Synergy of Atomistic Simulations and Experiments vs Multiscale Modeling

Science of Nanoscale Interfaces during Fabrication

Hanchen Huang

http://www.rpi.edu/~huangh

Department of Mechanical, Aerospace and Nuclear Engineering

NECIS Workshop on

Multidisciplinary Approaches to Science of Nanoscale Interfaces

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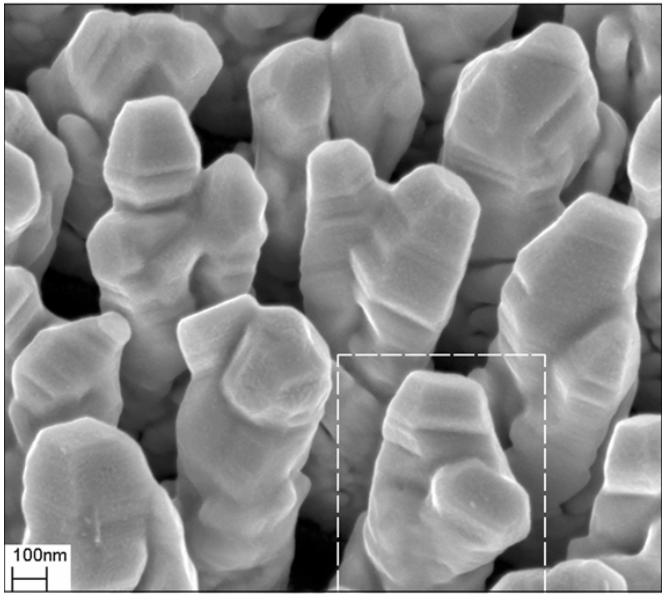
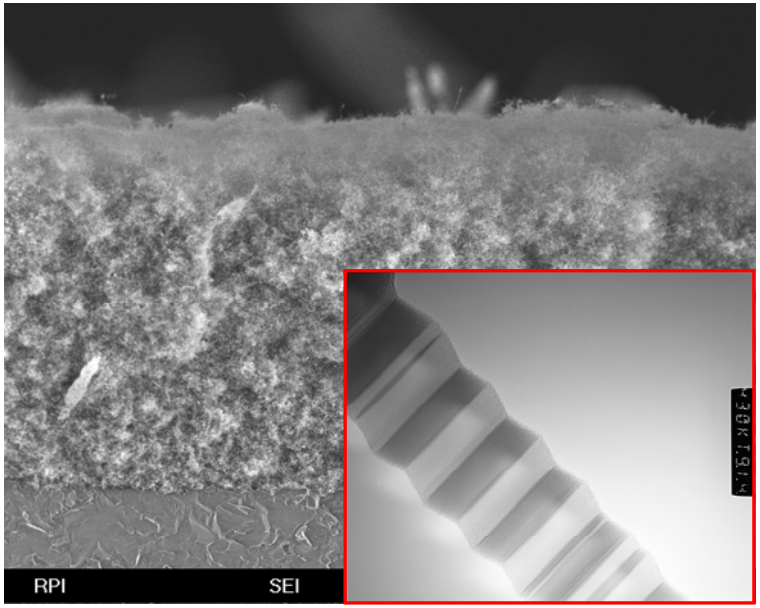
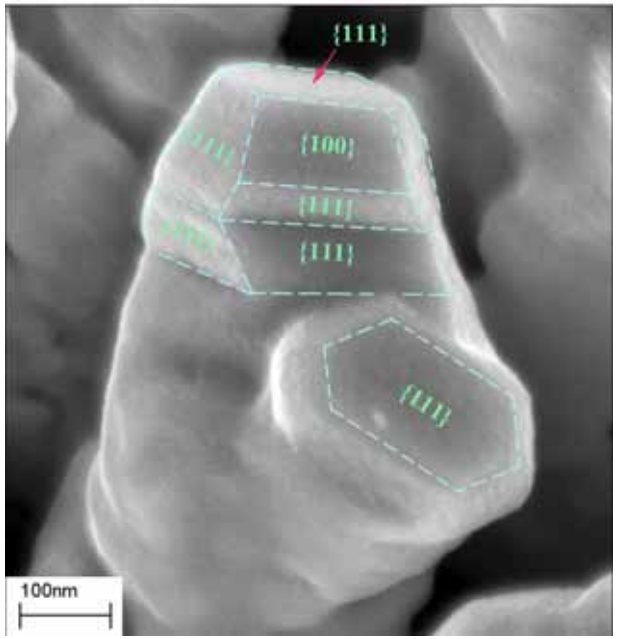
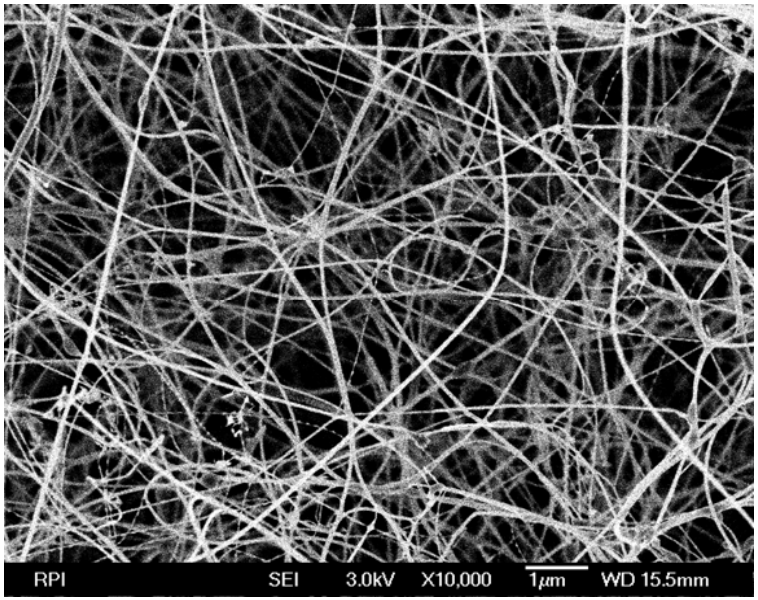
Nanoscale interfaces (nanometers)









