Joints de grains : couplage entre modélisation et microscopie électronique haute résolution

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Lab. d'Étude des Matériaux par Microscopie Avancée (Lemma), *idem*

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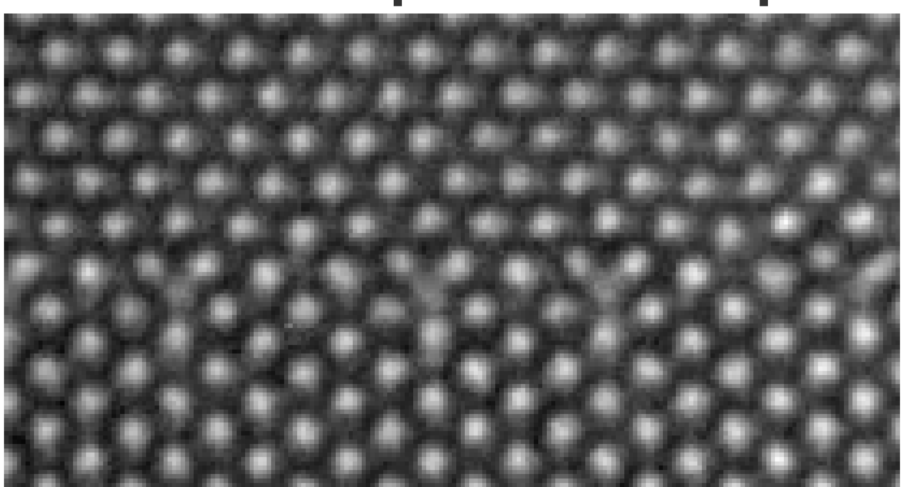
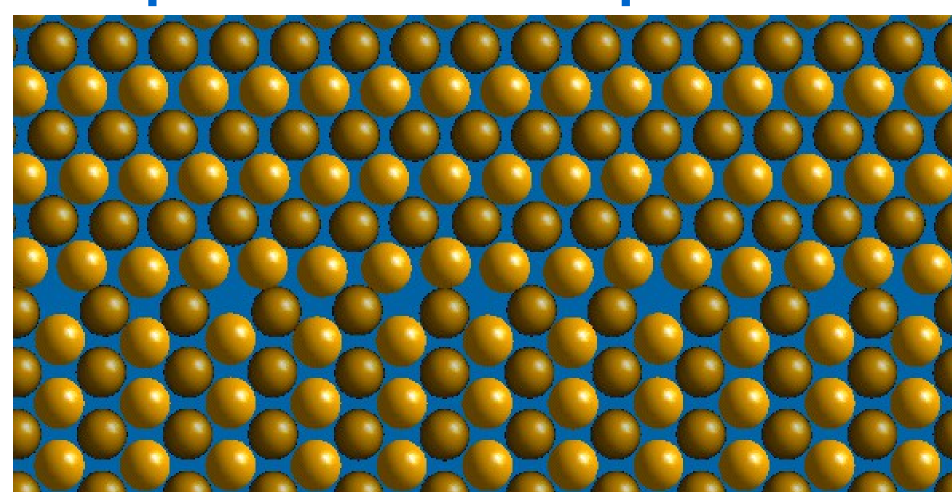
National Center of Electron Microscopy, LBNL, **Berkeley**, USA

Joint de grain incommensurable

Microscopie électronique ↔ **Expérience numérique**





○ **L_Sim** : Laboratoire de simulations atomistiques

○ **INAC** → Institut de Nanosciences et Cryogénie

○ **CEA-Grenoble**

Chercheurs L_Sim : 7 permanents,
4 doctorants,
5 post-doctorants

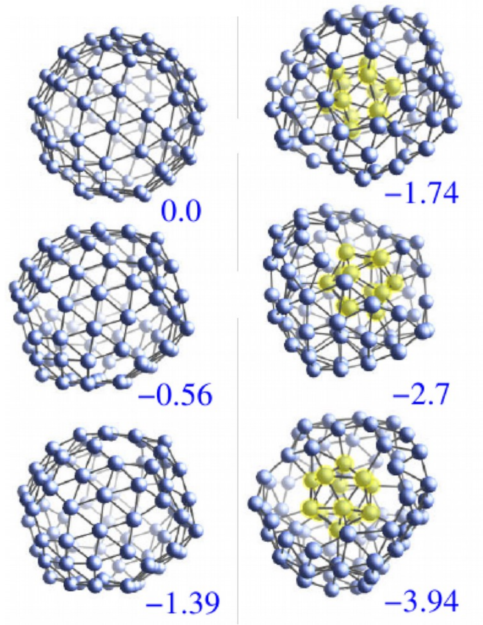
- Méthodes ab initio (BigDFT) : Thierry Deutsch, Luigi Genovese, Laura Ratcliff
- Modélisation des matériaux (batterie, matériaux sp2-sp3, défauts Si) : Damien Caliste, Pascal Pochet, Eduardo Machado-Charry, Sridevi Krishnan, Gilles Brenet, Dilyara Timerkaeva
- Nano-électronique et liaisons fortes : Ivan Duchemin, Yann-Michel Niquet, Manuel Cobian, Viet-Hung Nguyen
- Modélisation photo-voltaïque organique (coll. X. Blase, code Fiesta) : Carina Faber
- Nano-exploration : (structures atomiques et magnétisme) : Frédéric Lançon, Giovanni Vinai

L_Sim : développement de méthodes originales pour simulation à l'échelle atomique

BigDFT
ab initio, DFT, ondelettes
Couplage avec ART

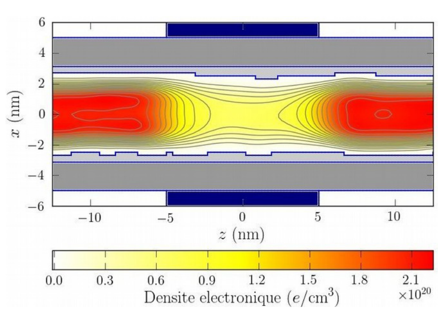
Cinétique, croissance, caractérisation
cages, défauts ponctuels

