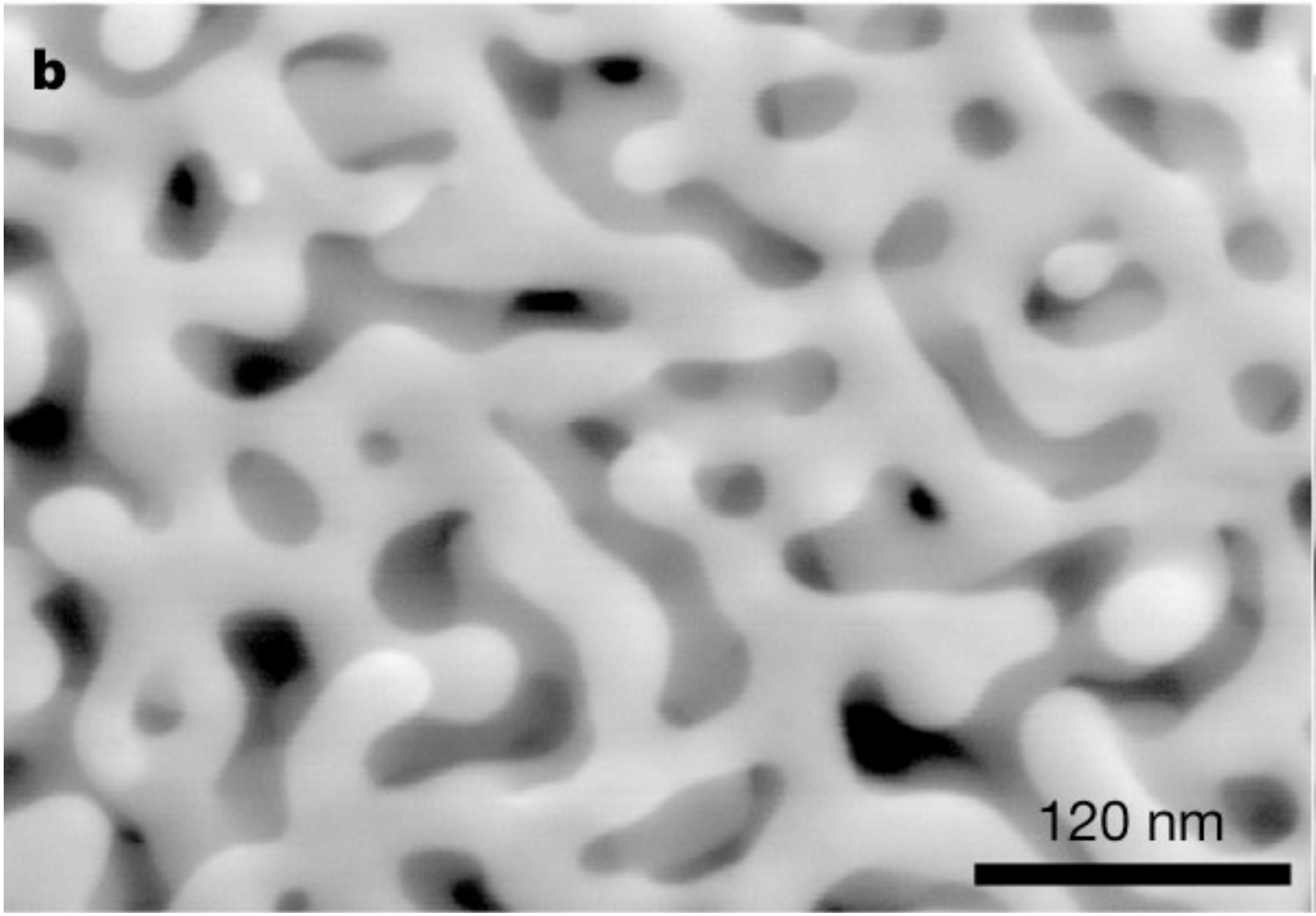
Nanoporous Gold



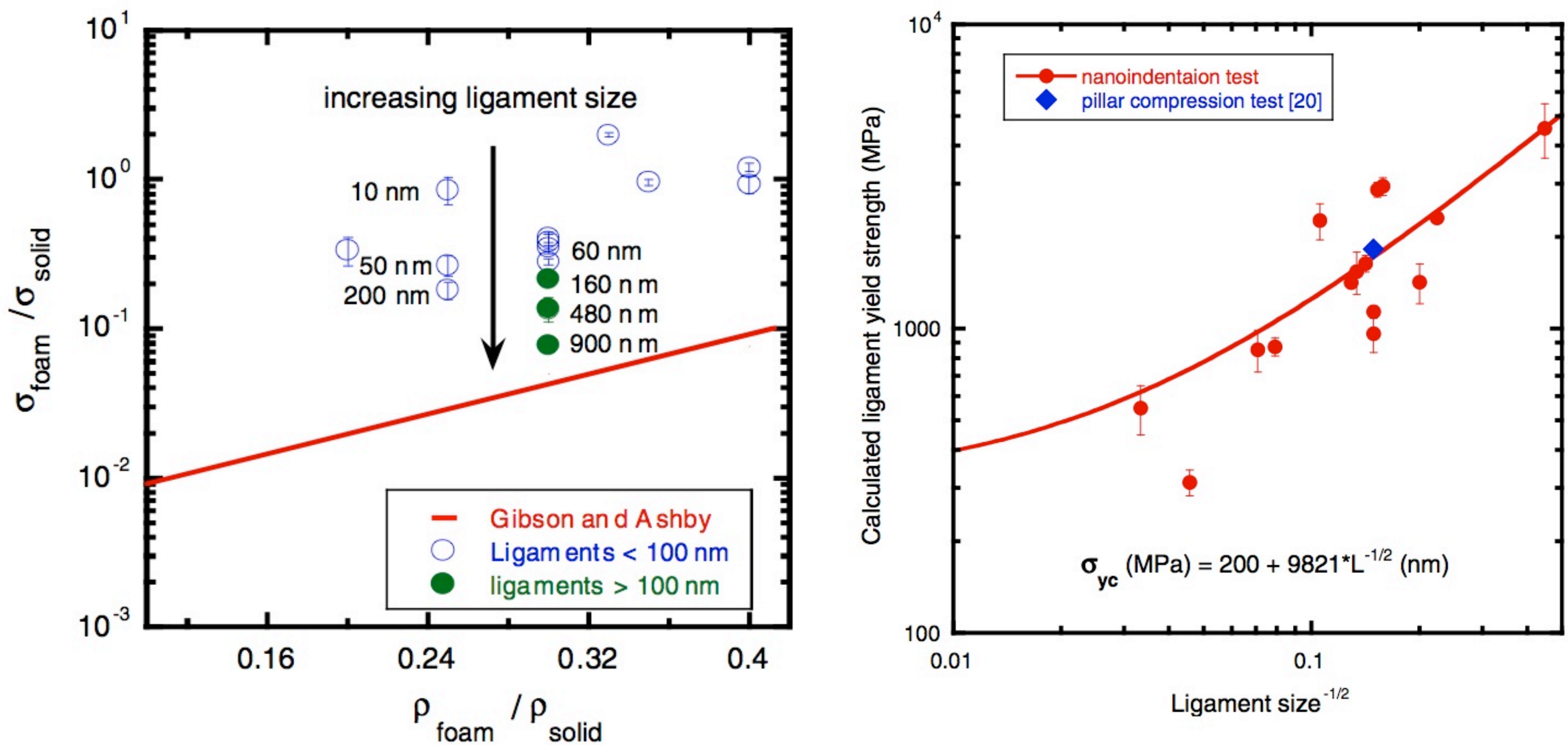
Source: Erlebacher, J., et al. "Evolution of Nanoporosity in Dealloying."
Nature 410 (2001): 450-53.

J. Erlebacher *et al.*, Nature **410**, 450 (2001)

Nanofoams made of other metals

Figures removed due to copyright restrictions.

Nanofoams are stronger than regular foams due to increased yield strength of ligaments (a “size effect”)



Source: Hodge, A.M. et al. *Acta Materialia* 55 (2007): 1343-9.
Courtesy Elsevier. Used with permission.
http://www.sciencedirect.com/science/article/pii/S1359645406007221

A. M. Hodge *et al.*, Acta Mater. **55**, 1343 (2007)

..