A story of atomistic simulations + experiments

- Understanding of three pieces of fundamental physics
  - ^ surface kinetics
  - ^ geometrical shadowing
  - ^ stacking fault
- Conceptual design by integrating the pieces of physics
- Atomistic simulations based on the design
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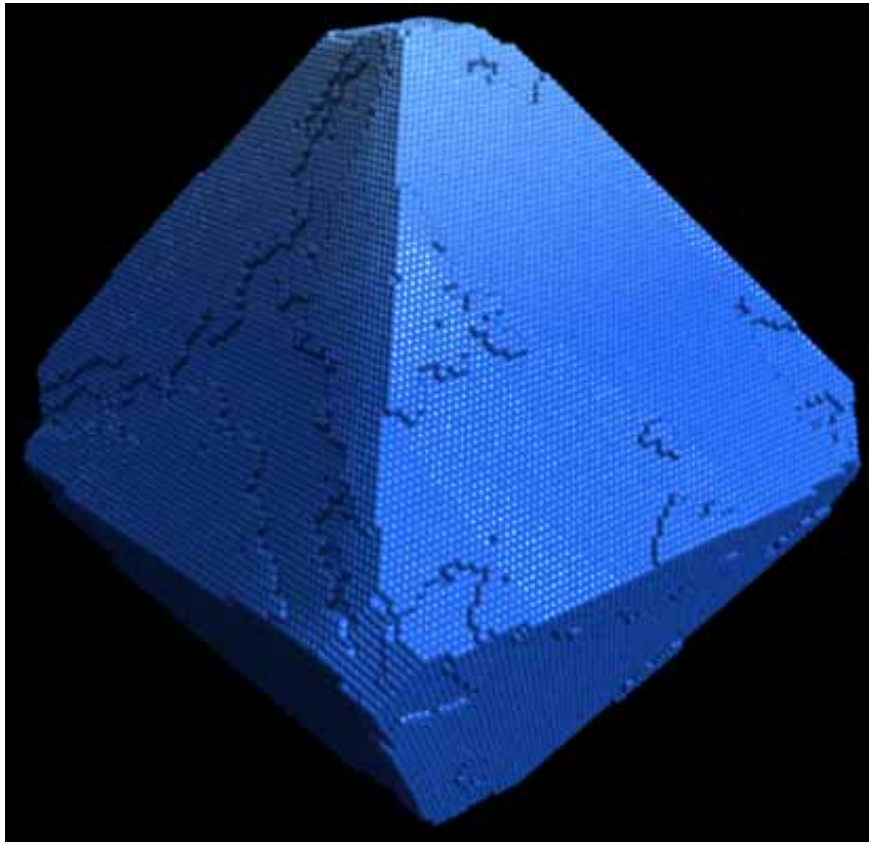
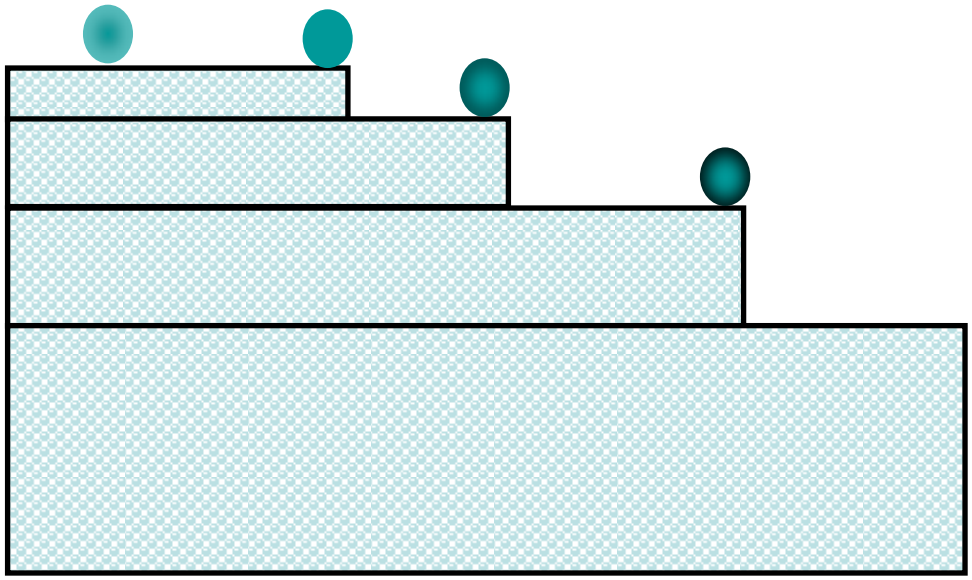
3D ES barrier - concept

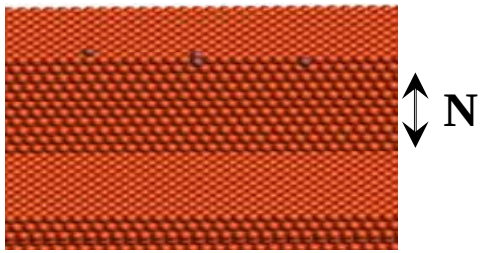




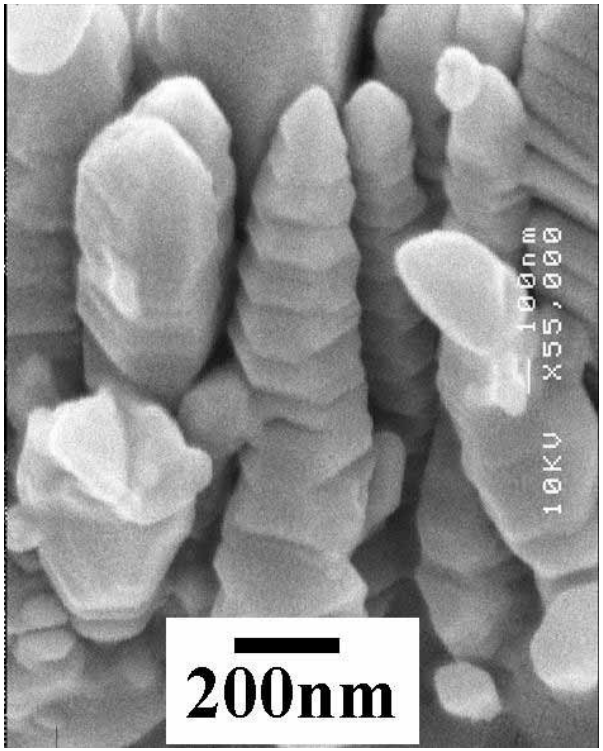
APL 2002; NATURE 2002

There may be 3D effect in diffusion down steps??