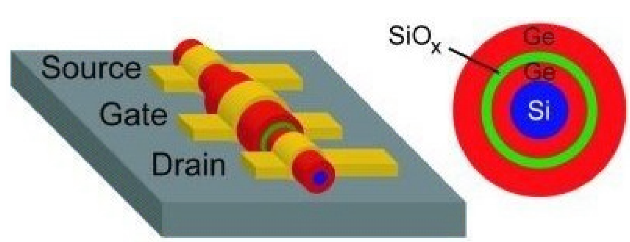
Énergies renouvelables
Batteries, Photovoltaïque

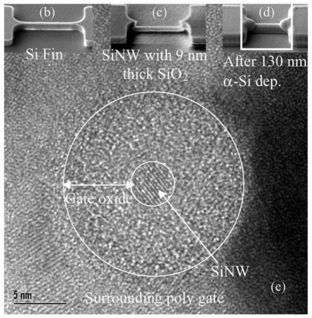


TB_Sim
Transport électronique
Couplage électron-phonon
onctions de Green hors-équilibre

Nano-électronique
Nanofils, transistors ultimes
(électron unique, blocage de Coulomb)

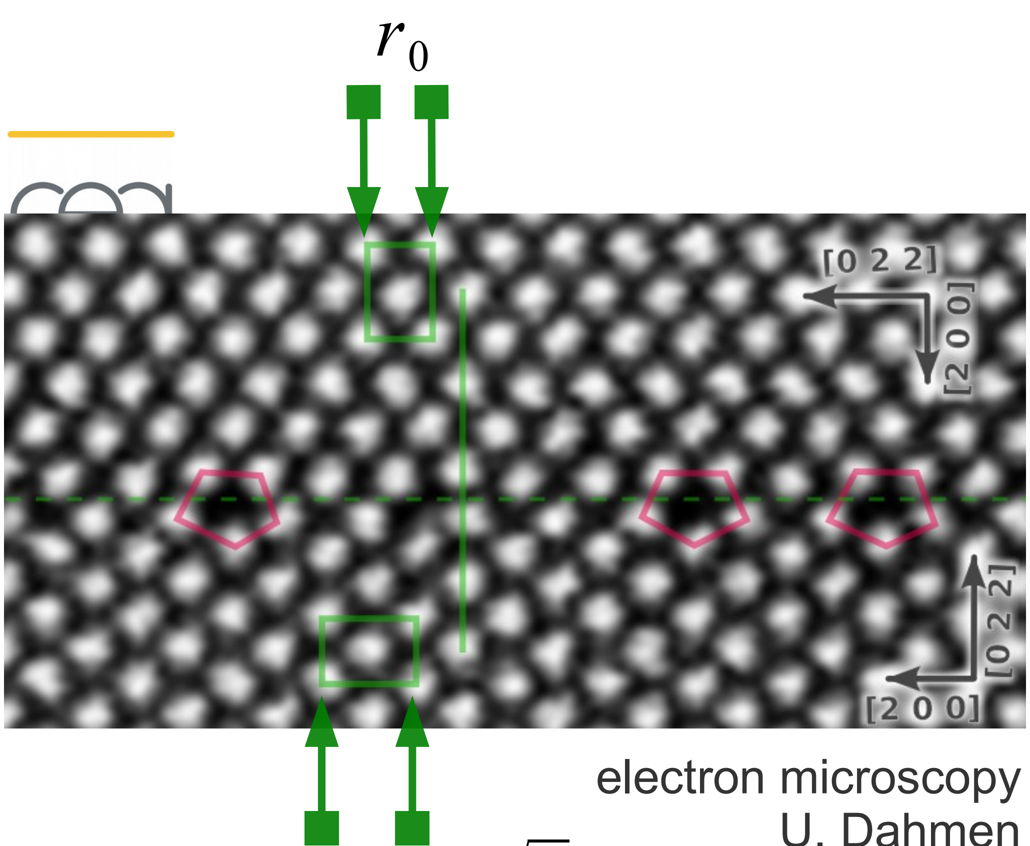






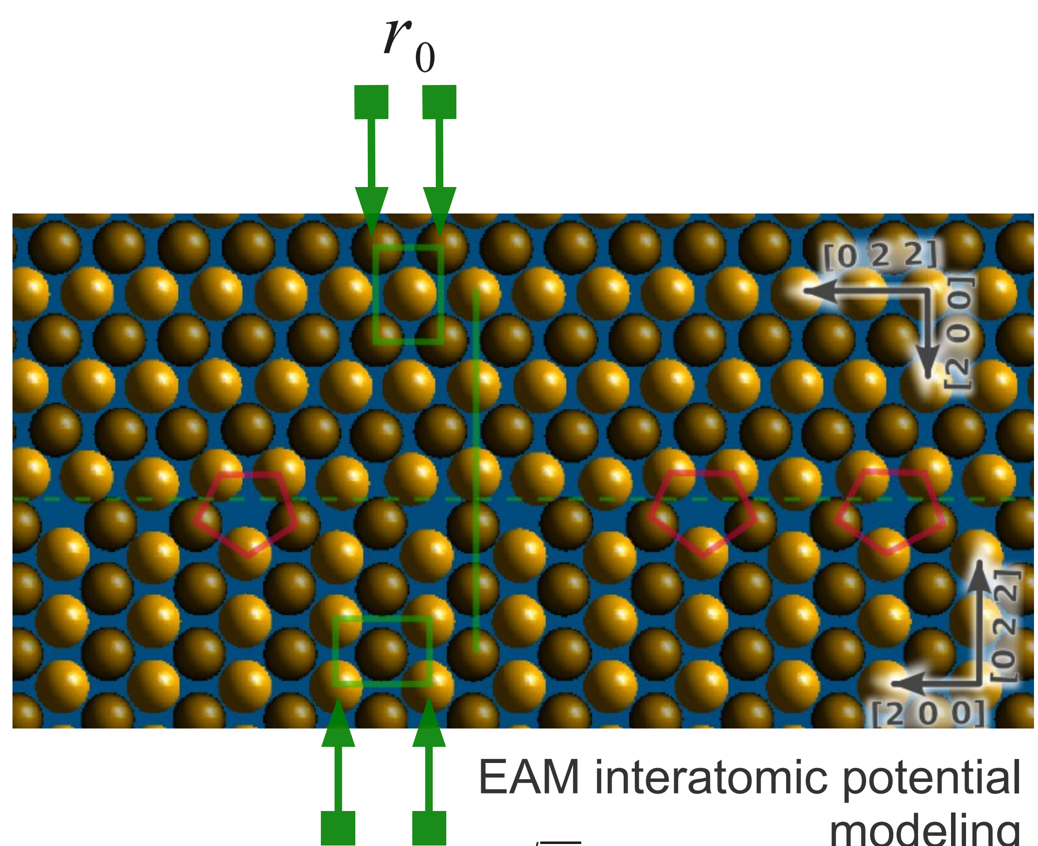
V_Sim, Mi_Magnet, d3_Sim, …

Au / Au incommensurate 90° <110> tilt grain boundary



$$a_{FCC} = \sqrt{2}\, r_0$$

electron microscopy
U. Dahmen
(Berkeley)



$$a_{FCC} = \sqrt{2}\, r_0$$

EAM interatomic potential
modeling
(Grenoble)

