Films and Crystals:
Search for the Perfect Structure

BROOKHAVEN NATIONAL LABORATORY

Seminar at AMSC, February 1 2007.

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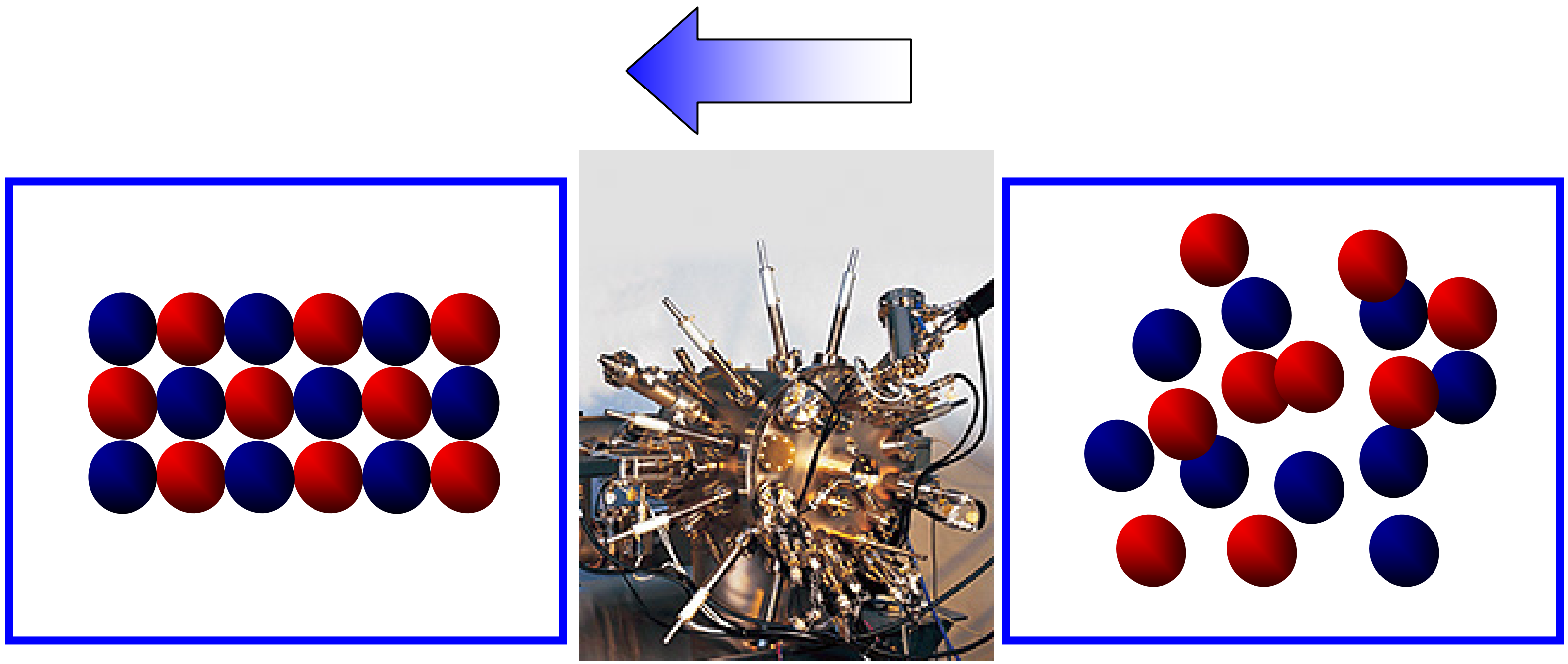
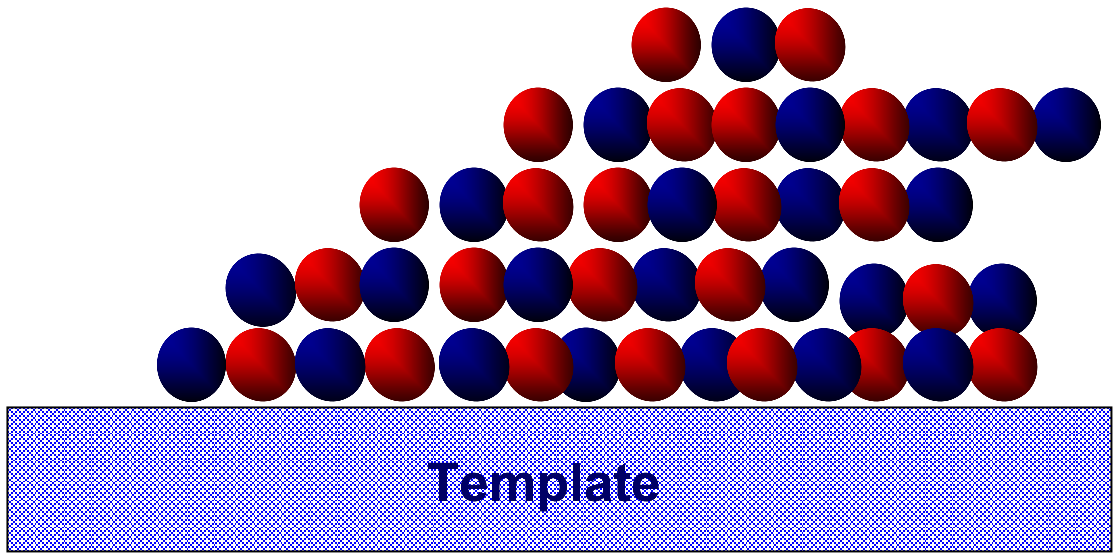
How we make materials



Low entropy state | Processing system (Veeco MBE) | High entropy state

- **Material making is a process of local entropy reduction by heating the outside world.**

Can we make perfect materials in bulk?



- If we wait long enough, can we make 1” thick perfect film?

Case 1: Low-temperature epitaxy of Ge and Si

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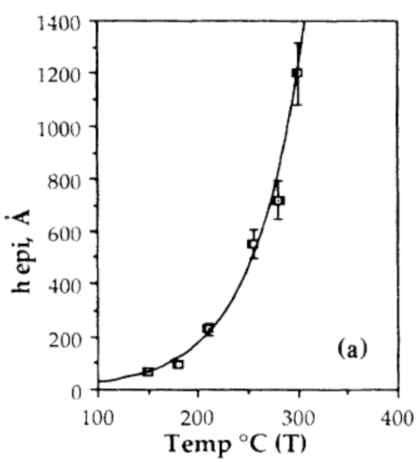
Si on Si

Ge on Ge



K. A. BRATLAND *et al.* PHYSICAL REVIEW B **67**, 125322 (2003)

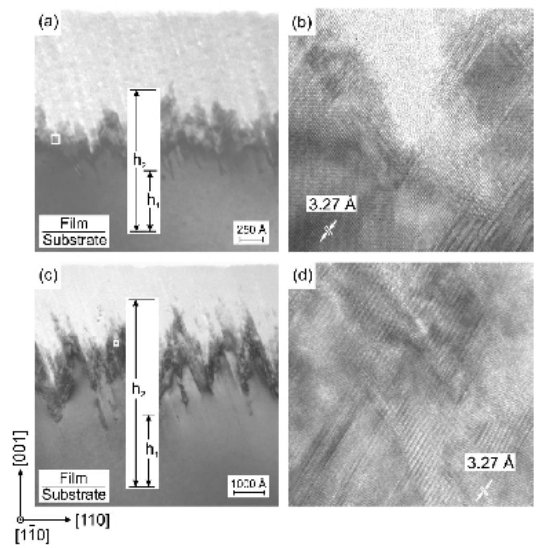
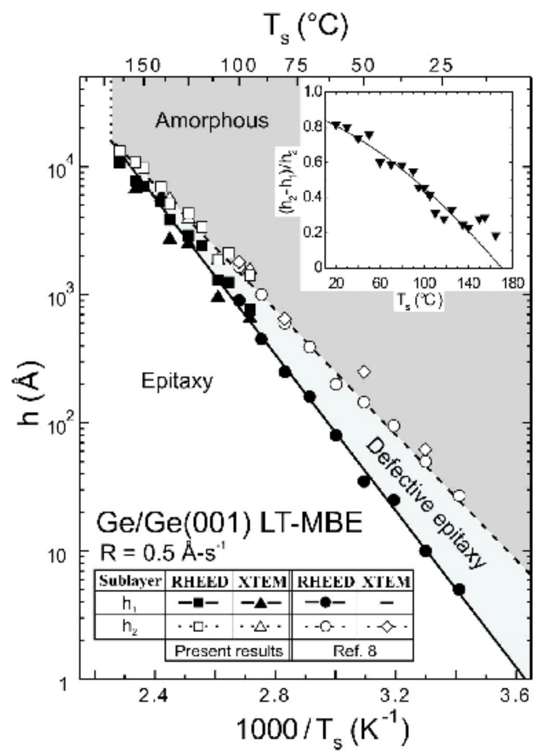