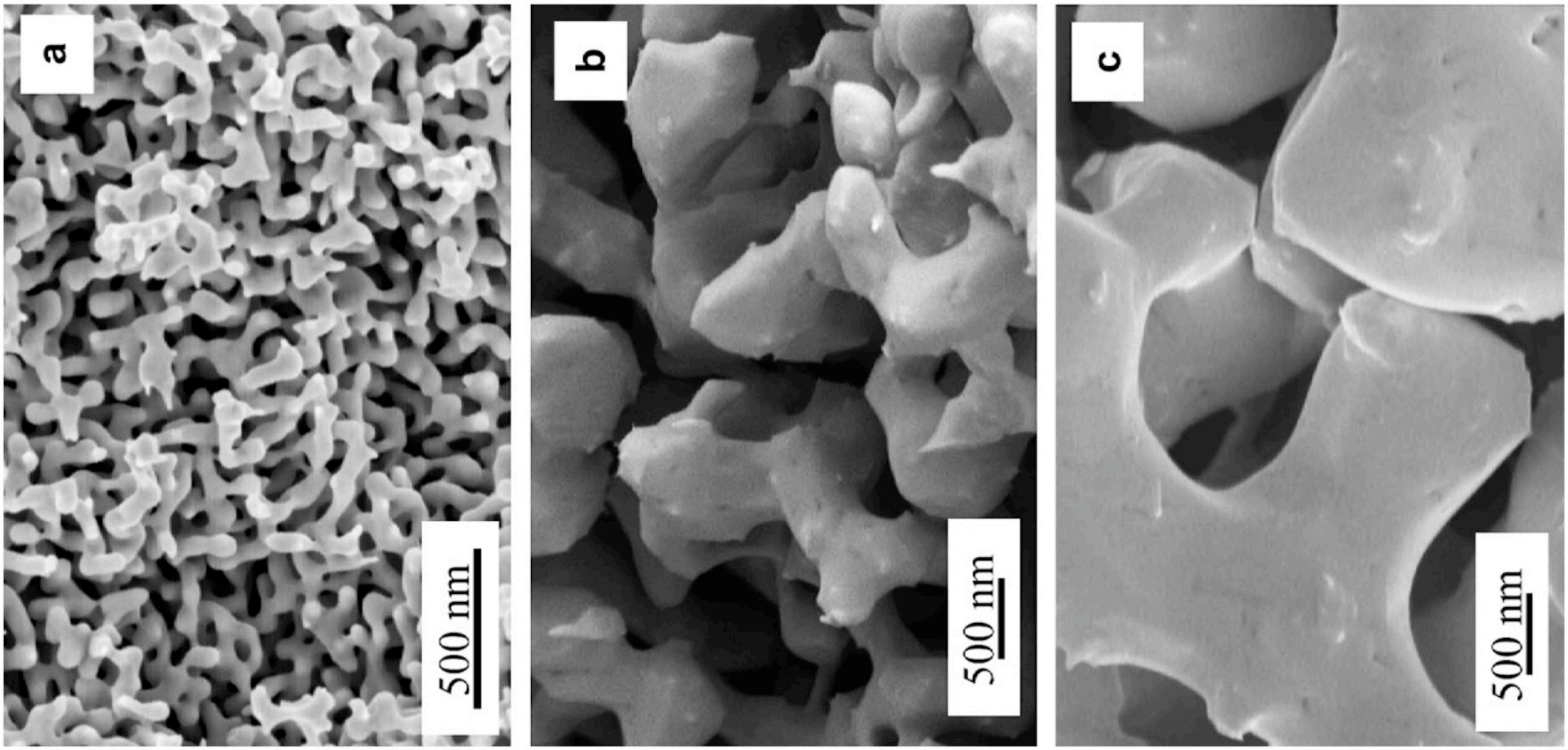
Tunable mechanical properties

Figures removed due to copyright restrictions. See Figs. 1a and 3: Jin, H. J., and J. Weissmüller. *Science* 332 (2011): 1179-82. http://www.sciencemag.org/content/332/6034/1179

H. J. Jin and J. Weissmüller, Science **332**, 1179 [2011]

Coarsening of nanofoams upon annealing: driven by reduction in surface area

As-prepared | Annealed for 2h at 400C | Annealed for 2h at 600C



A. M. Hodge *et al.*, Acta Mater. **55**, 1343 (2007)