Simulations with a EAM potential (type: tight binding - 2nd moment app.)

N-body potentials: $$E_{pot} = \sum_{i,j}^{N} \phi(r_{ij}) - \sum_{i}^{N} F(\rho_i)$$

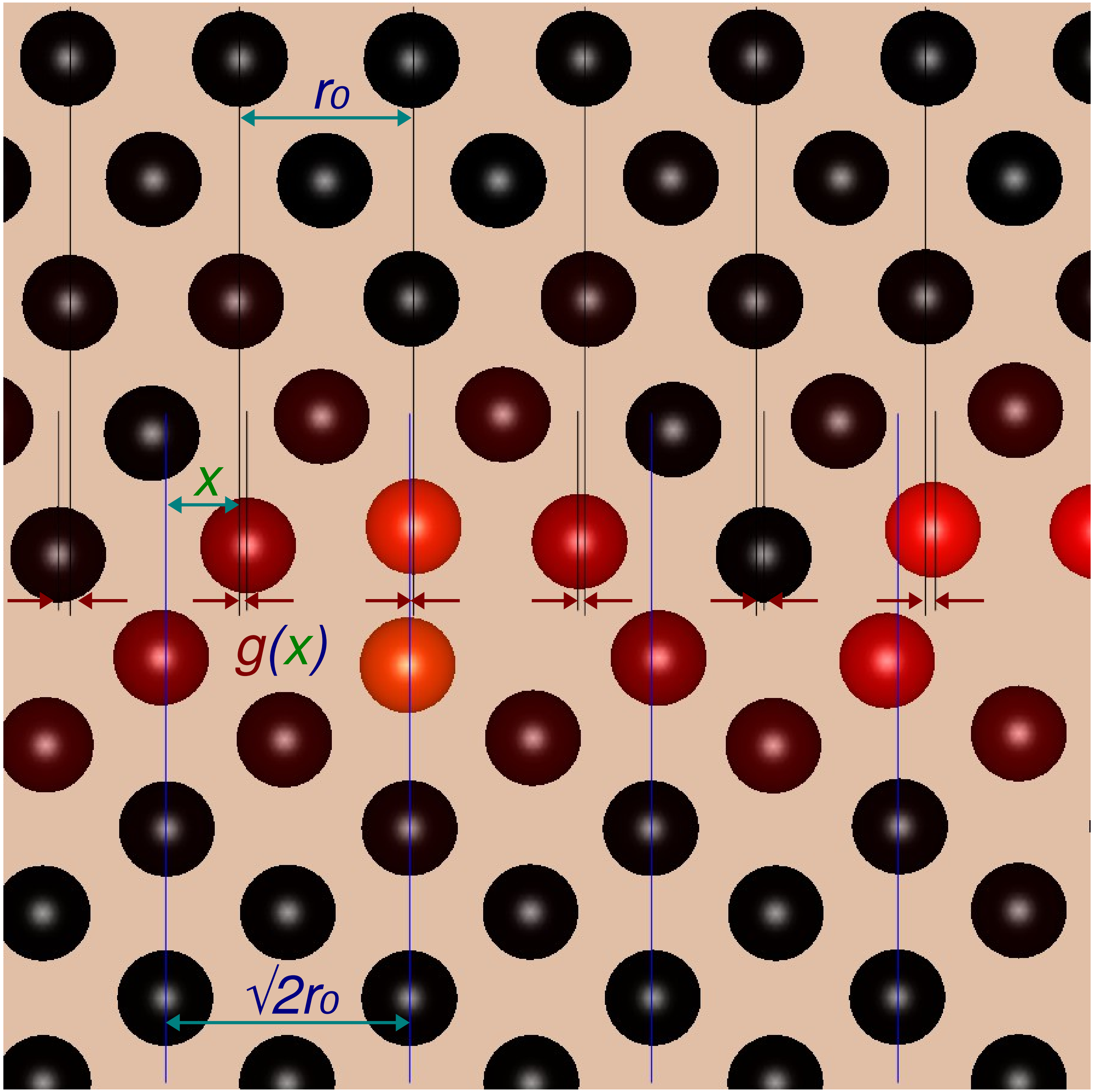
$$\underbrace{F(\rho),\quad \phi(r),\quad \psi(r)}_{\text{functions to be fitted}}$$

$$\underbrace{\rho_i = \sum_{j \neq i} \psi(r_{ij})}_{\text{local "e}^{-}\text{ density"}}$$

$$E = \sum_{\{i,j\}} A_{ij} \exp\left\{-p_{ij}\left(\frac{r^{ij}}{r_0}-1\right)\right\} - \sum_{i}\left[\sum_{j} \beta_{ij}^2 \exp\left\{-2q_{ij}\left(\frac{r^{ij}}{r_0}-1\right)\right\}\right]^{1/2}$$

The fits have been done using experimental data.