FIG. 2. [110] bright-field zone-axis XTEM micrographs of Ge(001) layers grown by LT-MBE at T_s with $R = 0.5$ Å s^{-1} to thicknesses h. (a) $T_s = 95$ °C, $h = 2100$ Å and (c) $T_s = 135$ °C, $h = 6750$ Å. (b) and (d) are HR-XTEM images of the regions outlined by the small open white squares in (a) and (c), respectively.

initiated by double-positioning defects on {111} facet planes and microtwins. Examples are shown in Figs. 2(b) and 2(d)



➢**At given temperature, there is a limit on the epi layer thickness.**

Evolution of Ge epitaxial growth front

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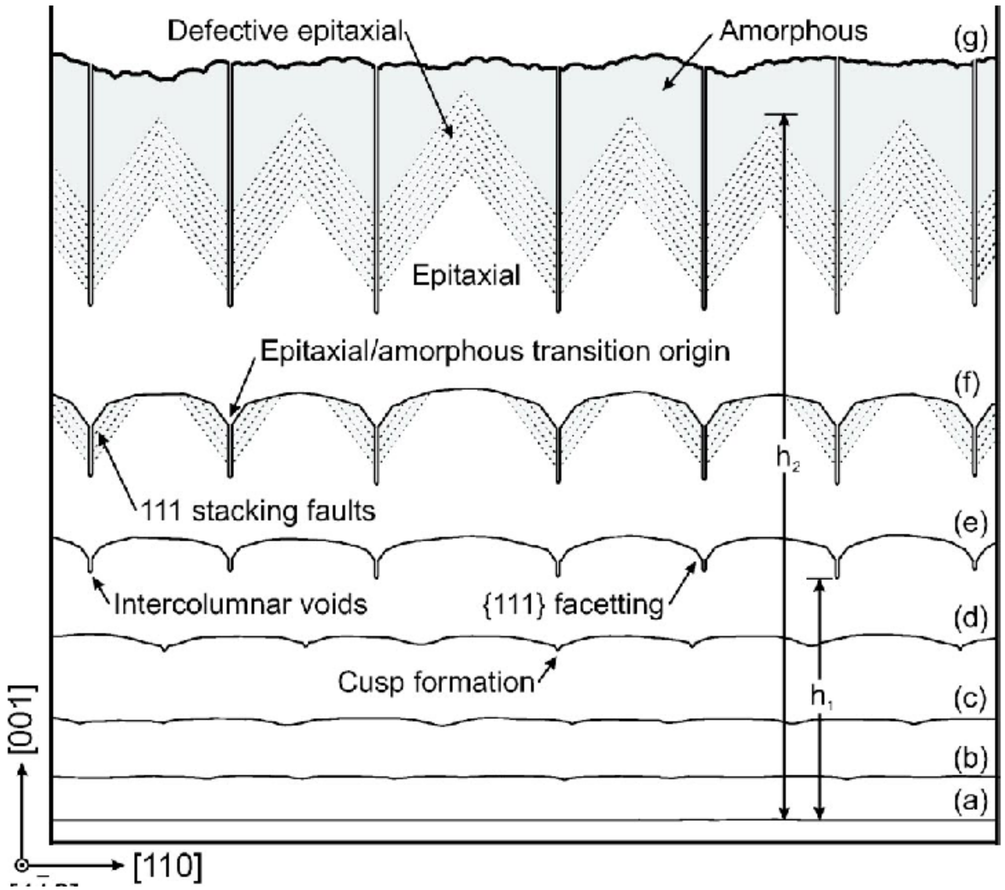
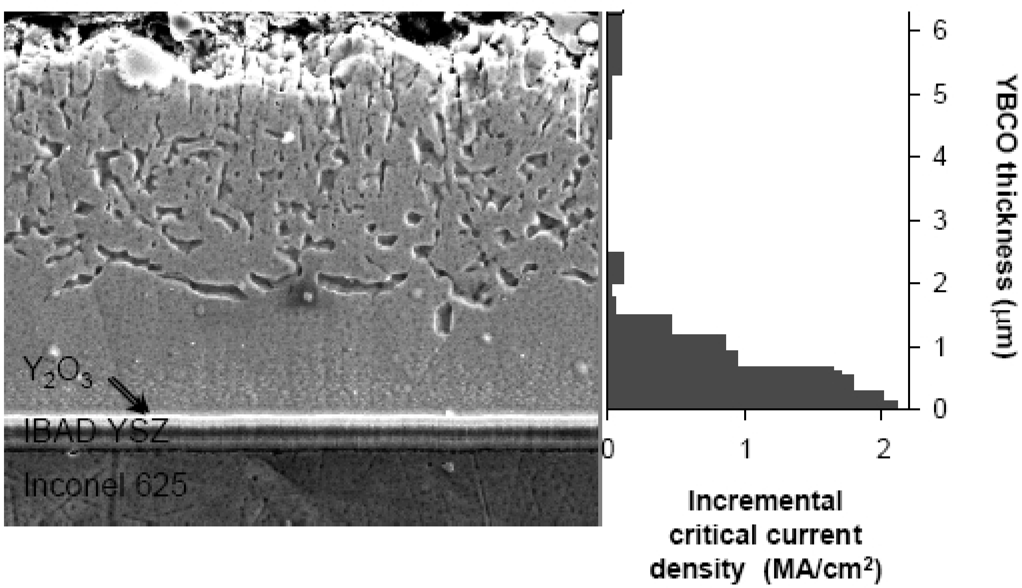


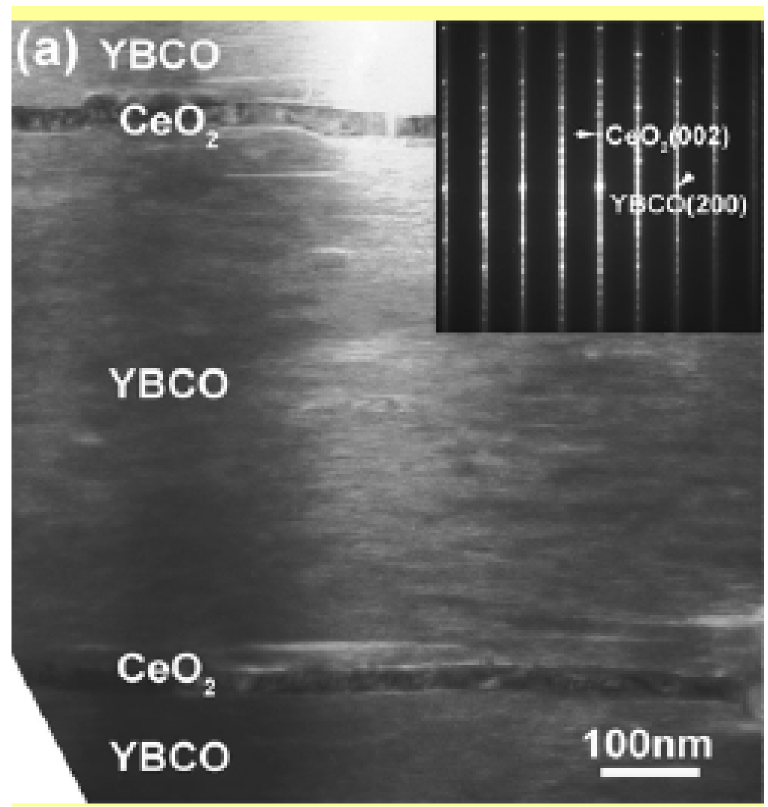
➢**Defects amplify as the thickness increases resulting in complete loss of epitaxy at the critical thickness.**