Questions concerning the surface diffusion coarsening model

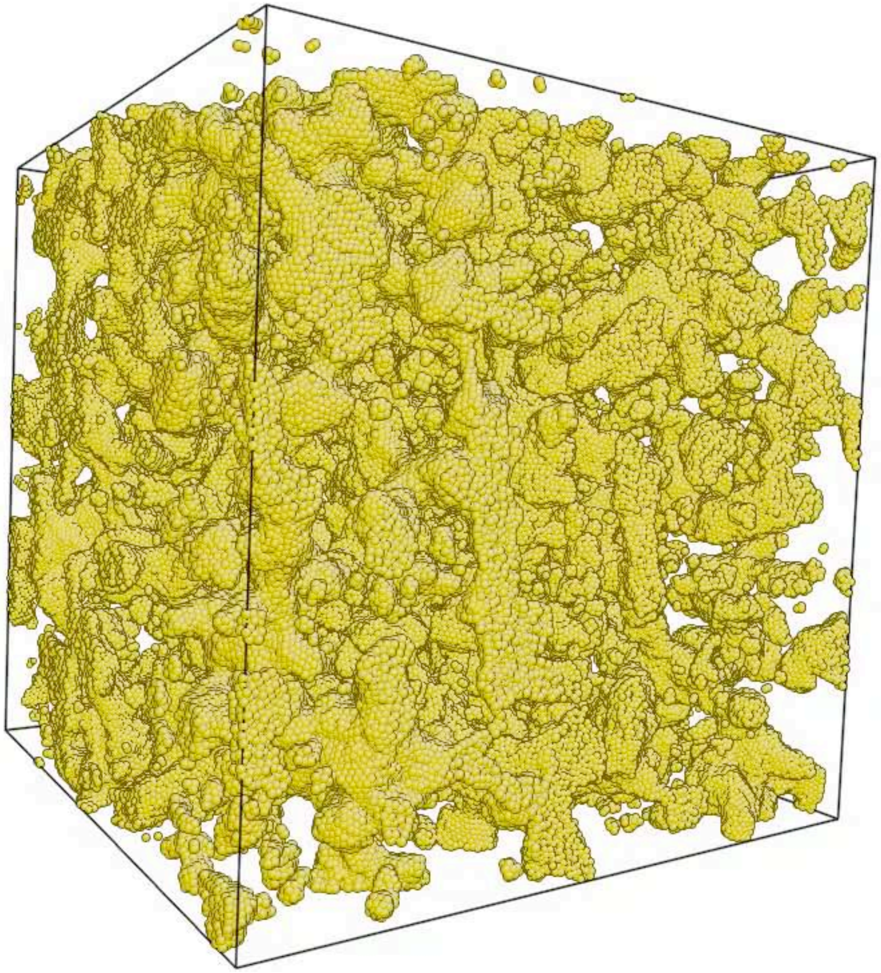
23% reduction in volume after dealloying and further reductions occur upon coarsening. In the surface diffusion model, however, the number of lattice sites is fixed and therefore the volume shouldn't change.

S. Parida *et al.*, Phys. Rev. Lett. **97**, 035504 (2005)

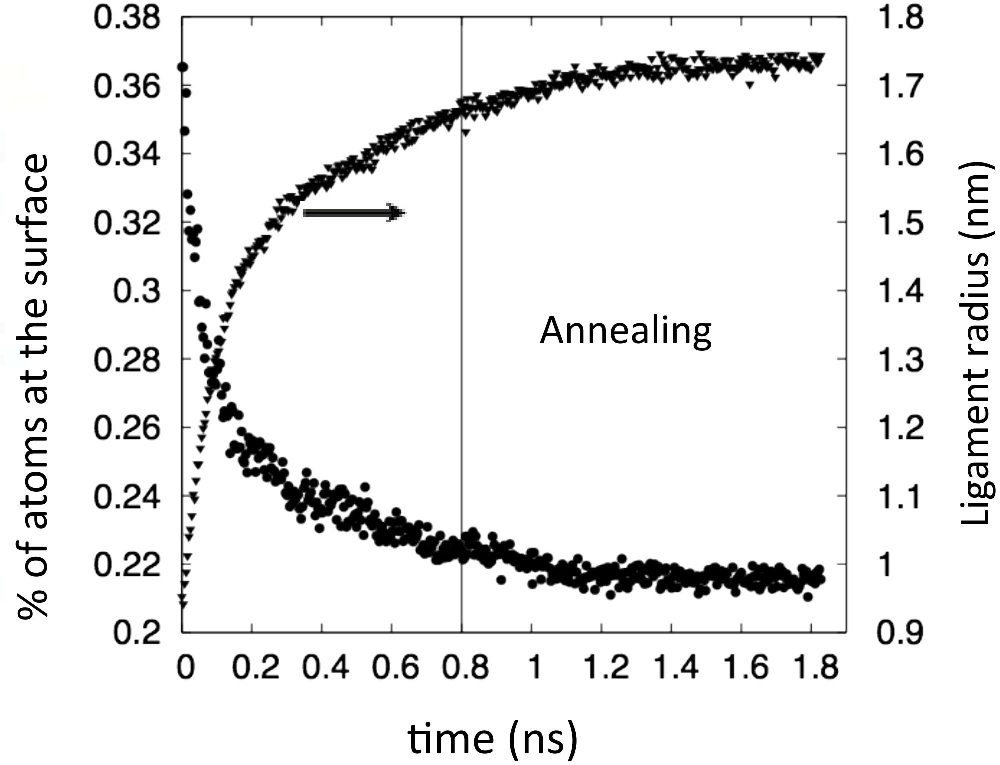
How to explain the occurrence of voids enclosed in ligaments?