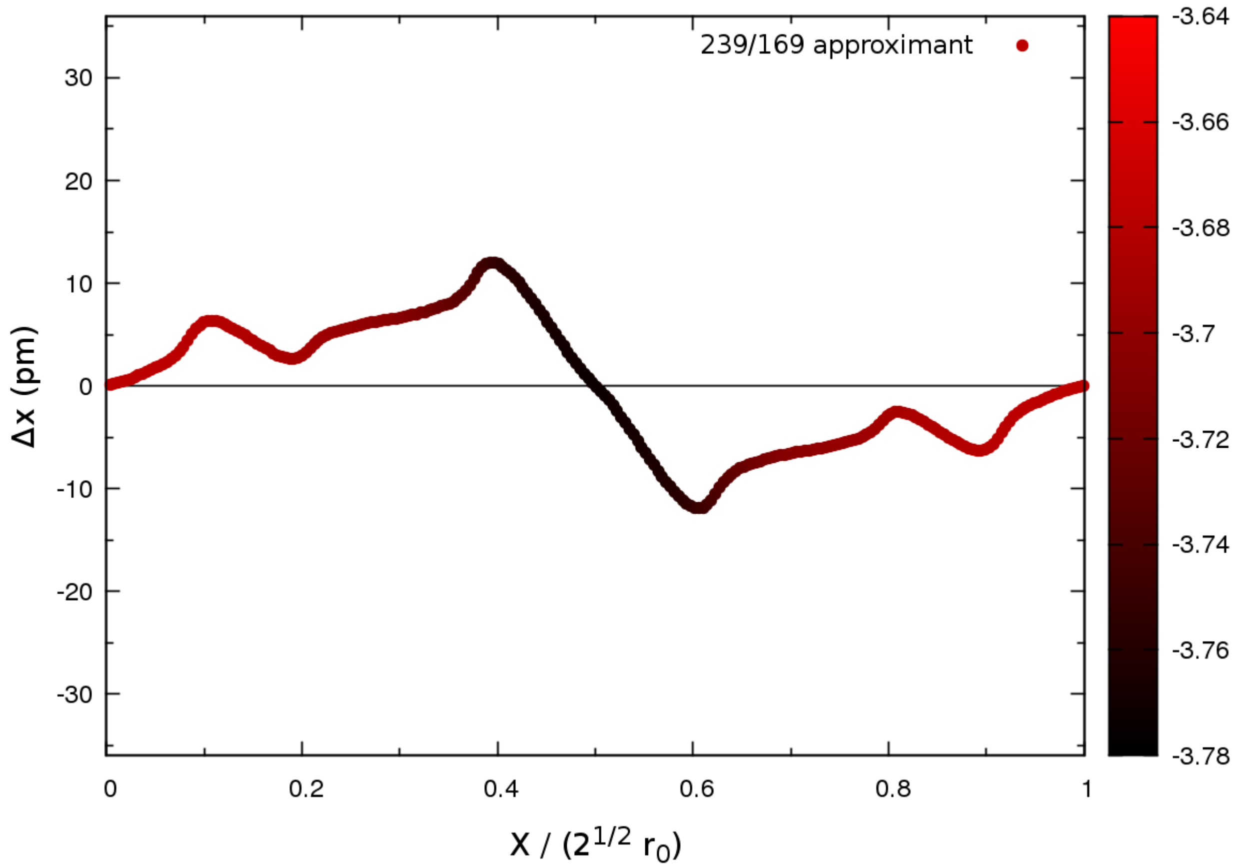
Au: Deutsch *et al*, JOP: C.M. **7** (1995) 6407.



Let us generalize, for incommensurate grain boundaries, the **hull function** introduced by Serge Aubry (1978) to analyze the Frenkel-Kontorova model (1D harmonic chain in an external periodic potential):

- ground state $\{x_i\}$
- $x_i = i\, r_0 + \alpha + g(i\, r_0 + \alpha)$
- $g(x) = g(x + \sqrt{2}\, r_0)$
- $g(x)$ is the modulation hull function
- $\alpha \in \mathbb{R}$ and indexes the ground states.

Incommensurate grain boundary in Gold : Au | Au



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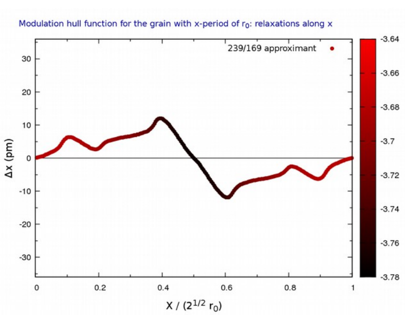
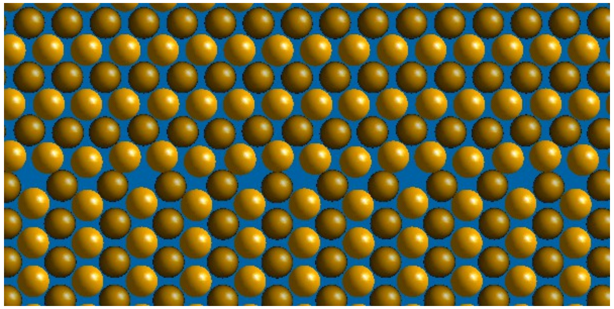
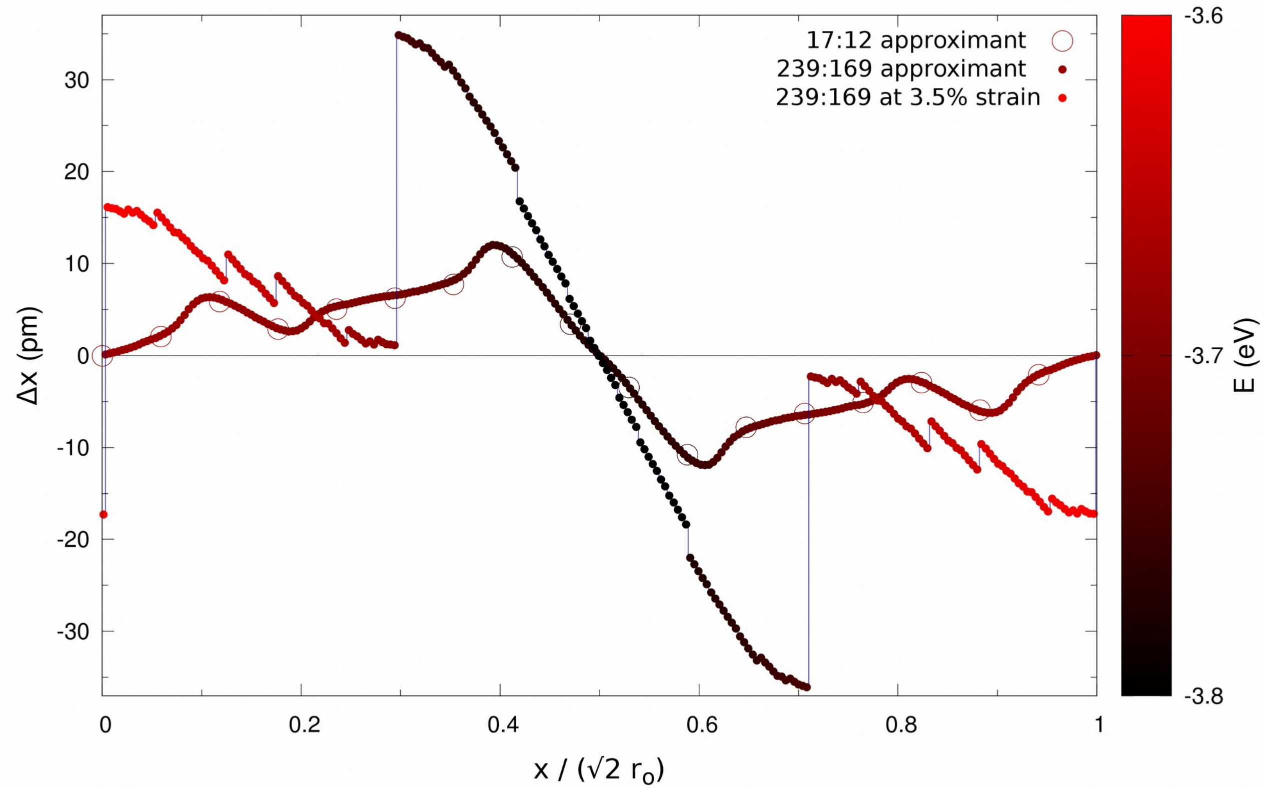