Case 2: epitaxial growth of thick YBCO film by PLD (Los Alamos result)

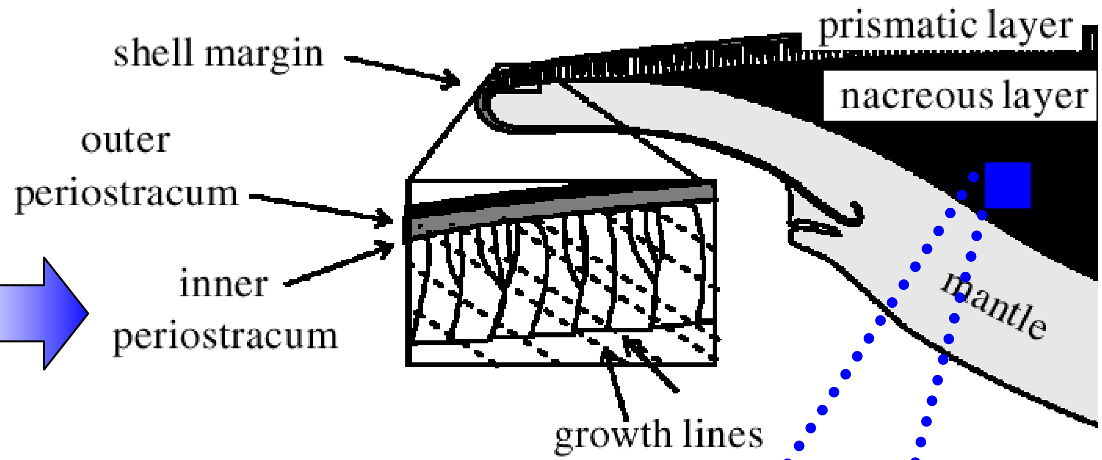
Single-layer

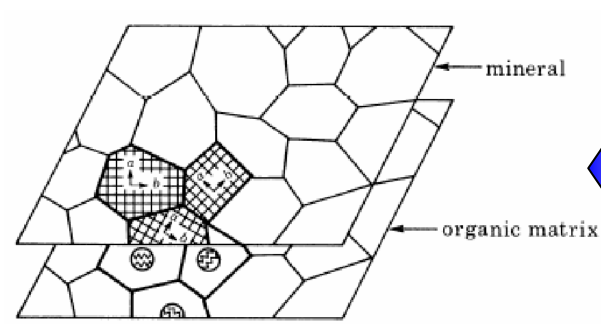


Solution: Multi-layer

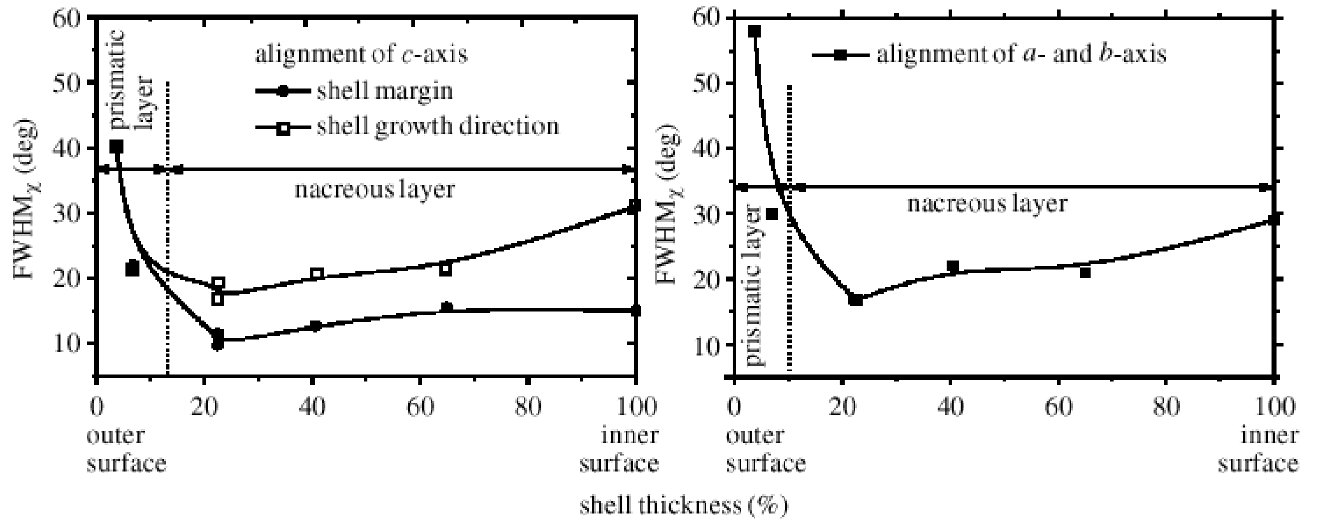


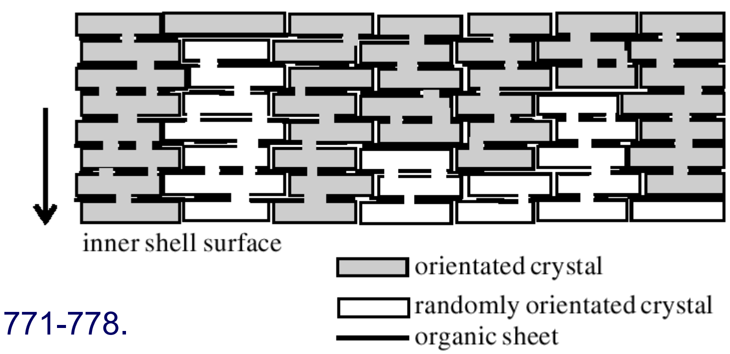
Case 3: growth of nacreous (mother of pearl) layer in a clam shell





Degradation of texture in the shell's nacreous layer

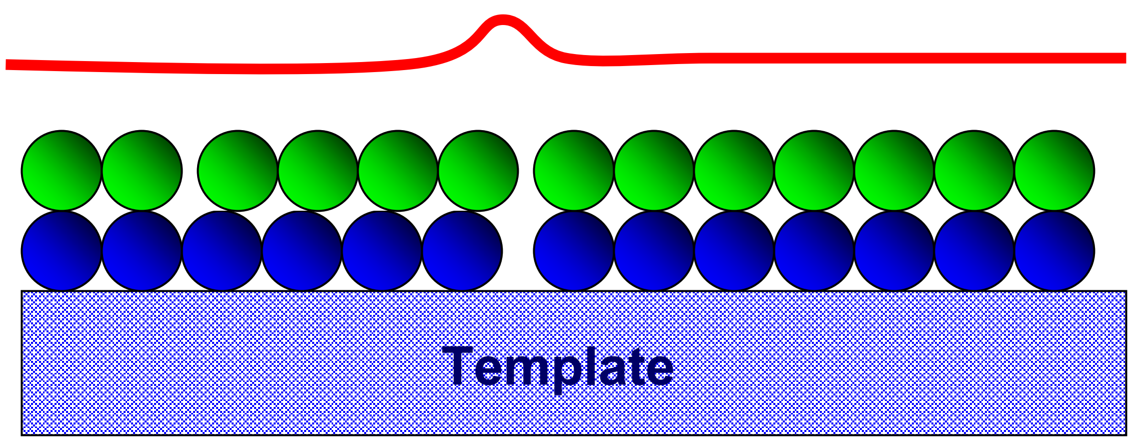




Antonio, G. Checa, Alejandro, RodrÃguez-Navarro,
Proceedings of the Royal Society B: Biological Sciences, vol. **268** (2001), pp. 771-778.