3D ES barrier - values



Process	N=1	N=2	N=3	N≥4
{111}→<110>/{111}	**0.08**	**0.29**	**0.30**	**0.30**
{111}→<110>/{100}	0.28	0.38	0.40	0.40
{100}→<110>/{111}	0.57	0.74	0.75	0.75
{100}→<100>/{100}	0.32	0.07	0.17	0.17



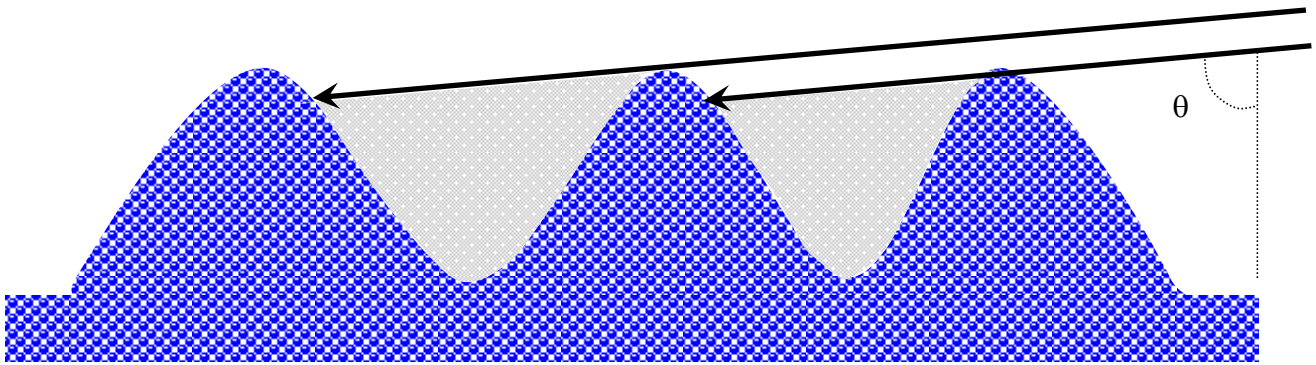
$$v = v_0 e^{-E/kT}$$

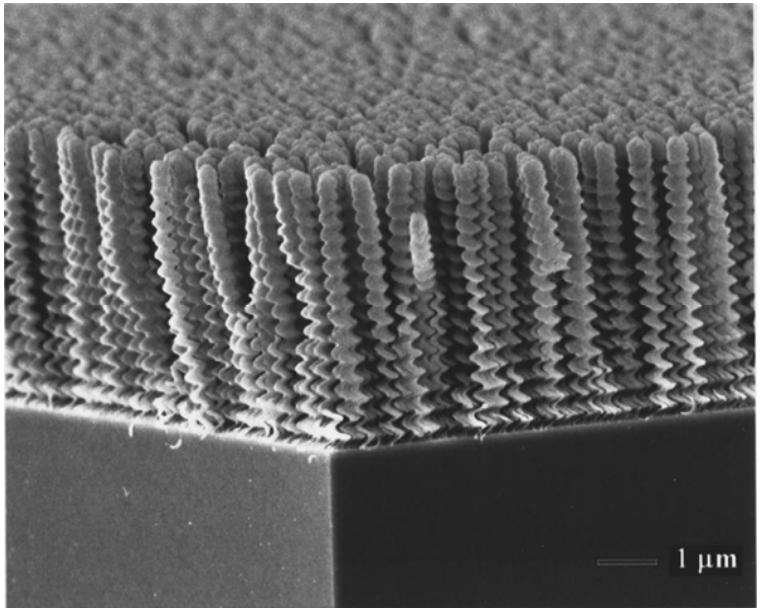
***kT* = 0.025 eV @RT**

With surface diffusion barrier, *l*=80,000 nm
With conventional ES barrier, *l*=65,000 nm
With 3D ES barrier, *l*=200 nm

Finally, we got the order of magnitude right!