H. Rosner *et al.*, Adv. Mater. **9**, 535 (2007)

Spontaneous formation of model nanoporous gold (computer simulations)



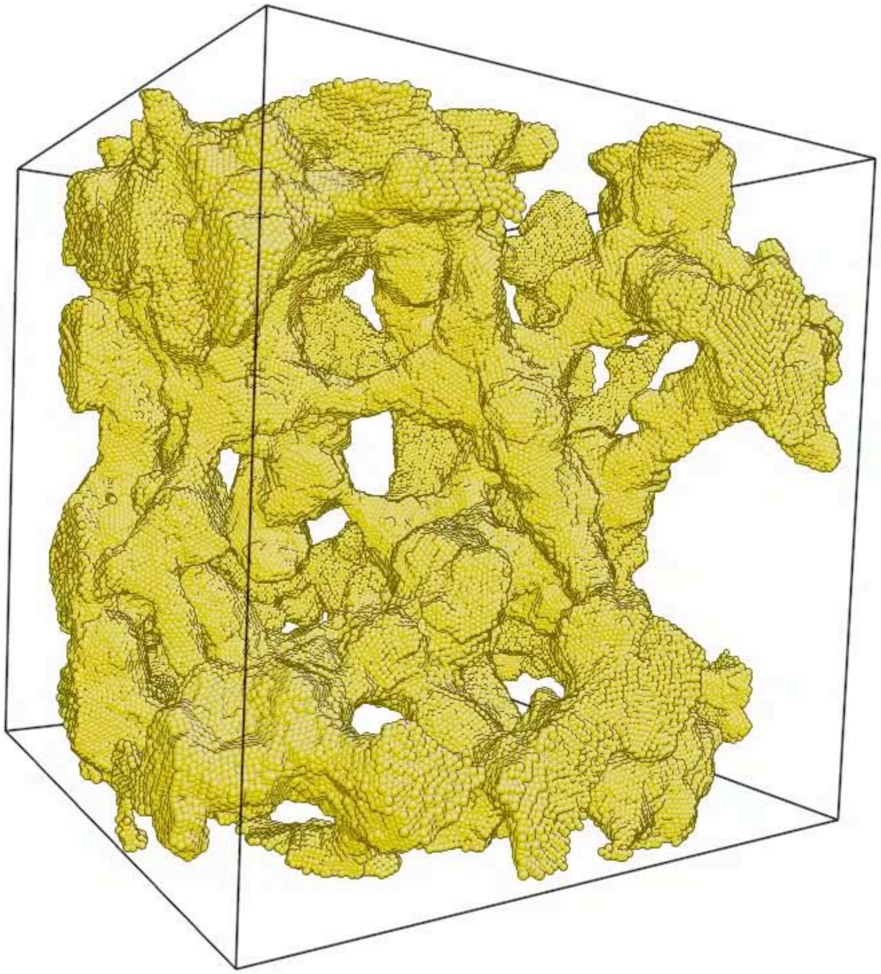
with_clusters.mov



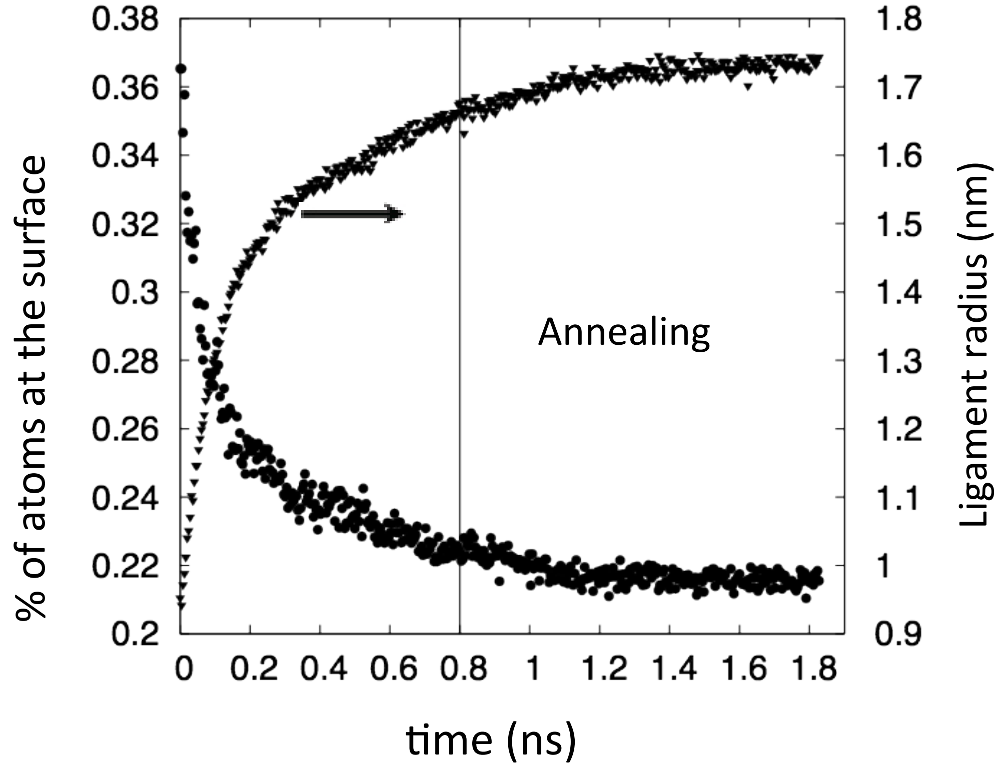
Source: Kolluri, K., and M. J. Demkowicz. *Acta Materialia* 59 (2011): 7645-53.

