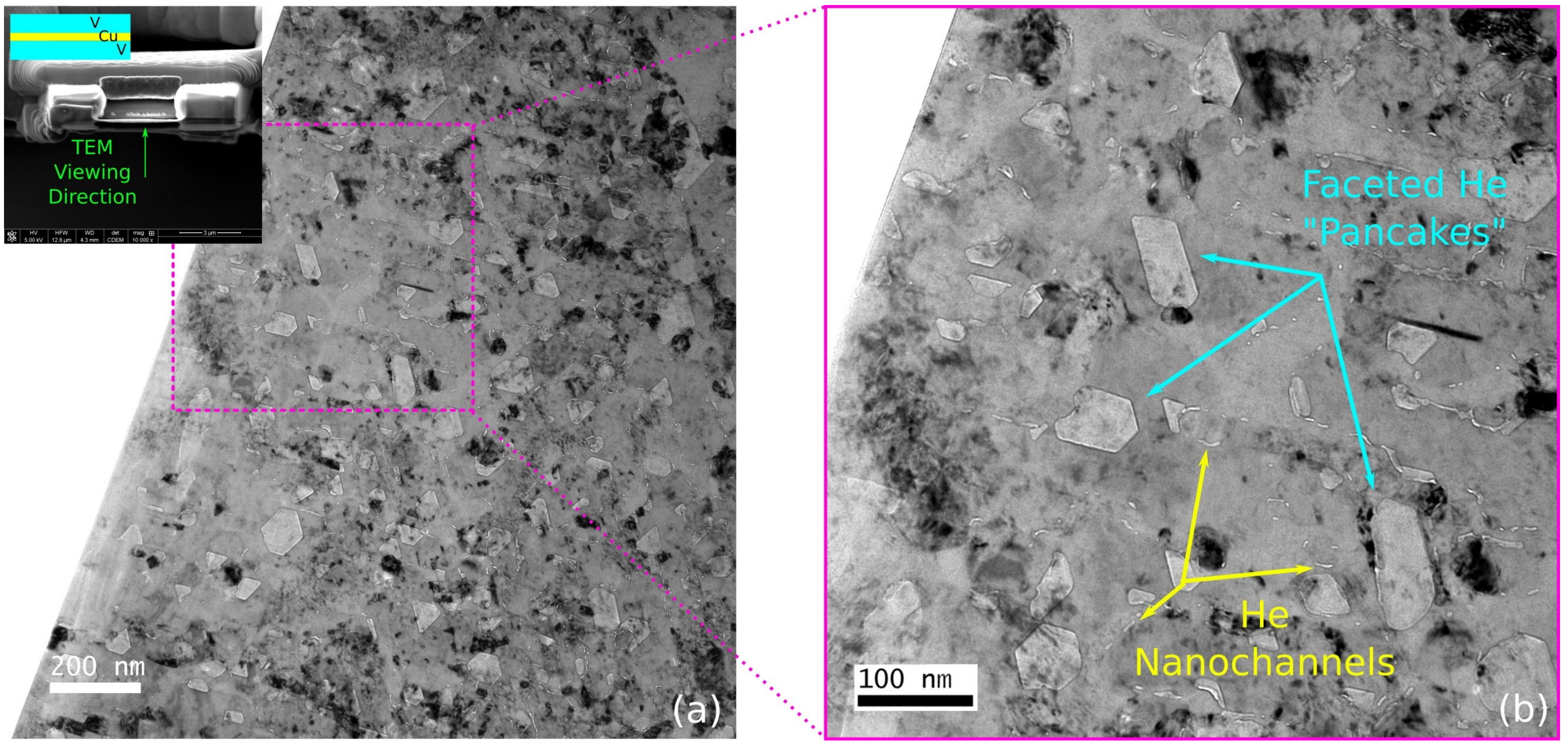
Wetting ribbons are templates that guide He precipitates to coalesce into elongated channels as they grow

Bubble growth on wetting ribbons



Similar sequences of coalescence into elongated channels occur for a wide range of wetting angles and wettable region configurations (ribbons, patches, etc.)