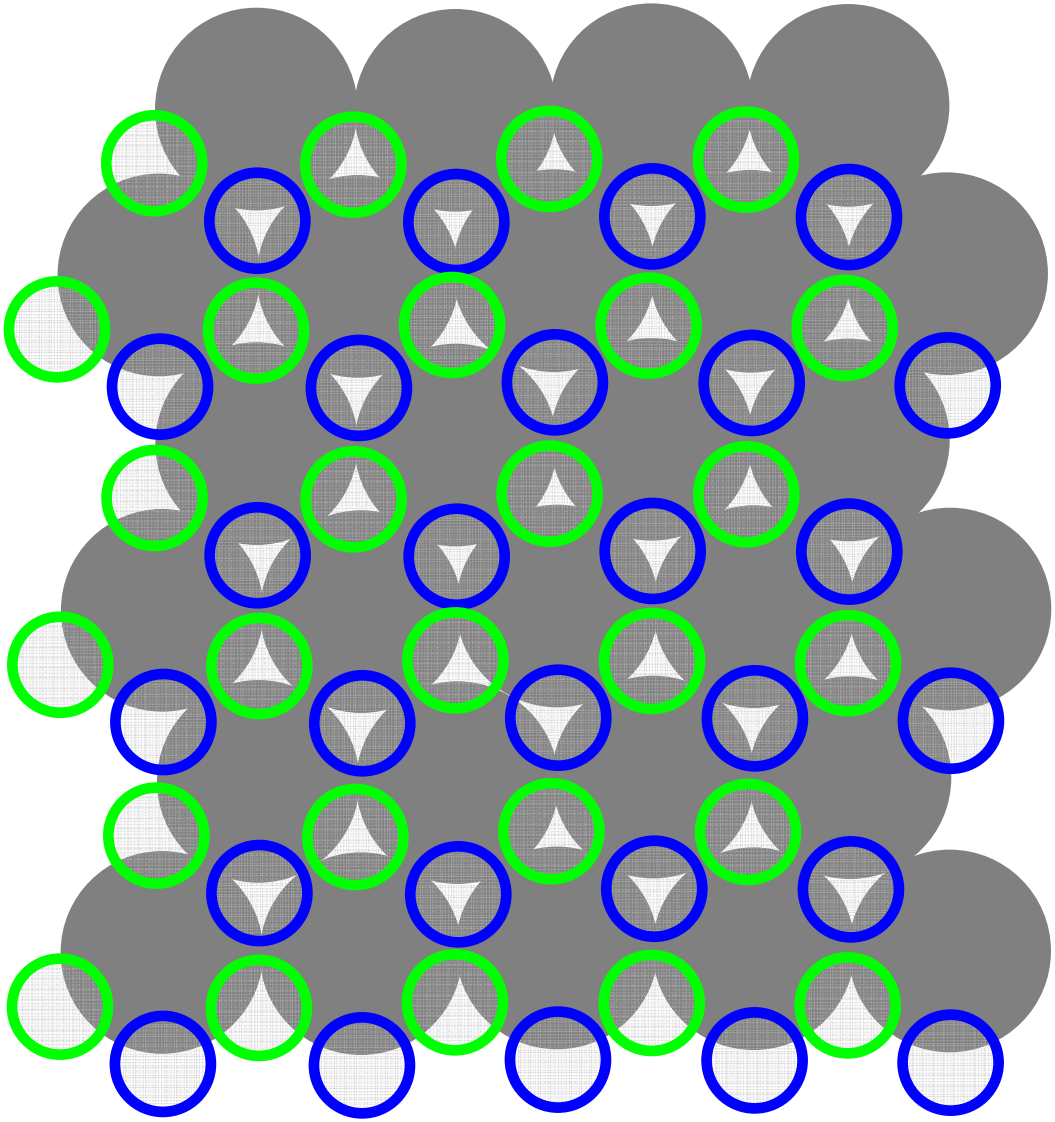
Geometrical shadowing

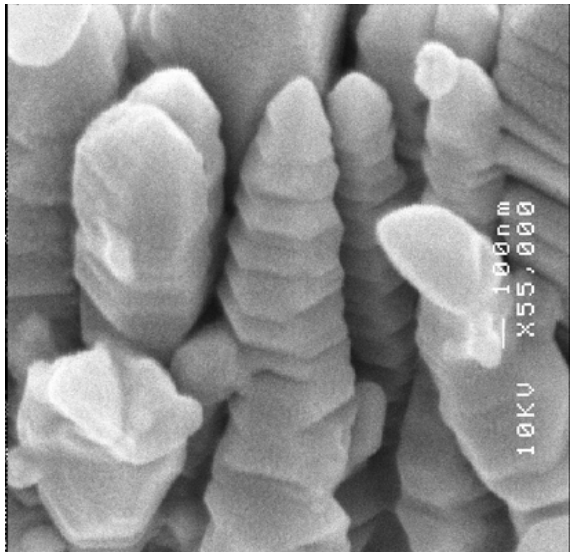


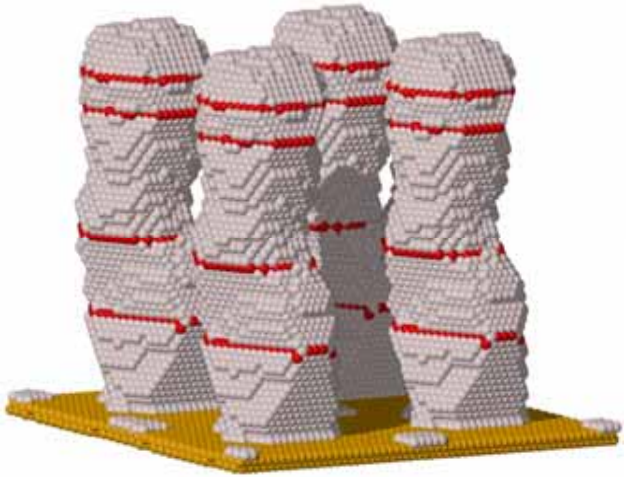


K. Robbie and M. J. Brett
J. Vac. Sci. Technol. A 15 (1997)

Stacking fault formation







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