Incommensurate grain boundary in Gold : Au | Au



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- ground state $\{x_i\}$
- $x_i = i\, r_0 + \alpha \;+ g(\, i\, r_0 + \alpha\,)$
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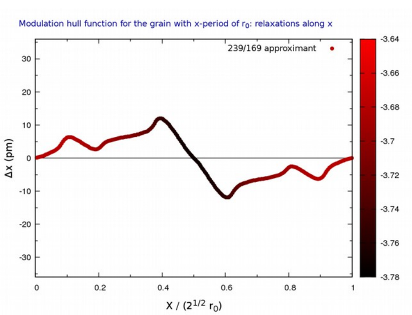
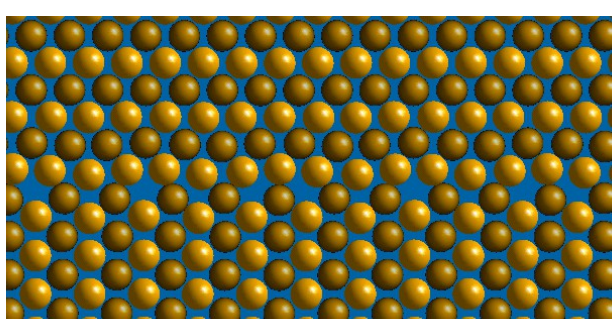
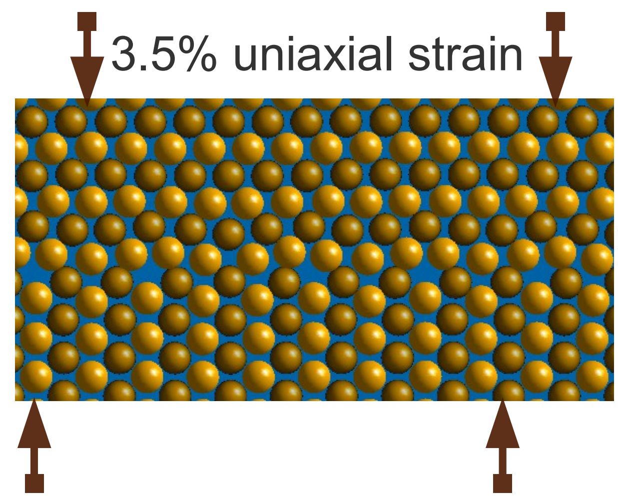
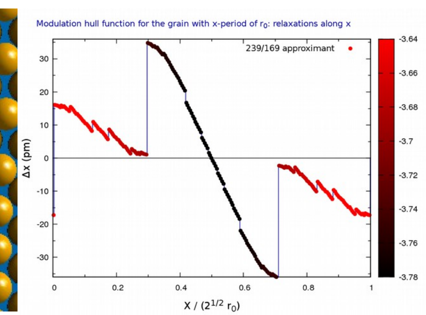