Conversion of channels into "pancakes"



B. K. Derby *et al.*, JOM **72**, 145 (2020)

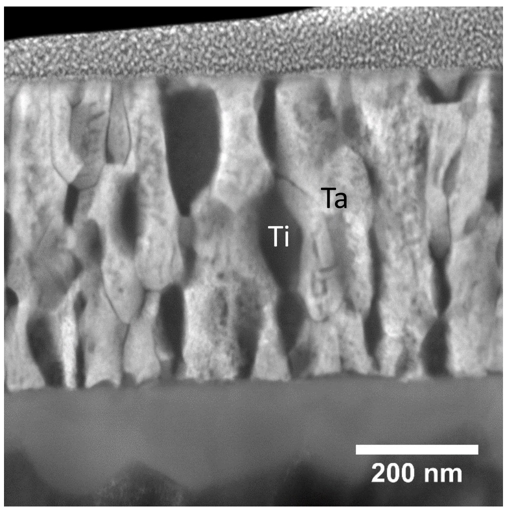
This change is driven by reduction in surface area per unit volume of the He-filled cavities

Outline

- A primer on He research in metal multilayers
- Self-organization of He bubbles into nano-channels
- ***Outlook for future applications***

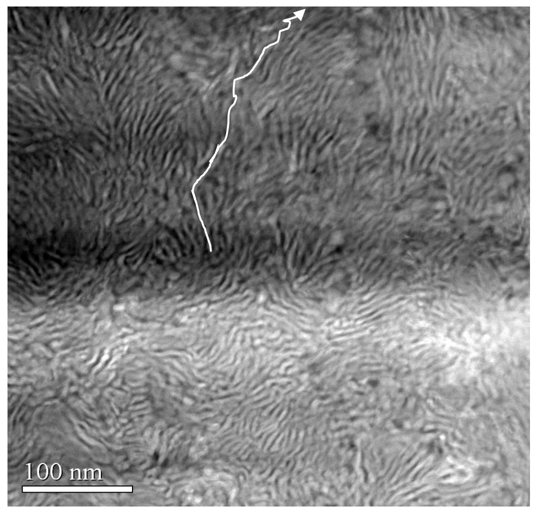
He outgassing through self-organized "vascular" networks in bicontinuous nanocomposites?

Phase-separated Ta/Ti



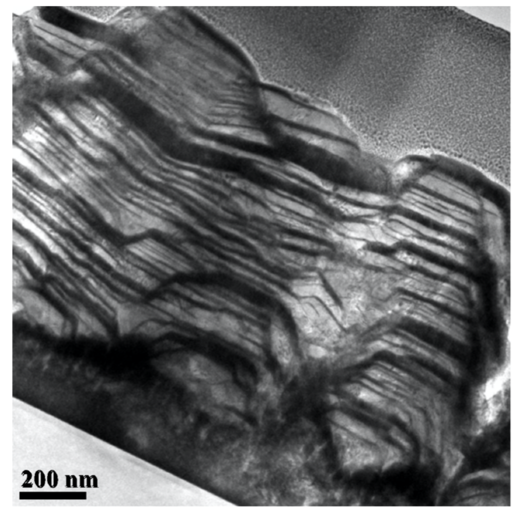
S. Xiang *et al.*, Phil. Mag. Lett. **100**, 307 (2020)

Spinodally-decomposed Cu/Mo



B. K. Derby *et al.*, Scripta Mater. **177**, 229 (2020)

Self-assembled Cu/W "multilayers"



D. Yadav *et al.*, Scripta Mater. **194**, 113677 (2021)

We are exploring multiple composite types and finding a clear effect of microstructure morphology on He precipitate shapes and He retention

Conclusions

- We have demonstrated that He bubbles confined within a thin metal layer form elongated channels, which later transform into "pancakes"