http://www.sciencedirect.com/science/article/pii/S1359645411006148.

Coarsening of np-Au during annealing

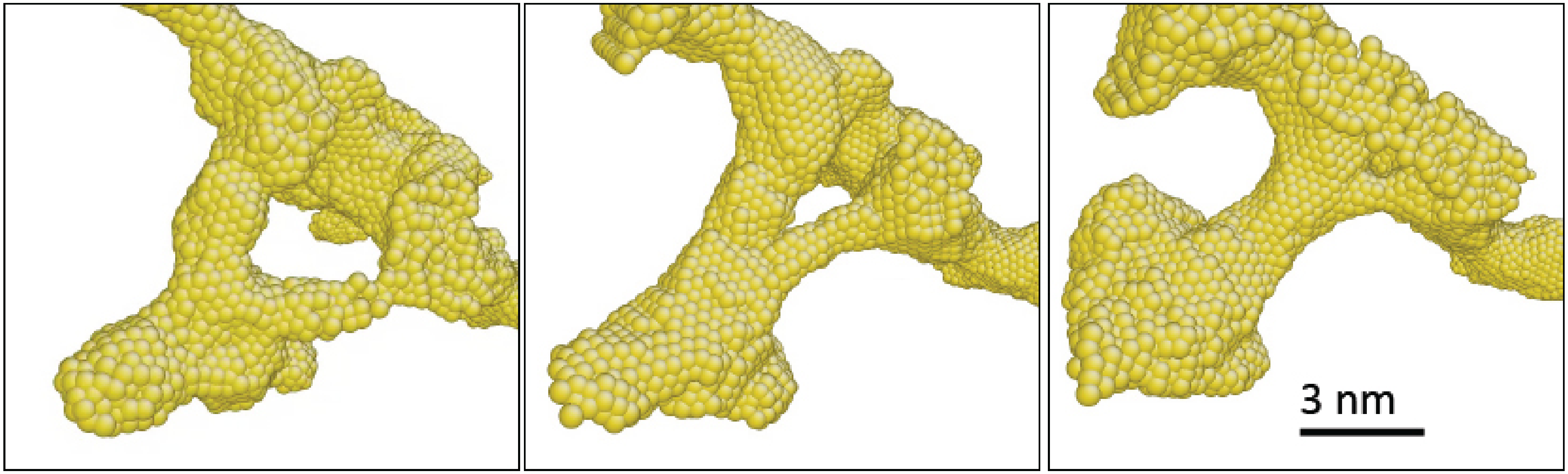


without_clusters.mov



Source: Kolluri, K., and M. J. Demkowicz. *Acta Materialia* 59 (2011): 7645-53.
Courtesy of Elsevier. Used with permission.
http://www.sciencedirect.com/science/article/pii/S1359645411006148.

Coarsening during annealing by collapse of ligaments

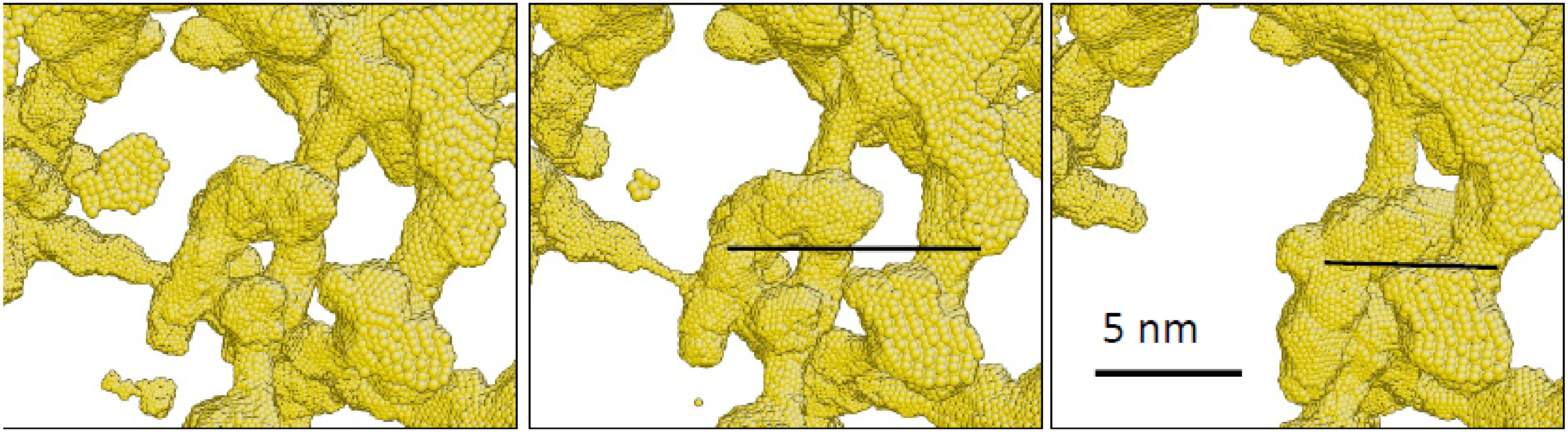


Source: Kolluri, K., and M. J. Demkowicz. *Acta Materialia* 59 (2011): 7645-53.
Courtesy of Elsevier. Used with permission.
http://www.sciencedirect.com/science/article/pii/S1359645411006148.