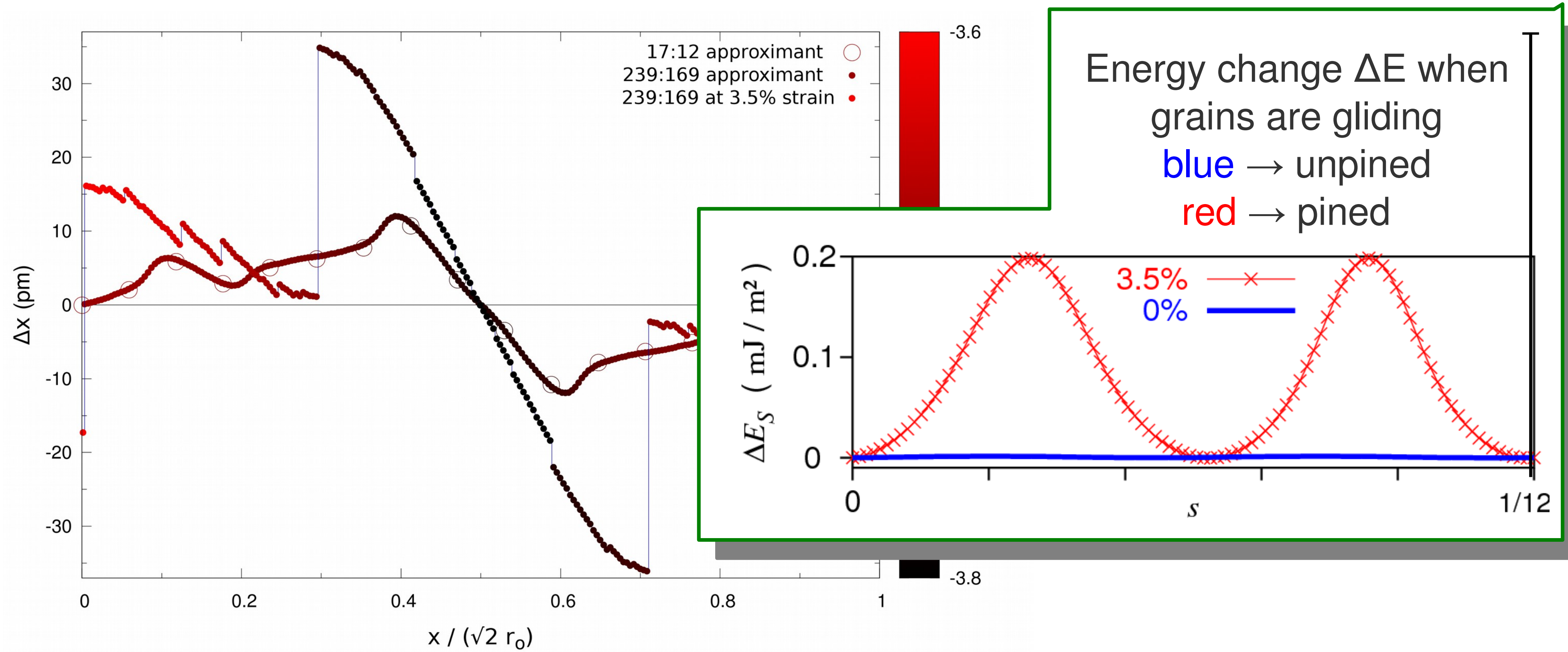


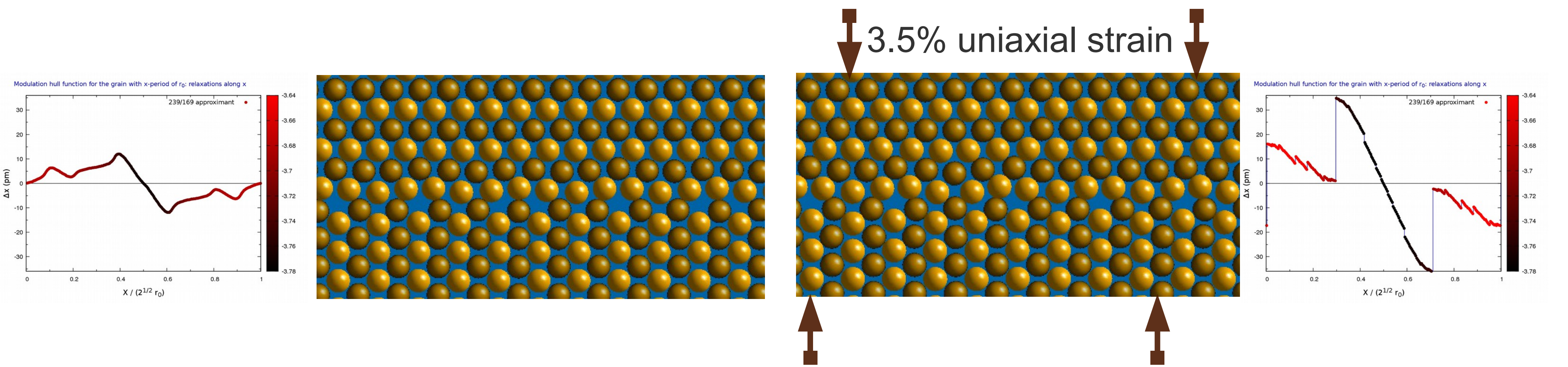
3.5% uniaxial strain



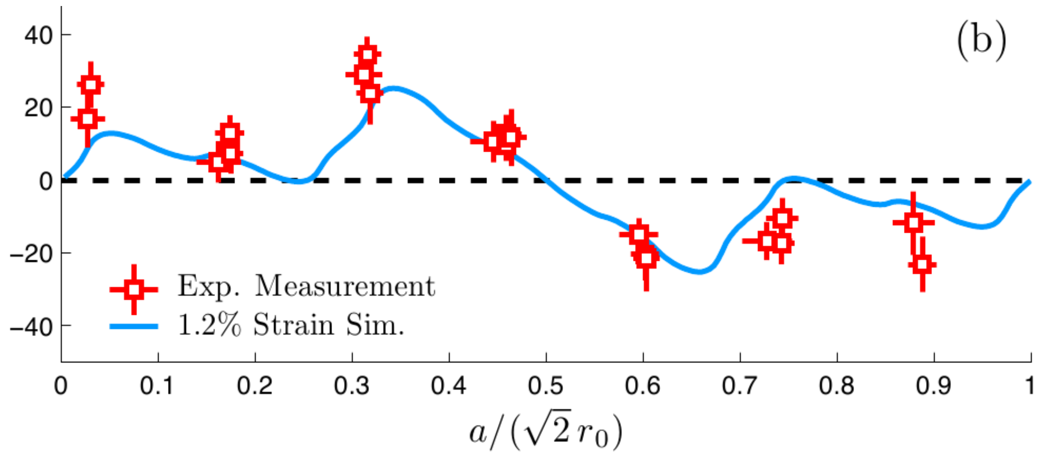


Incommensurate grain boundary in Gold : Au | Au





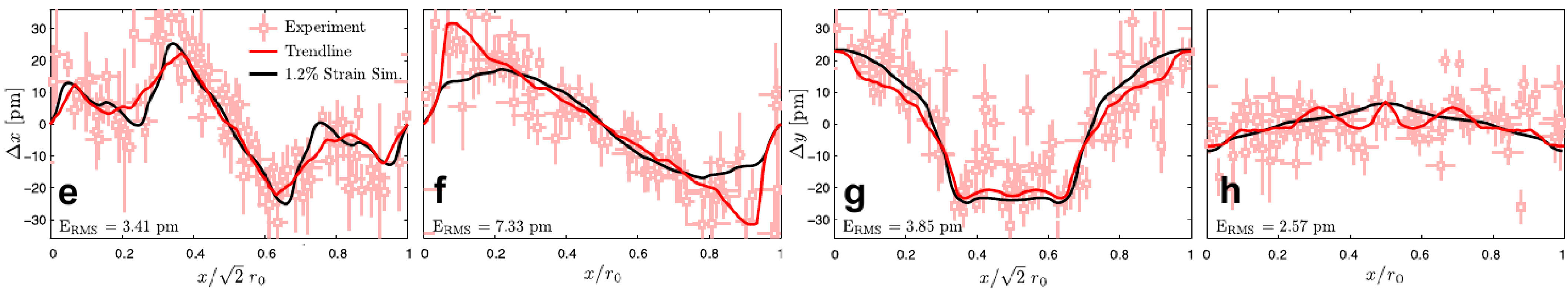
Incommensurate grain boundary in Gold : Au | Au