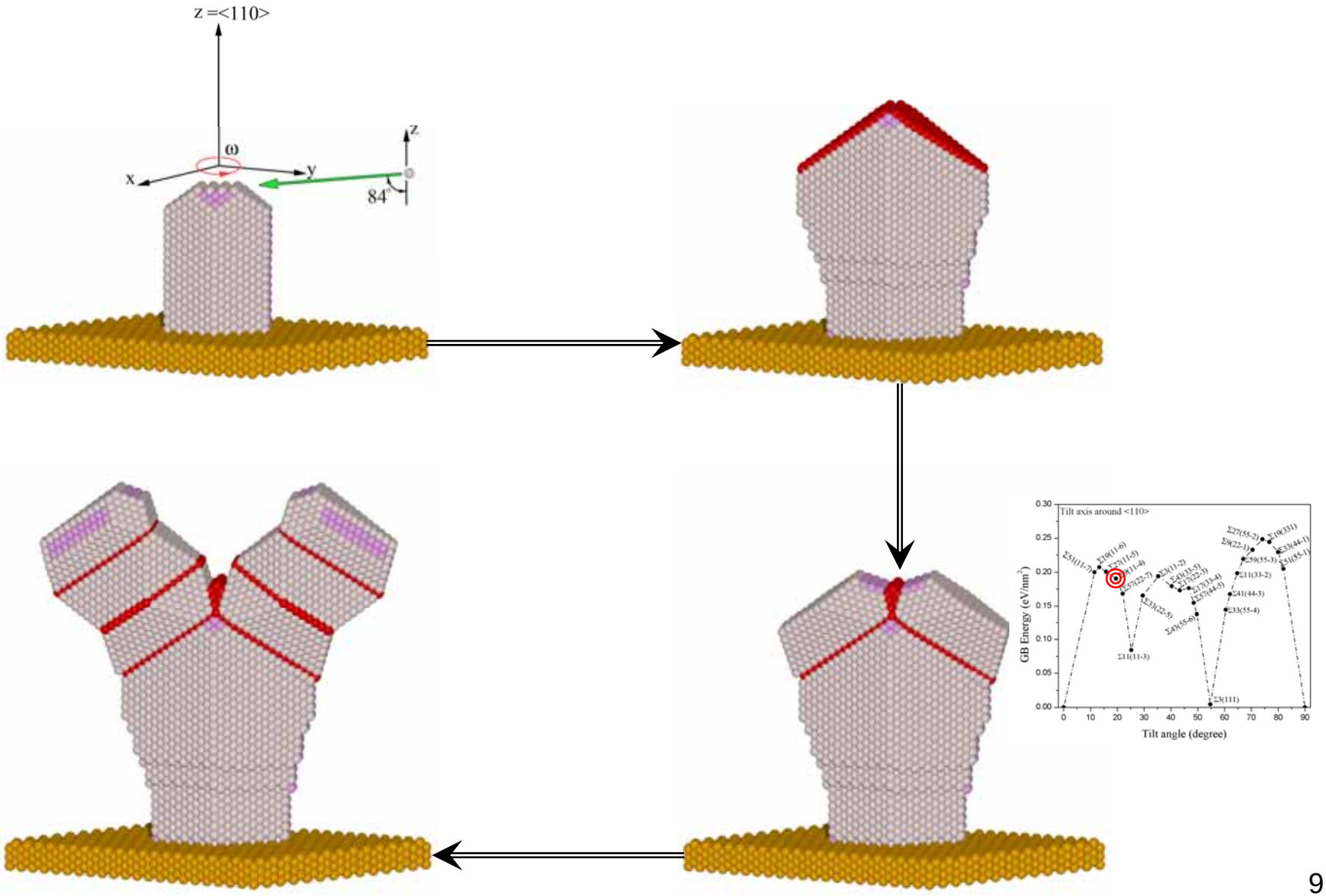
Design by integration



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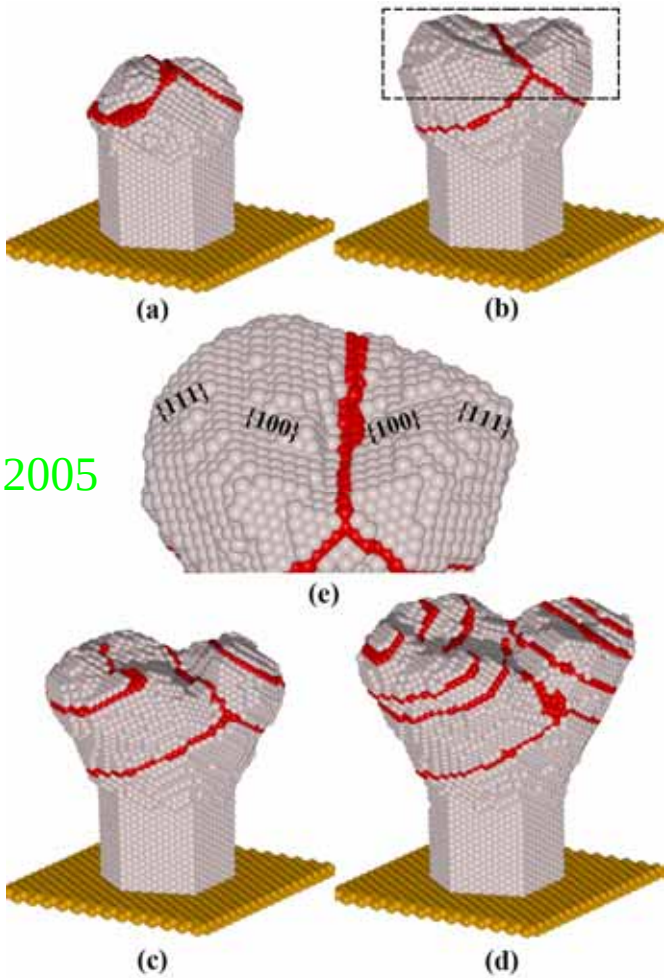
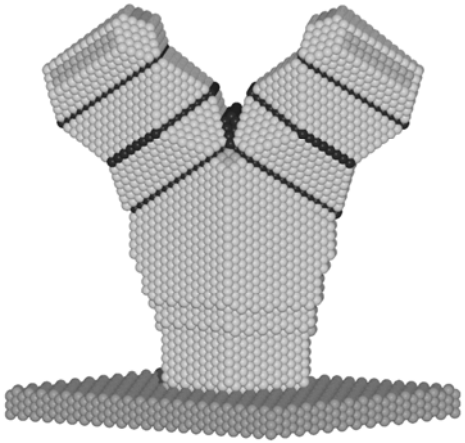
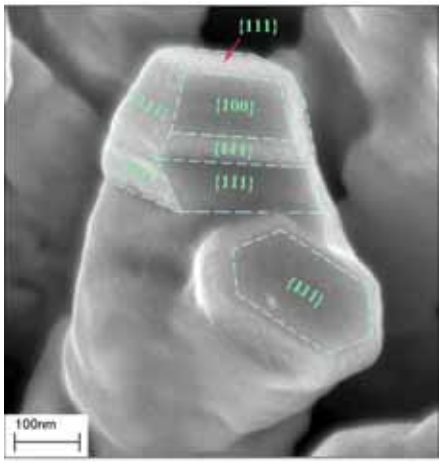
Nano Lett 2005







Simple physics works.