ligament_collapse.mov

- Shear at the bases of adjacent ligaments due to dislocation motion
- Subsequently, shear at the ligaments themselves
- Shear leads to “displacive” motion of ligaments towards each other and eventual collapse

Coarsening during annealing by collapse of ligaments



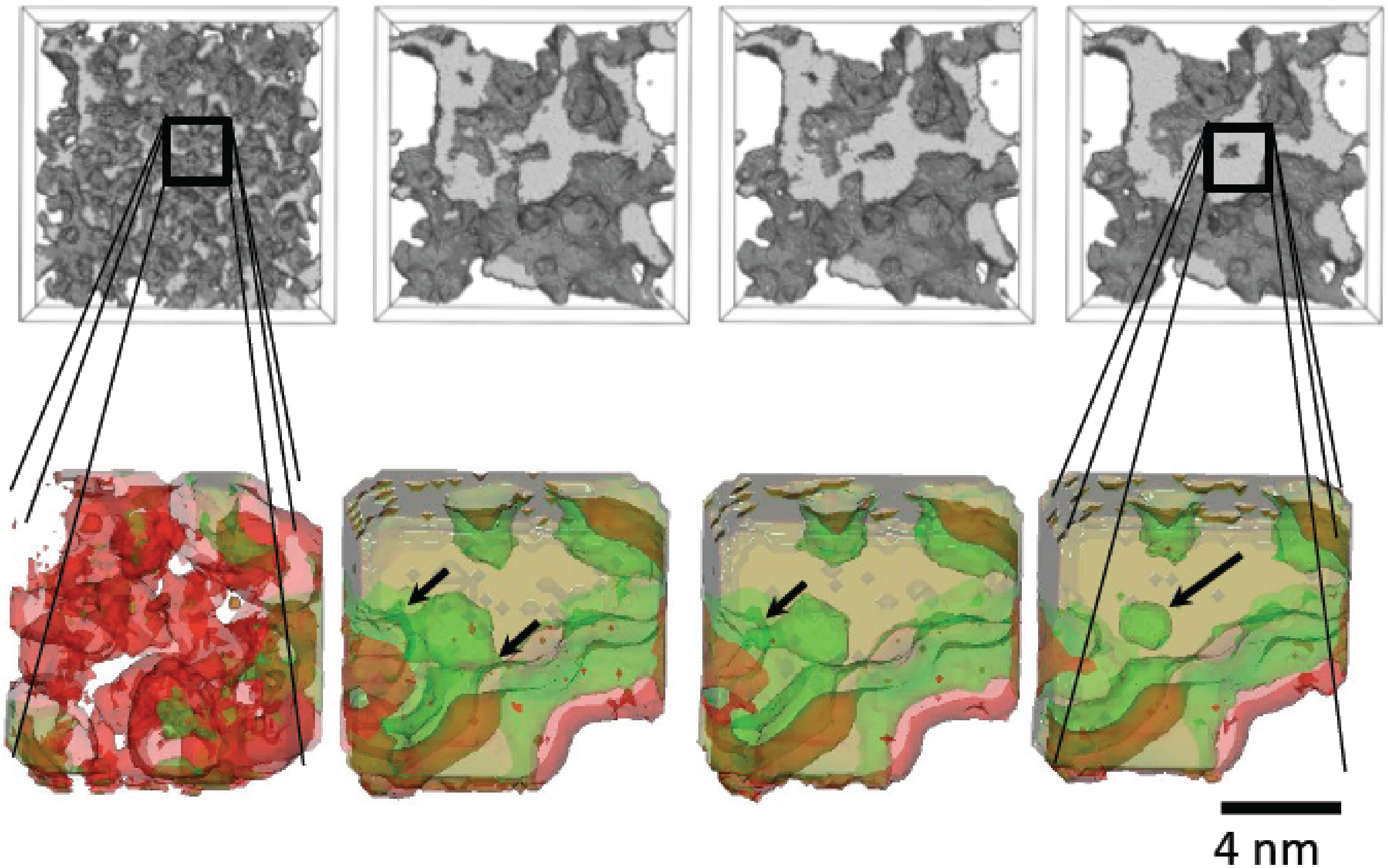
Source: Kolluri, K., and M. J. Demkowicz. *Acta Materialia* 59 (2011): 7645-53.
Courtesy of Elsevier. Used with permission.
http://www.sciencedirect.com/science/article/pii/S1359645411006148.