- **Defect accumulation leads to texture degradation of the nacreous layer**

Why defects accumulate?
We are paying price for making materials from atoms.



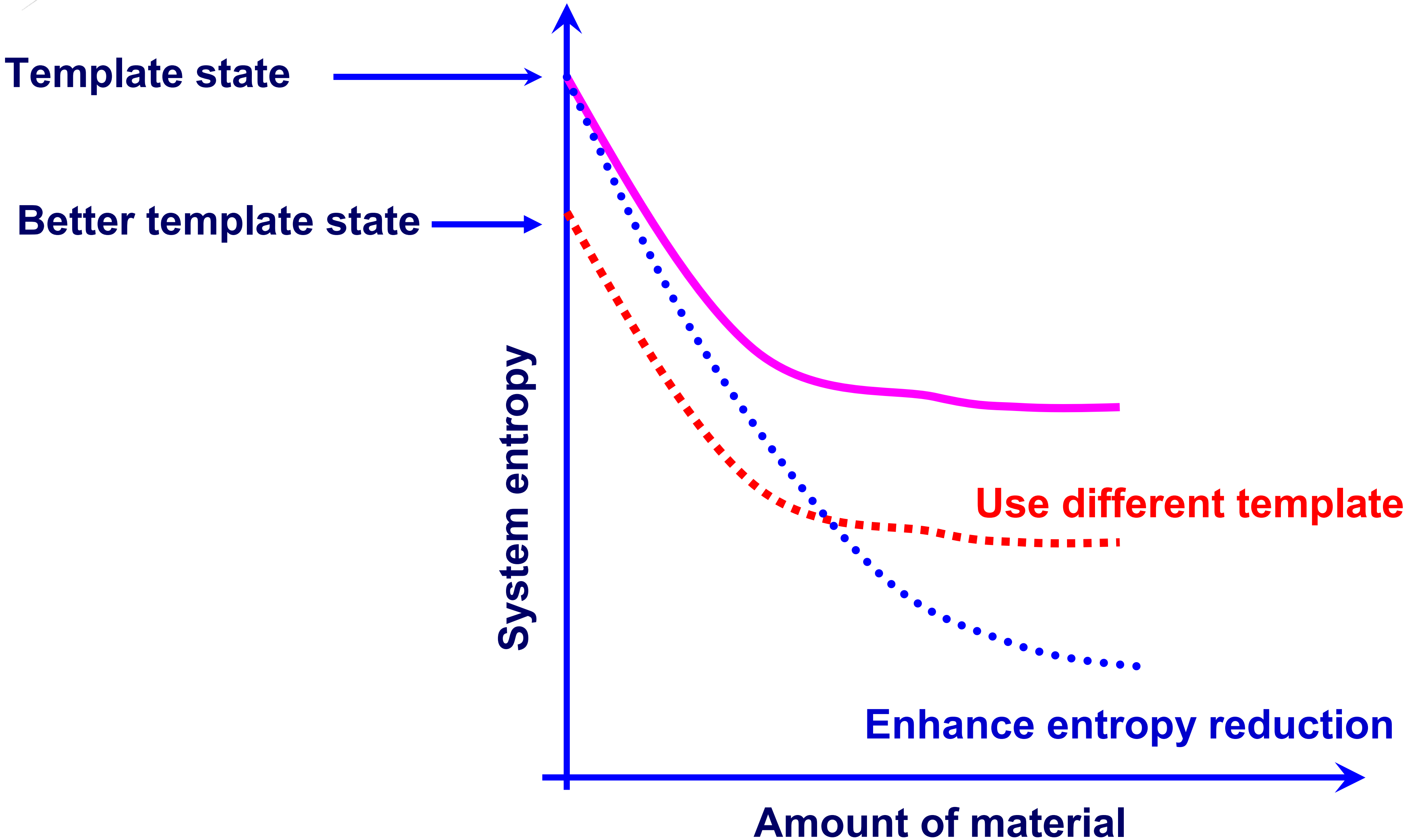
Surface term σ

Volume term σ

$\mu = \kappa T \ln(P/P_e)$

- **Homoepitaxy is sensitive to high-frequency fluctuation of the attraction potential.**
- **Heteroepitaxy is integrates the potential reducing effects of high-frequency harmonics.**

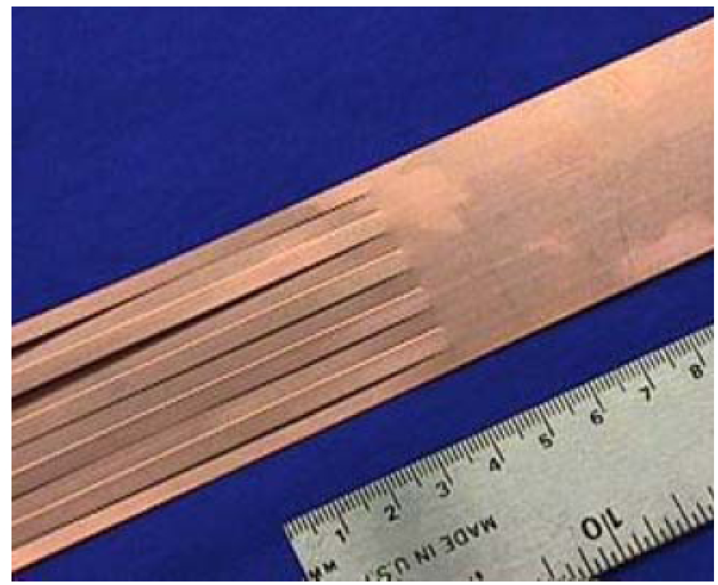
What can we do to make material more perfect?



Template factor: two very different substrates

Good, but expensive: $SrTiO_3$

Not so good, but cheap:
CeO_2 buffered tape.