Closing the story: synergy of atomistic simulations & experiments

From **physics understanding**

→ To **conceptual design by integration**

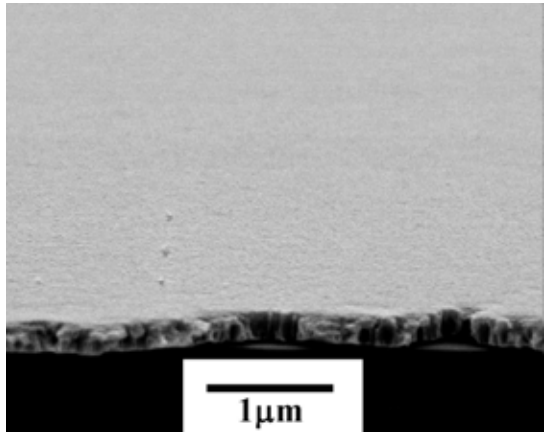
→ To **atomistic simulation**

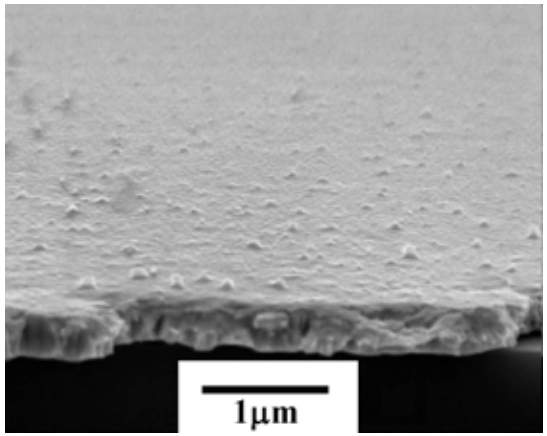
→ To **Experimental validation**

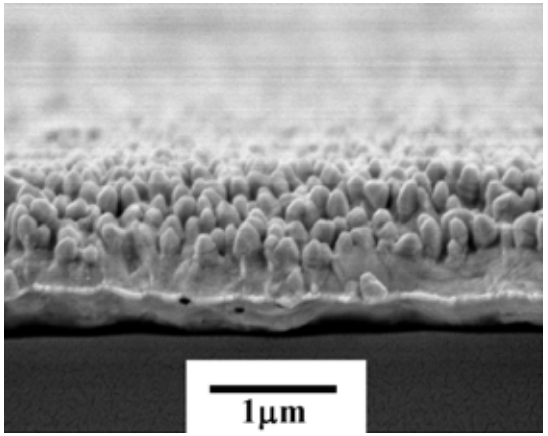
Another fabrication example calling for more work

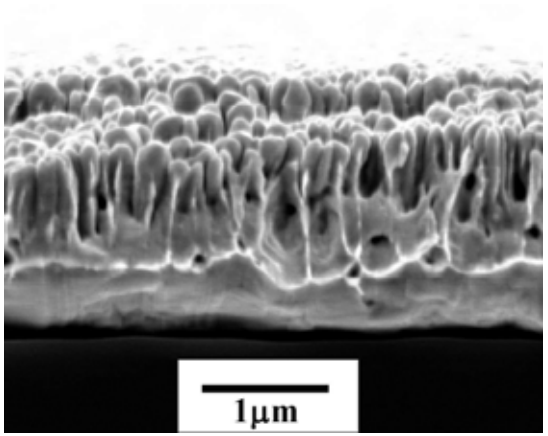
- Time scale (also)
- Length scale

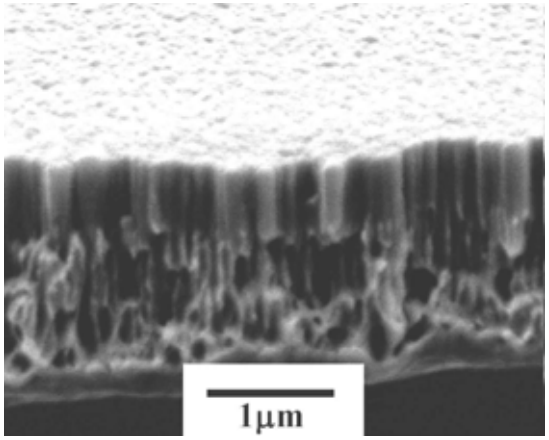
Cu thin film (microns)