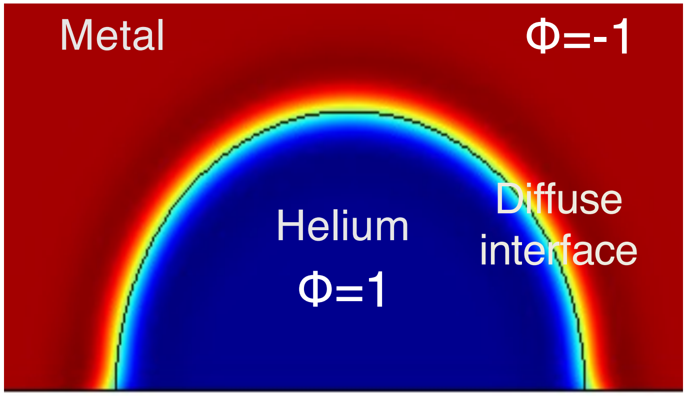
- Critical factors for the formation of these unusual shapes are
  - Confinement to a thin layer (prevents the Plateau-Rayleigh instability)
  - Coalescence guided by a precipitation "template" provided by the location-dependent internal structure of the interfaces bounding the layer
  - Coarsening over time driven by the reduction in surface area

- Channels may interconnect into "vascular" networks through which He may outgas without damaging the surface => opportunity for designing novel, He damage-resistant composite materials

The phase field method

Cahn-Hilliard Equation:

$$\frac{\partial \phi}{\partial t} = \nabla \cdot M \nabla \frac{\partial F}{\partial \phi}$$

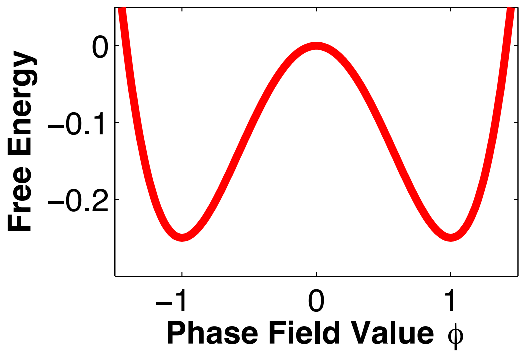


Defining the free energy:

$$F = \int_V \left[f(\phi) + \frac{\varepsilon}{2} |\nabla \phi|^2 \right]$$

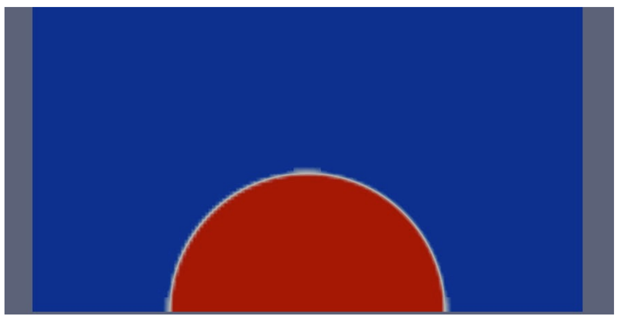
Bulk energy

Gradient energy



Modeling wetting and non-wetting behavior

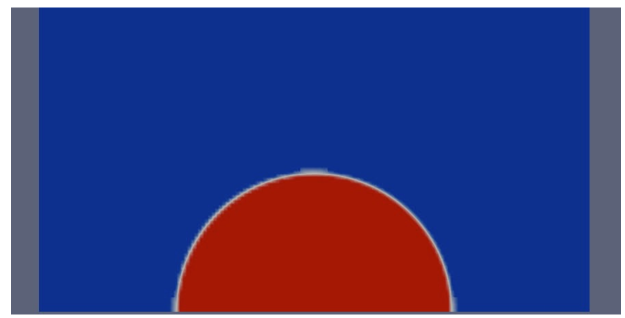
Non-wetting regions



$$\phi = -1$$

$$\hat{n} \bullet \nabla j = \cos(q) \left| \nabla j \right|$$

Wetting regions



$$\hat{n} \cdot \nabla \phi = cos(\theta) |\nabla \phi|$$