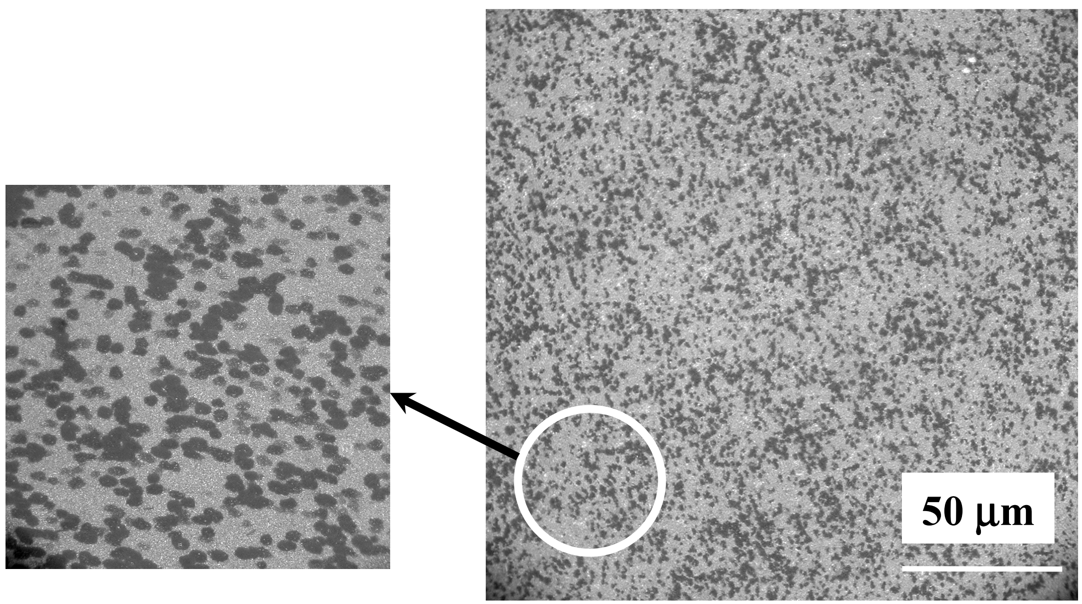


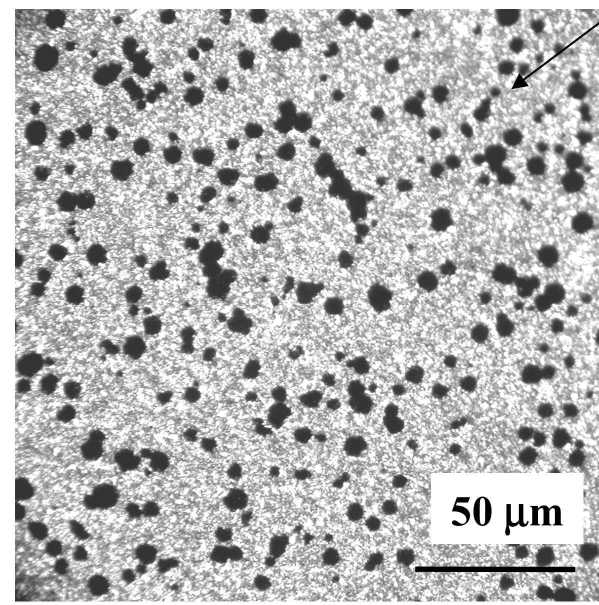
Nucleation efficiency of these two very different templates

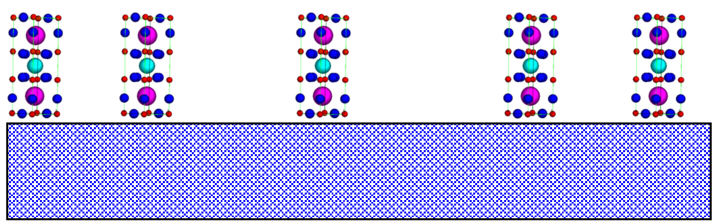
Good, but expensive: $SrTiO_3$

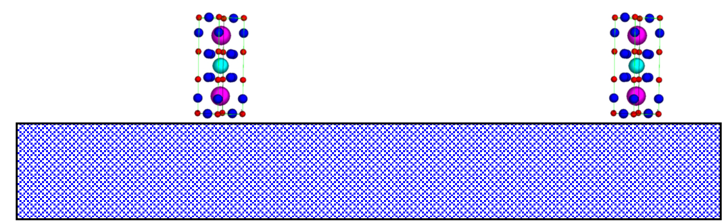
Not so good, but cheap: CeO_2 buffered tape.