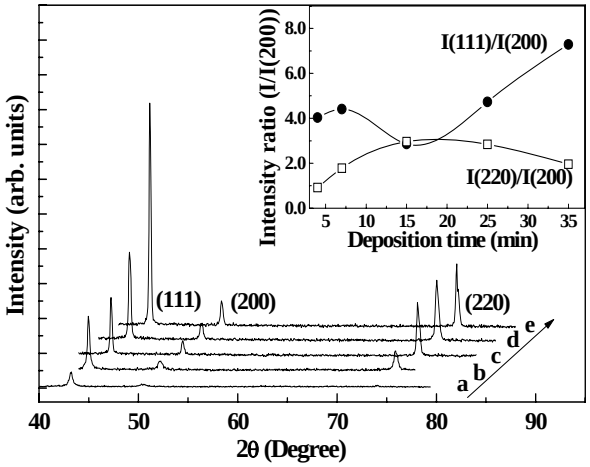








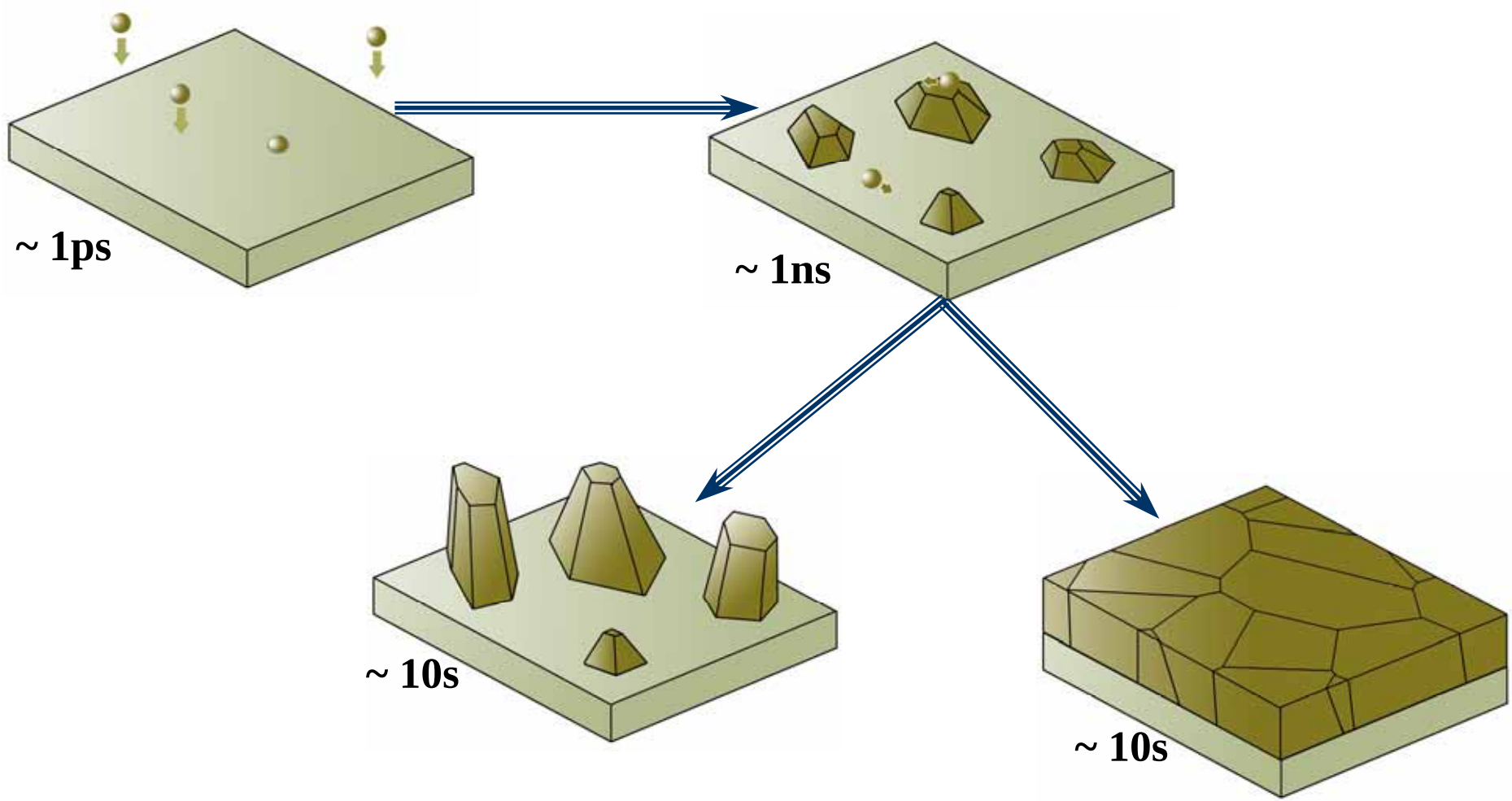




APL 2003

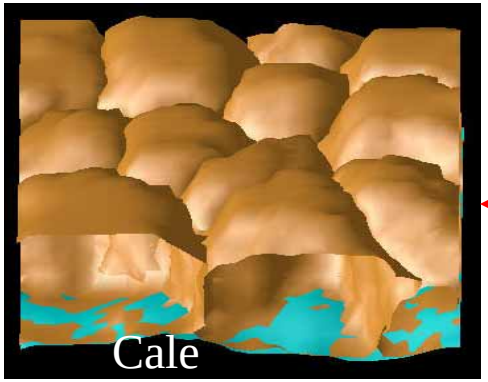
Texture development can be unexpected.

Challenge to atomistic simulations – multiple time scales

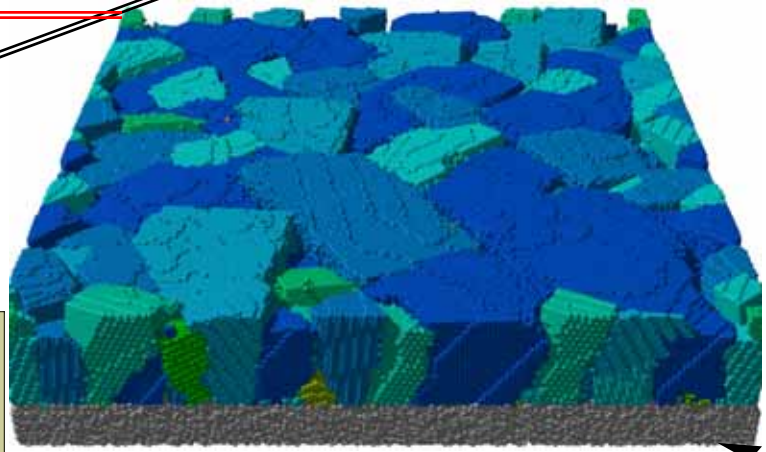


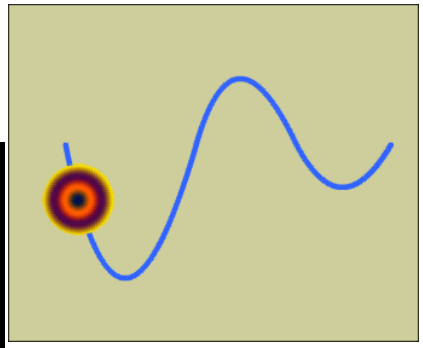
Multiple time scales from 1ps to 10s

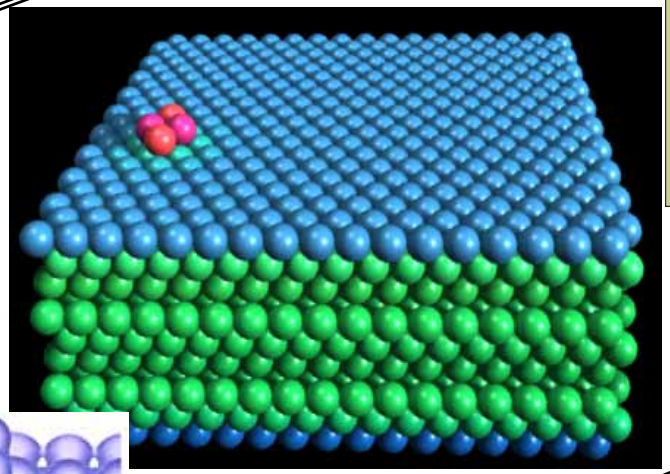
Necessary physics ingredients in a model