- Ligament pinch-off assisted by plastic deformation
- Ligament pinch-off causes collapse of other nearby ligaments

- Pinch-off of a ligament creates additional surface

- However, surface area lost by ligament collapse more than compensates the surface area created by pinchoff

Void formation during ligament collapse

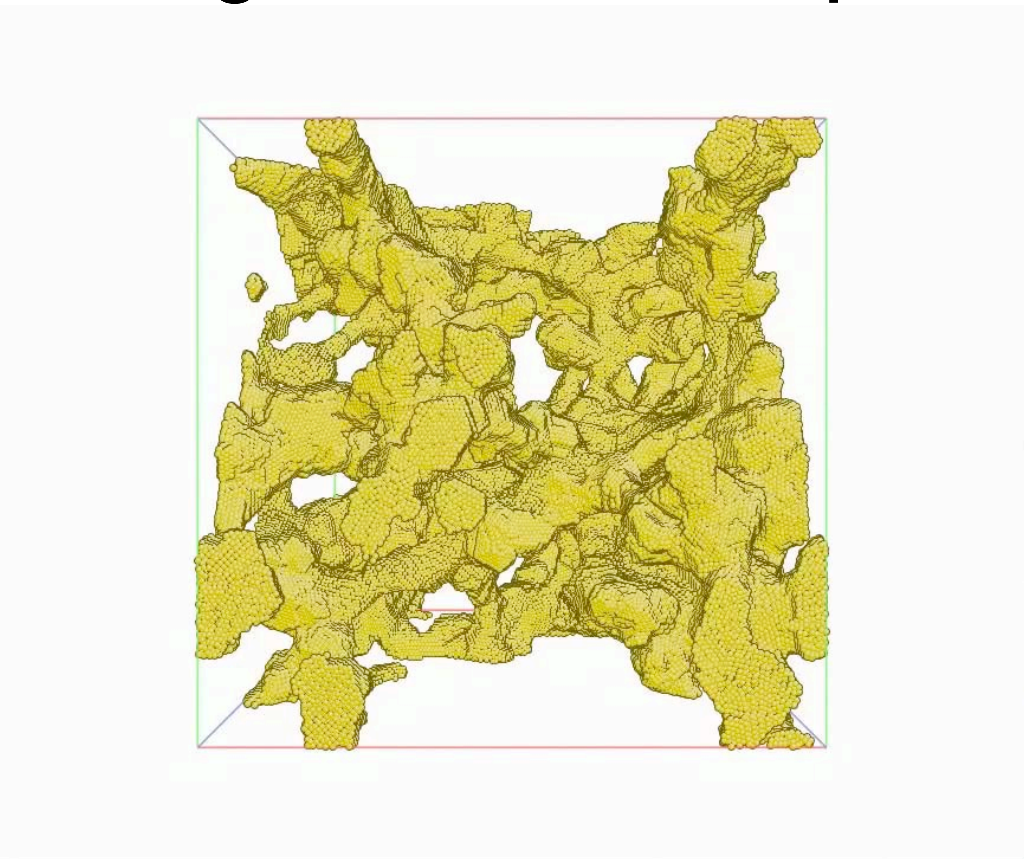


Source: Kolluri, K., and M. J. Demkowicz. *Acta Materialia* 59 (2011): 7645-53.
Courtesy of Elsevier. Used with permission.
http://www.sciencedirect.com/science/article/pii/S1359645411006148.

If ligament collapse is not contiguous, voids form

For details, see K. Kolluri and M. J. Demkowicz, Acta Mater. **59**, 7645 (2011)