←(squares) Experimental measurement on one segment of the grain boundary.
←(line) model.

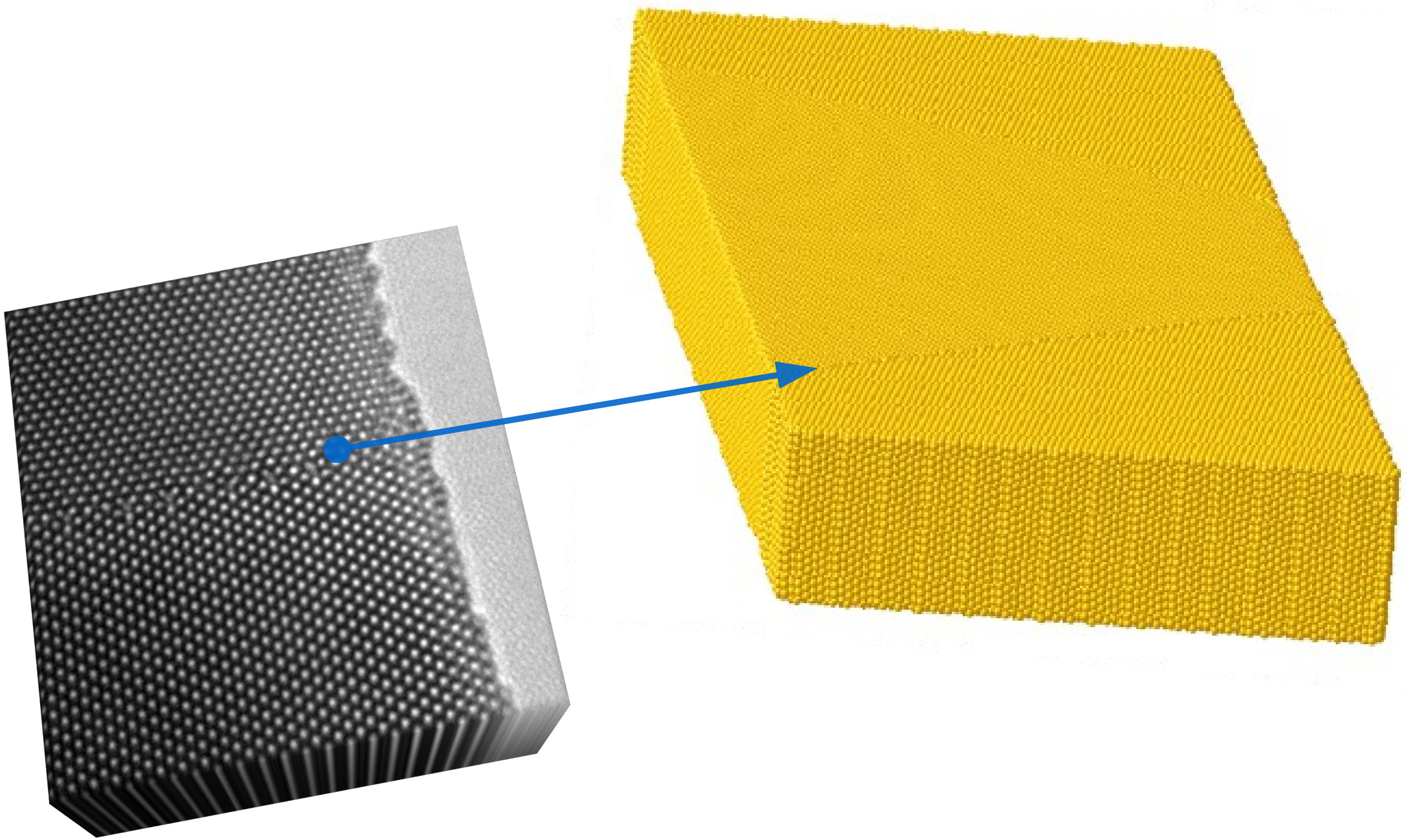
- each experimental image corresponds to **one** value of the ground state index α ...
… but with the same hull function *g(x)*.