YBCO



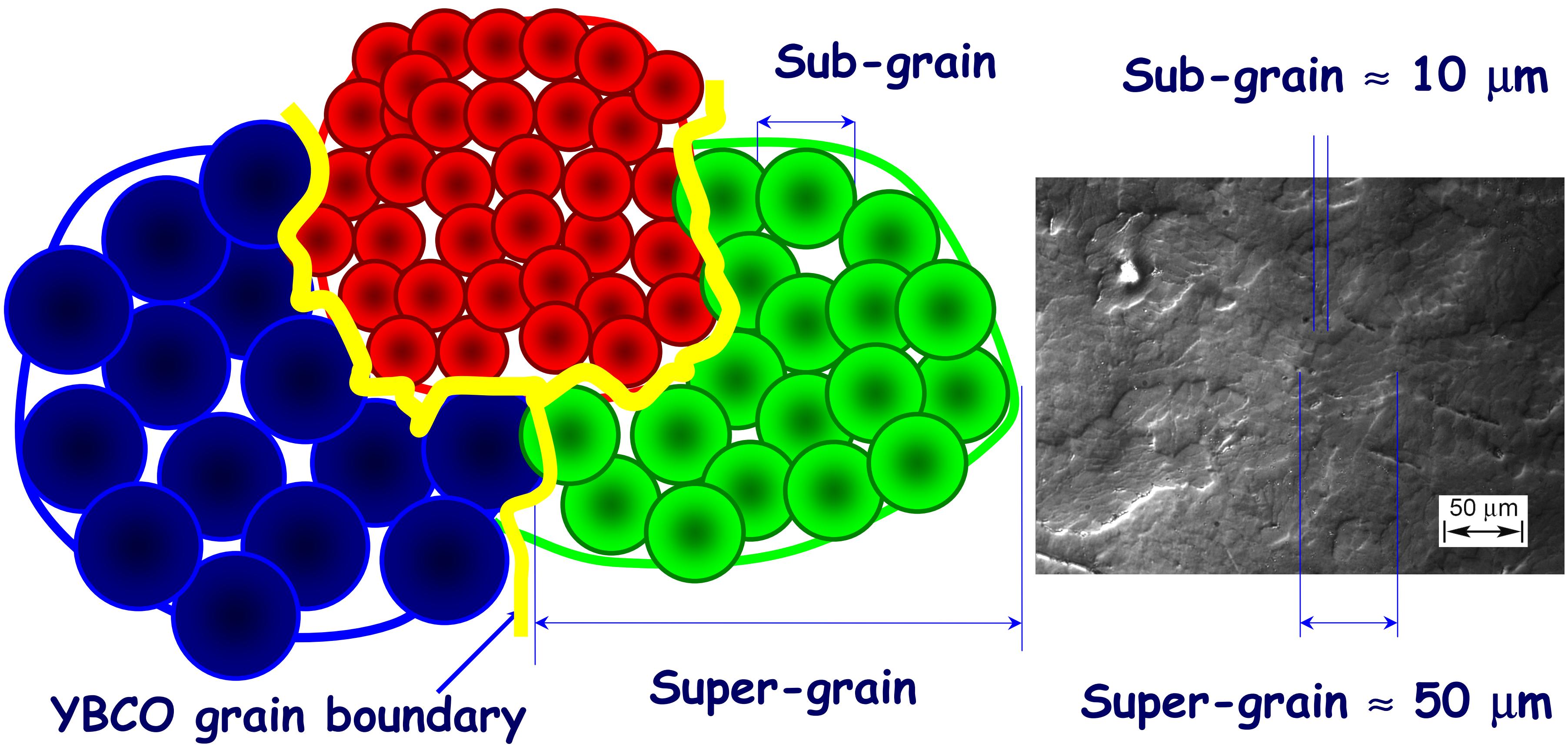






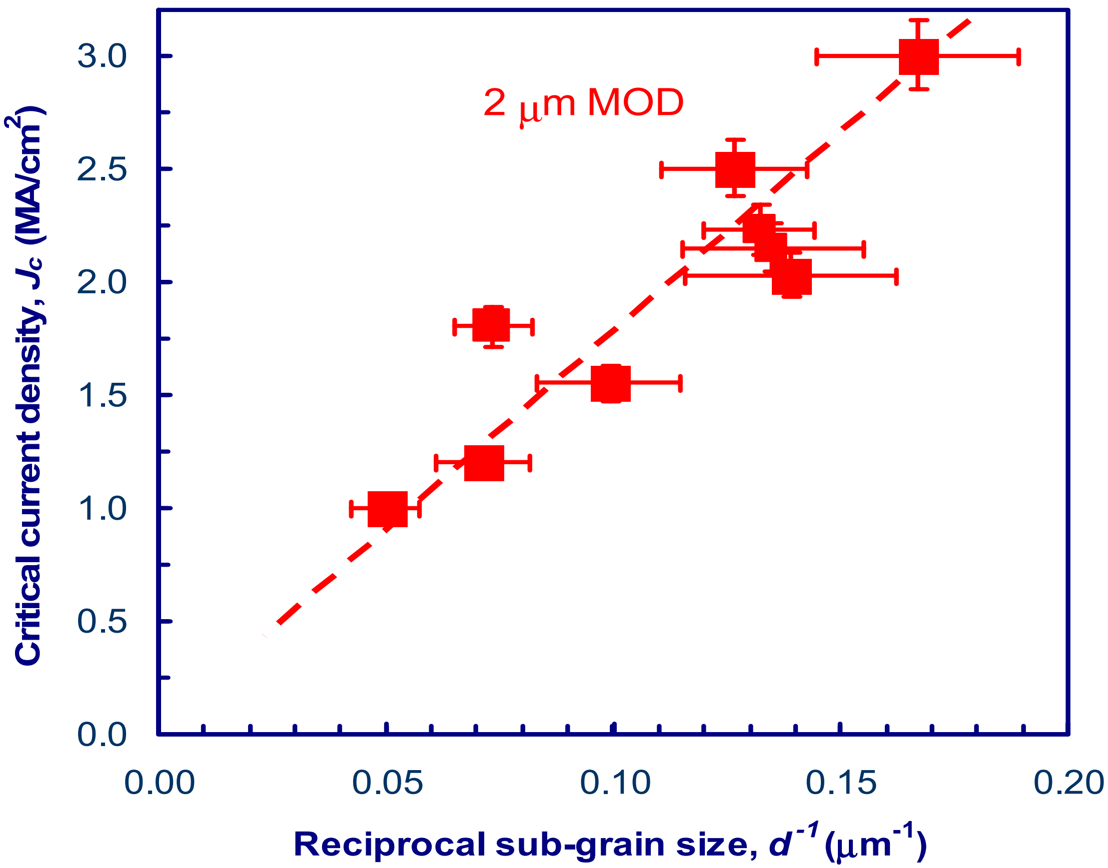
What makes "good" YBCO layer?

Complete YBCO layer



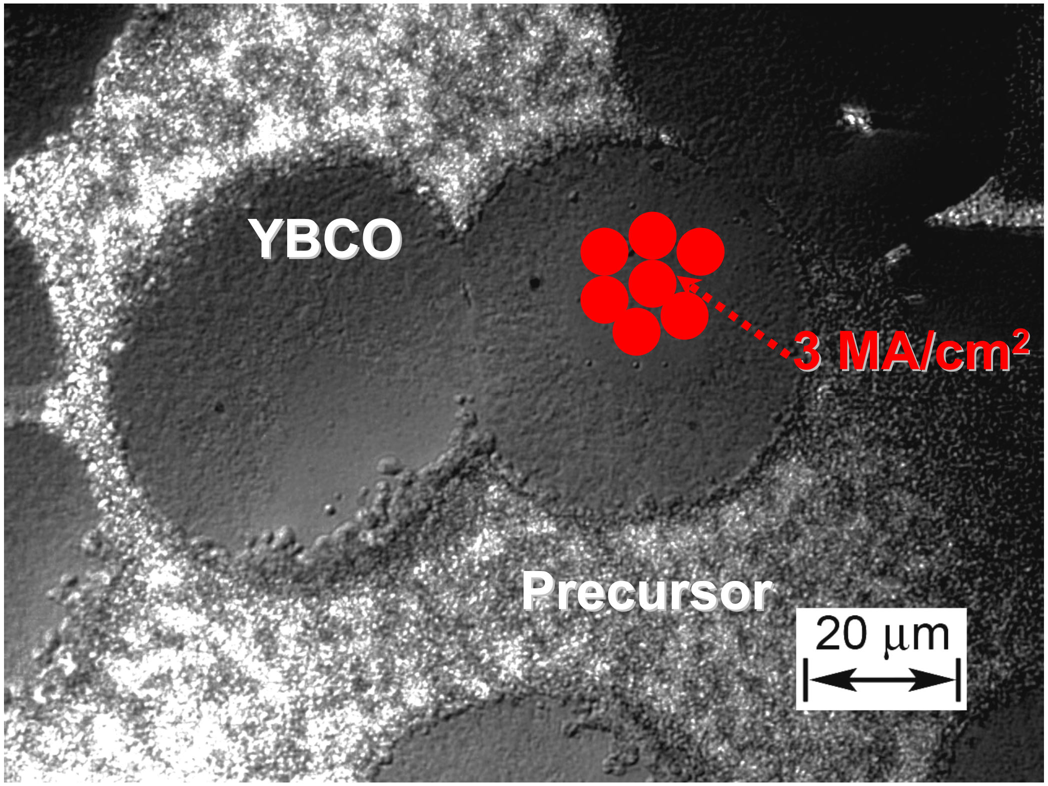
➢ **Small sub-grains make good YBCO layer!**

Sub-grain size effect on J_c



- **J_c is inversely proportional to the sub-grain size!**

Why small grains make good material? *or* Why large grains make bad material?



- Structure degrades when the nuclei expand laterally.

Accumulation of dislocations in expanding YBCO island during PLD deposition

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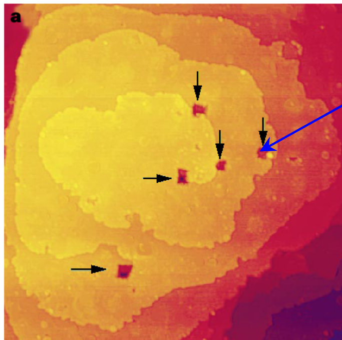
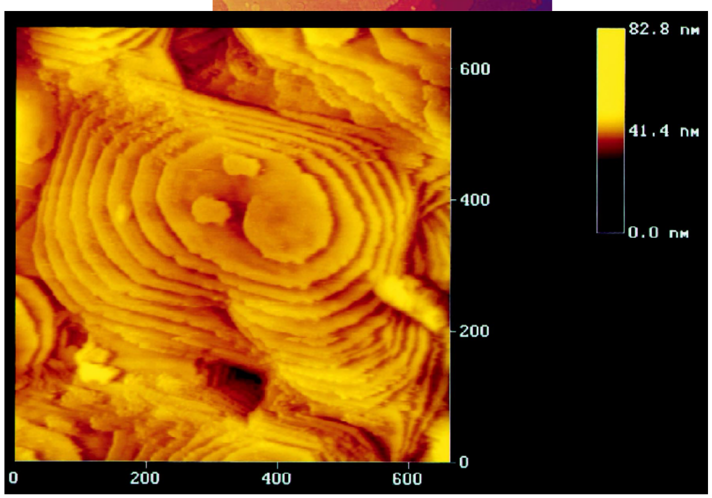
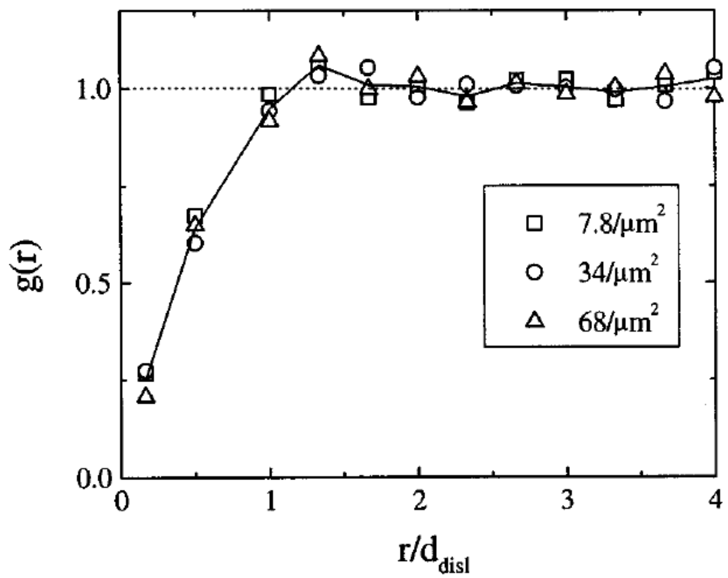