Plastic deformation under volume conserving uniaxial compression

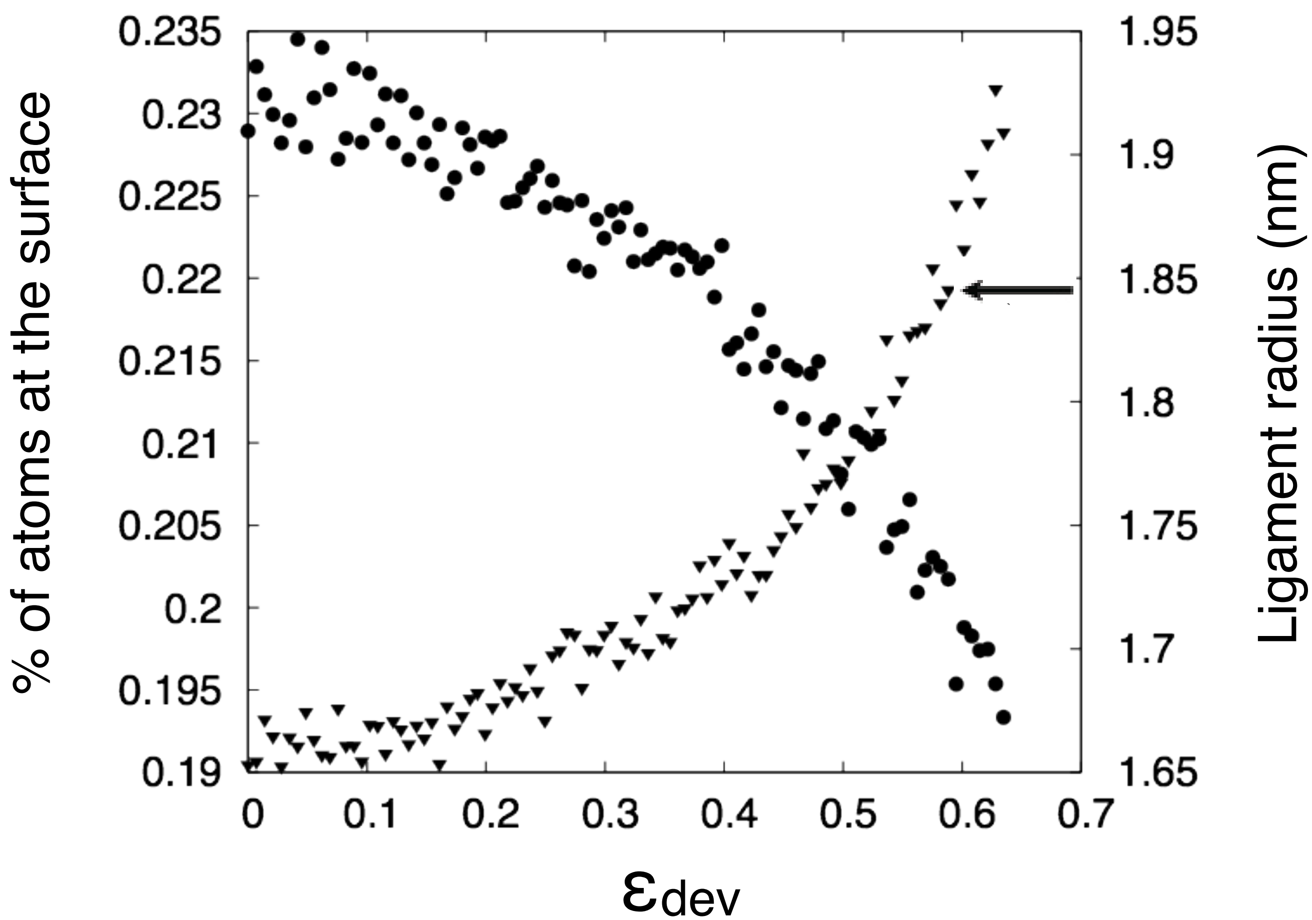


- Model np-Au structure is initially mechanically stable at T=0K
- Volume-conserving deformation: $\varepsilon_{zz} < 0$, $\varepsilon_{xx} = \varepsilon_{yy} > 0$
- Strain increments of 0.0099 (0.99%) up to a deviatoric strain of ~0.65
- Each Strain increment is followed by conjugate gradient minimization (T=0K)

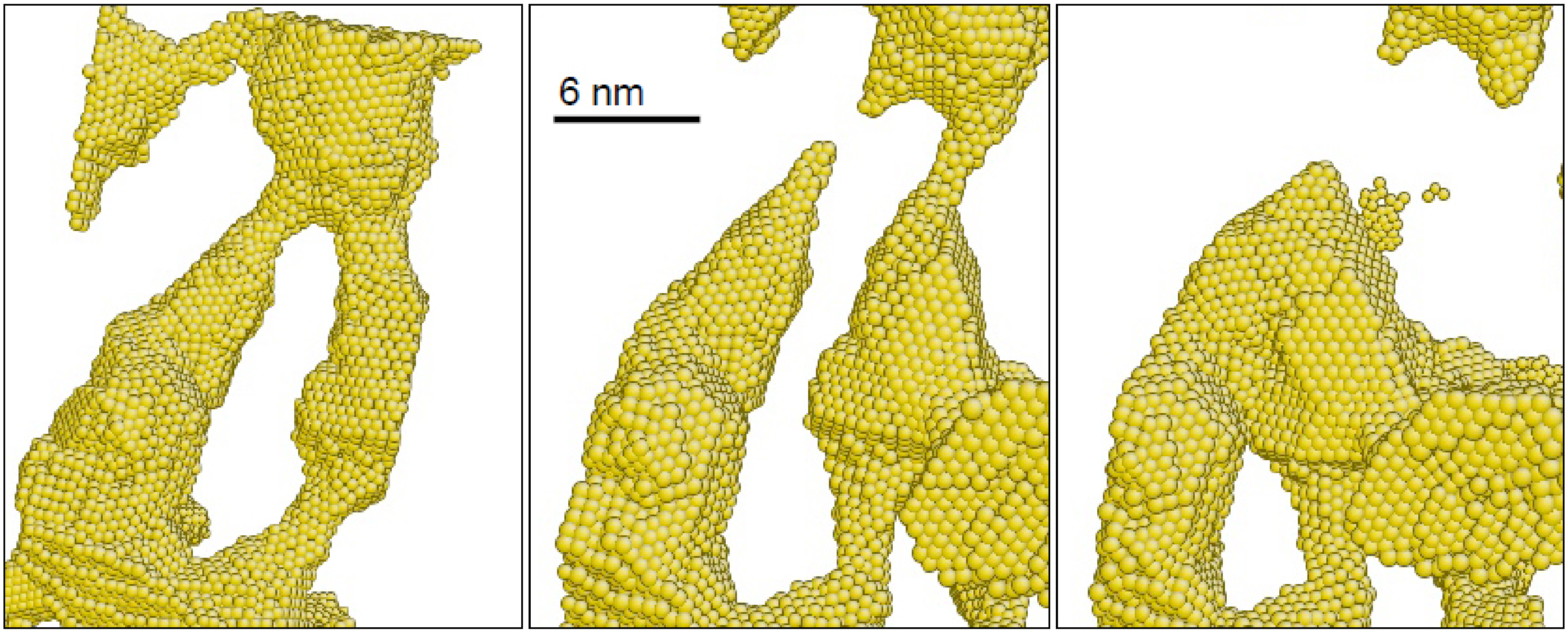
Mechanical response to volume conserving uniaxial compression

- Elastic-perfect plastic stress-strain response reminiscent of the compaction plateau of conventional foams
- Critical yield strength backed out from Gibson-Ashby equation is in excellent agreement with those obtained directly for the Au potential we used in this study
- When deformed under zero pressure the foams would densify; under constant volume, however, they begin to break up after $\varepsilon_{dev} \sim 0.3$

Coarsening during deformation



Coarsening during deformation by collapse of ligaments: example



- Ligament pinch-off assisted by plastic deformation
- Pinched-off ligaments collapse onto each other, leading to coarsening
- No surface diffusion (T=0K simulation)

Conclusions

- Atomistic modeling suggests that there may be a different mechanism of coarsening in np-Au besides surface diffusion: network restructuring by collapse of neighboring ligaments enabled by localized plasticity

- Indirect evidence:
  - Network restructuring gives rise to densification upon annealing
  - Voids enclosed in ligaments form during network restructuring
  - Critical ligament radius below which coarsening by network restructuring is predicted to occur spontaneously is greater than the ligament radii of np-Au samples in all studies we are aware of

- Improvements in high spatio-temporal resolution x-ray tomography will provide a means for direction verification?

3.054 / 3.36 Cellular Solids: Structure, Properties and Applications
Spring 2014