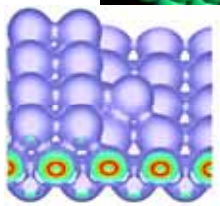


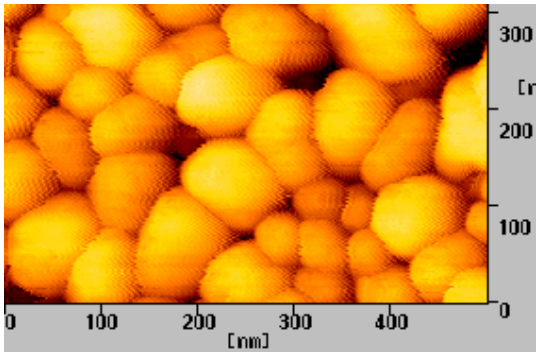
L>1 micron



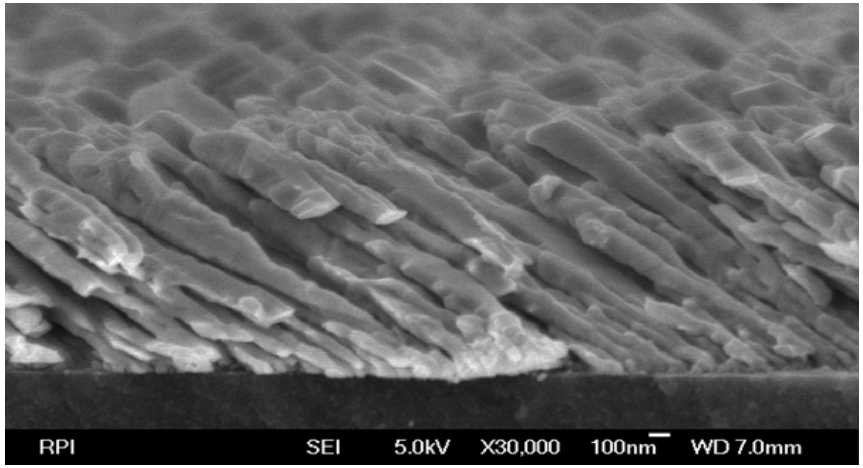




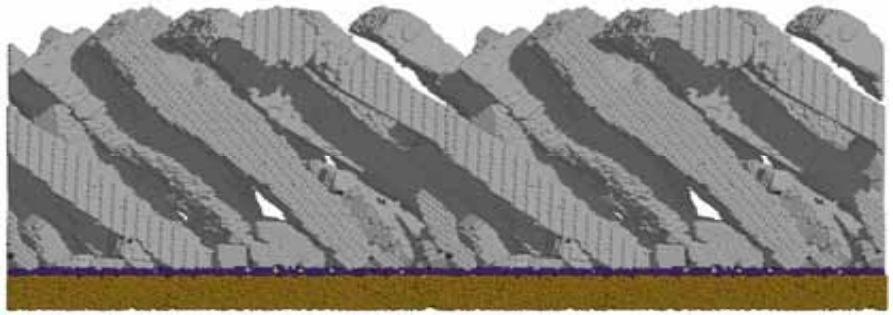


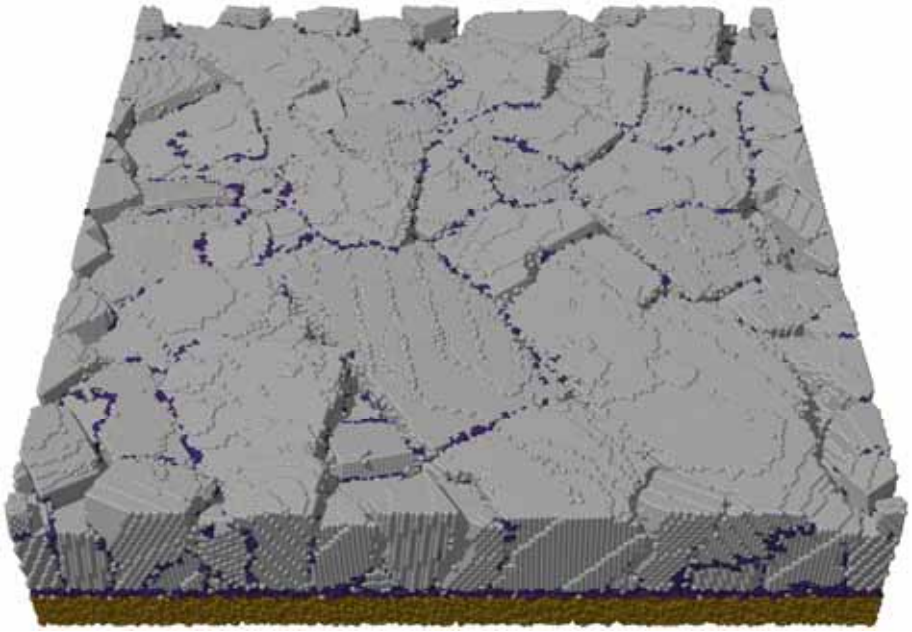


Textured nanorods and thin films



Courtesy of Wang-Lu @RPI





Handbook of Materials Modeling
Springer, 2005

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NCSA Supercomputer Center

Modeling and simulations

- Why do we do simulations
  - ^ “agree with experiments”
  - ^ replace experiments
  - ^ reveal mechanisms and augment experiments
  - ^ design/discover

- What are the important ingredients
  - ^ mathematics
  - ^ algorithms
  - ^ physics/chemistry