Dislocations revealed by etching

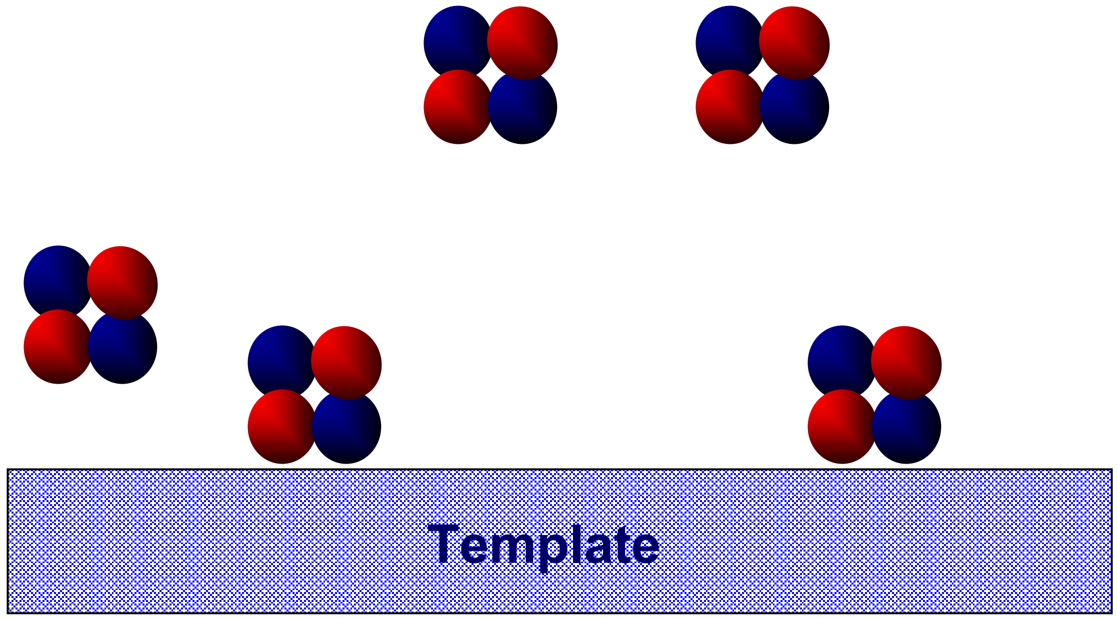




B. Dam, J. M. Huijbregtse, F. C. Klaassen et al., Nature 399 (6735), 439-442 (1999).

➢ **These dislocations may be responsible for high-field Jc of these films.**

Can nano-technology make a breakthrough?

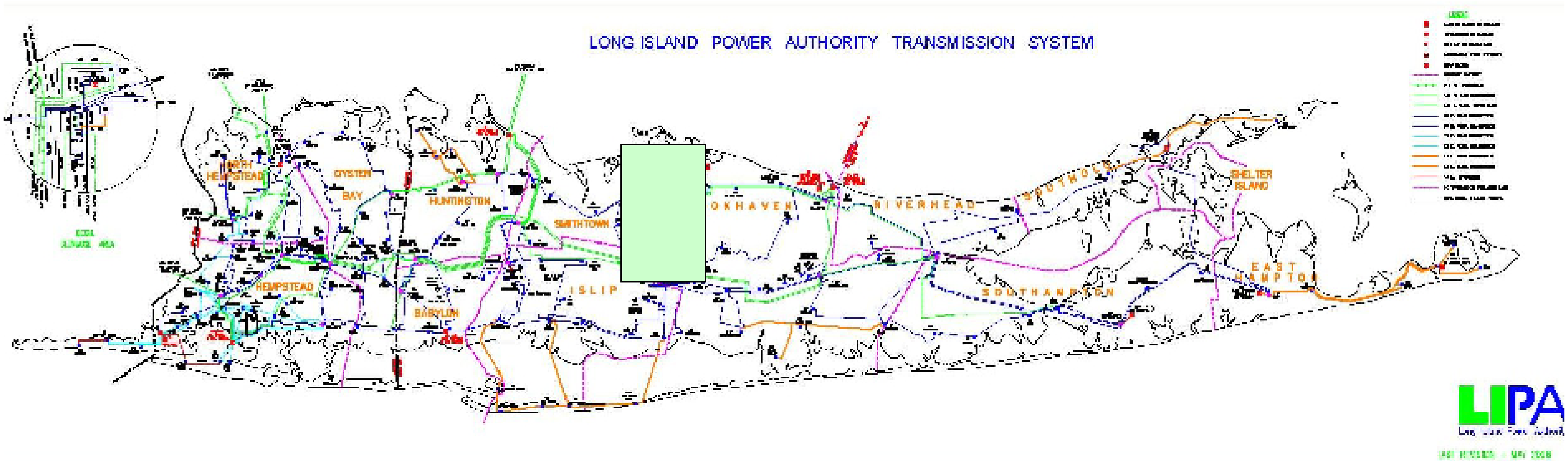


➢ **If we could make material from pre-assembled nano-blocks, we may avoid defect accumulation.**

Conclusion

- **Very difficult to make bulk perfect.**
- **Right epitaxial film has a potential to be far more perfect object than a crystal.**
- **In epitaxial growth right substrate (probably not off-shelf) is 90% of the success, very little we can do with thermal activation.**
- **Complex materials challenges:**
  - **No melting point**
  - **No reversibility**
  - **Competition from other phases (rich phase diagrams)**

Price of perfection and complexity: YBCO wires



American Superconductor

LIPA Long Island Power Authority

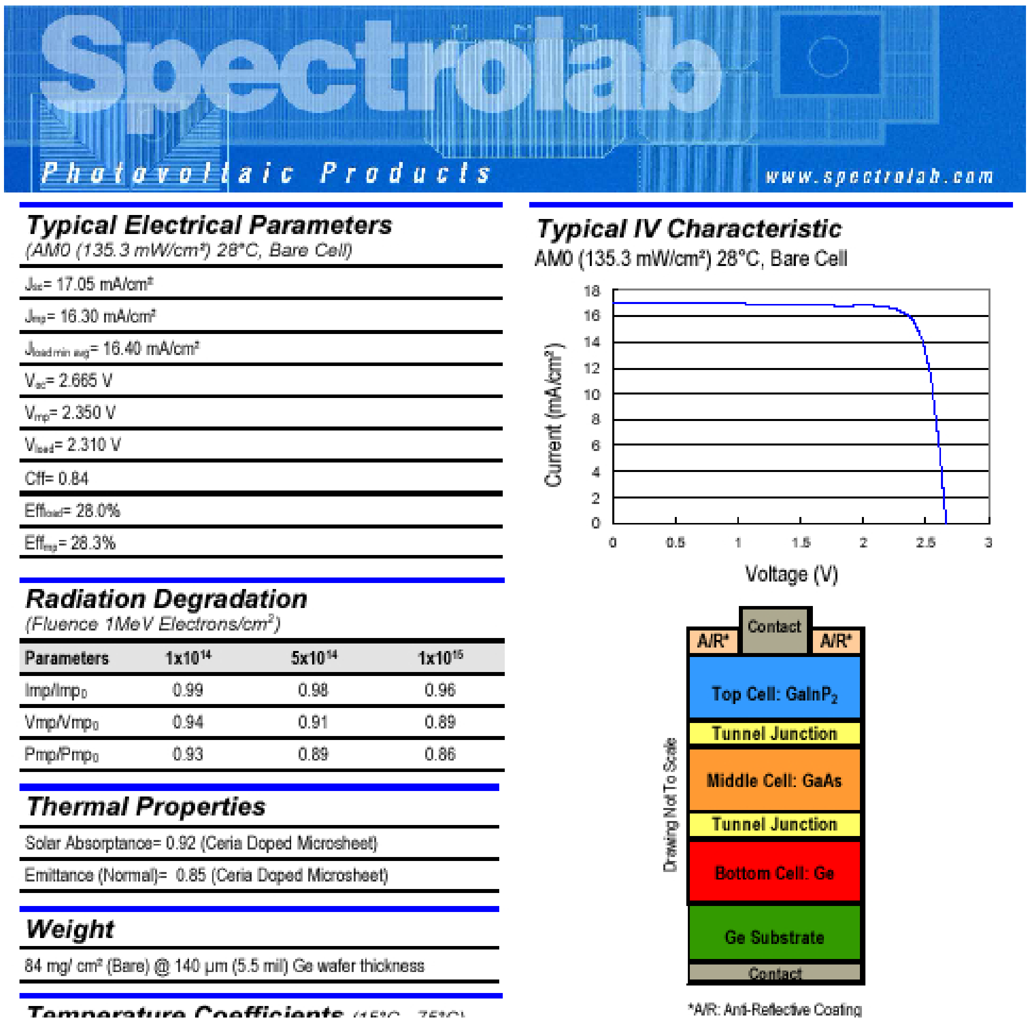
DEPARTMENT OF ENERGY • UNITED STATES OF AMERICA

AIR LIQUIDE

Nexans

- **Current wire price is $1,200 KA/m.**
It has to go down by a factor of 100.

Price of perfection and complexity: solar cells



Spectrolab

Photovoltaic Products

www.spectrolab.com

Typical Electrical Parameters

(AM0 (135.3 mW/cm²) 28°C, Bare Cell)

J_{sc}= 17.05 mA/cm²
J_{mp}= 16.30 mA/cm²
$J_{load\ min\ avg}$= 16.40 mA/cm²
V_{oc}= 2.665 V
V_{mp}= 2.350 V
V_{load}= 2.310 V
Cff= 0.84
Eff_{load}= 28.0%
Eff_{mp}= 28.3%

Radiation Degradation

(Fluence 1MeV Electrons/cm²)

Parameters	1x10¹⁴	5x10¹⁴	1x10¹⁵
Imp/Imp₀	0.99	0.98	0.96
Vmp/Vmp₀	0.94	0.91	0.89
Pmp/Pmp₀	0.93	0.89	0.86

Thermal Properties

Solar Absorptance= 0.92 (Ceria Doped Microsheet)
Emittance (Normal)= 0.85 (Ceria Doped Microsheet)

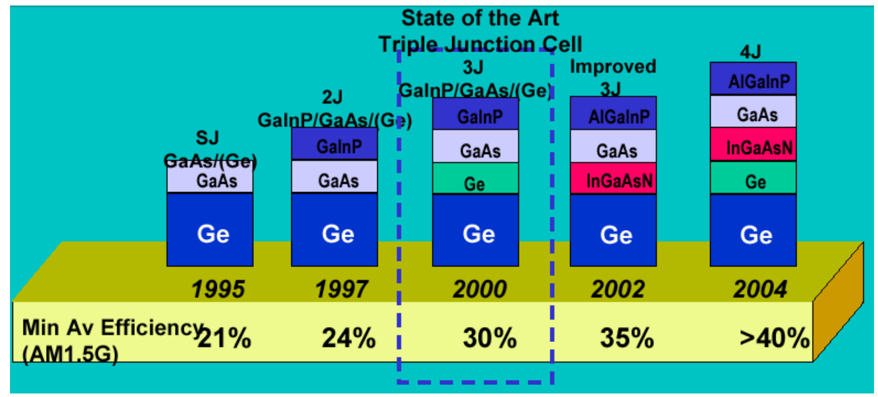
Weight

84 mg/ cm² (Bare) @ 140 μm (5.5 mil) Ge wafer thickness

***Temperature Coefficients** (15°C - 75°C)*

Typical IV Characteristic

AM0 (135.3 mW/cm²) 28°C, Bare Cell



Spectrolab:

Rectangular Dual Junction

GaAs/Ge solar cell:

1.23" x 2.72"

286 mA at 2.05 V

20.02% - above

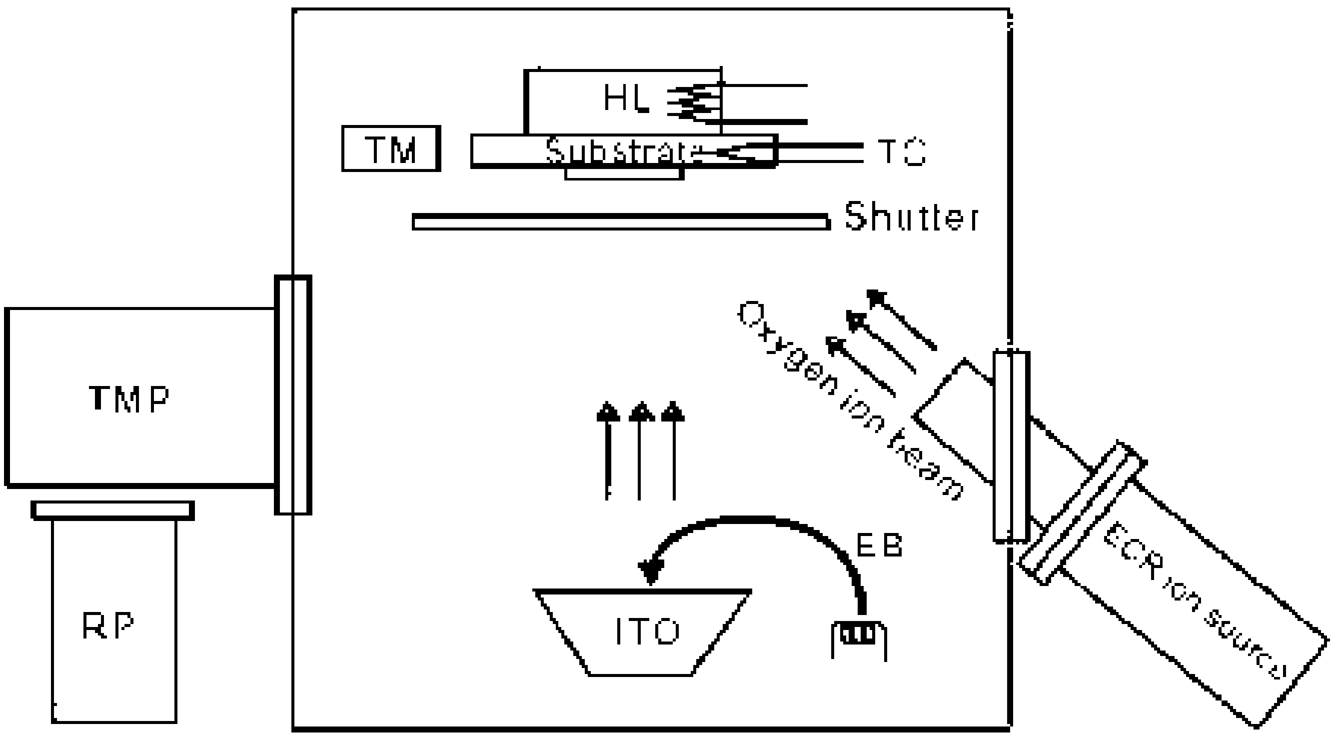
$630.00 for 50 cells

$22/Watt

1 kW = $22,000

Ion beam assistance (IBAD):
More effective entropy reduction

Dislocations revealed by etching



➢**IBAD allows use of non-epitaxial substrate.**