Δ*x* — top grain   Δ*x* — bottom grain   Δ*y* — top grain   Δ*y* — bottom grain

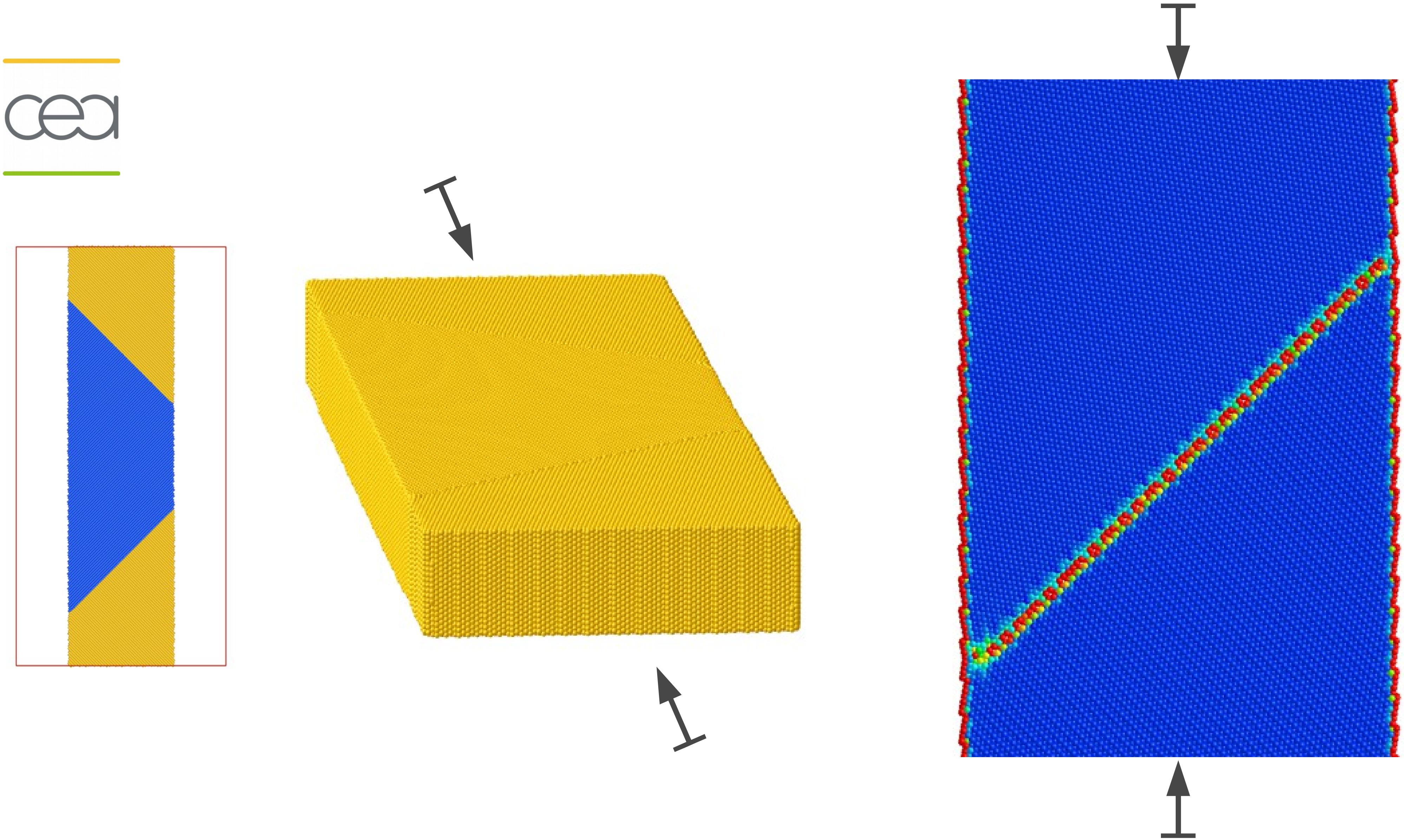


— *Atomic Structure Characterization of an Incommensurate Grain Boundary* ;
A. Gautam[1], C. Ophus[1], F.Lançon[2], V. Radmilovic[1] and U. Dahmen[1] ; submitted at Acta Materialia (January 2013)

Incommensurate grain boundary: testing the supergliging property

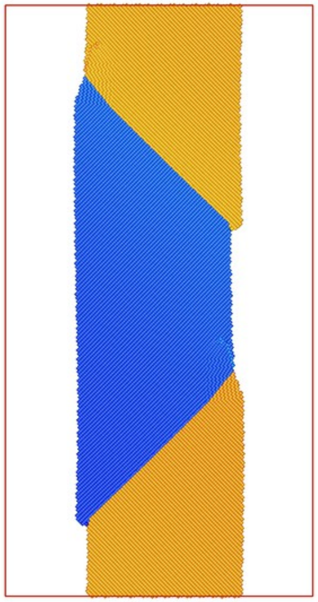


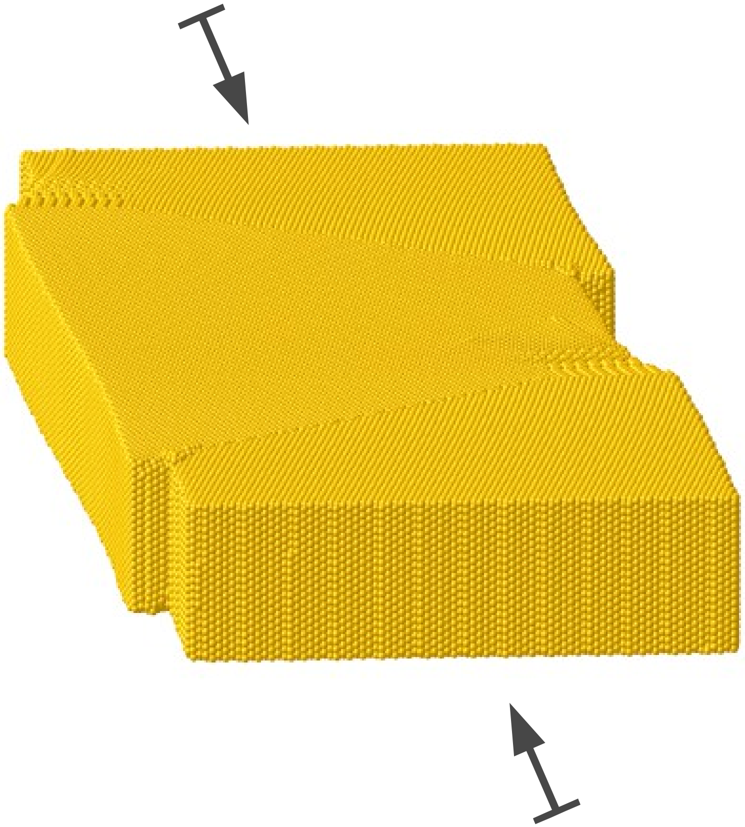
Nano-mechanical test: simulation

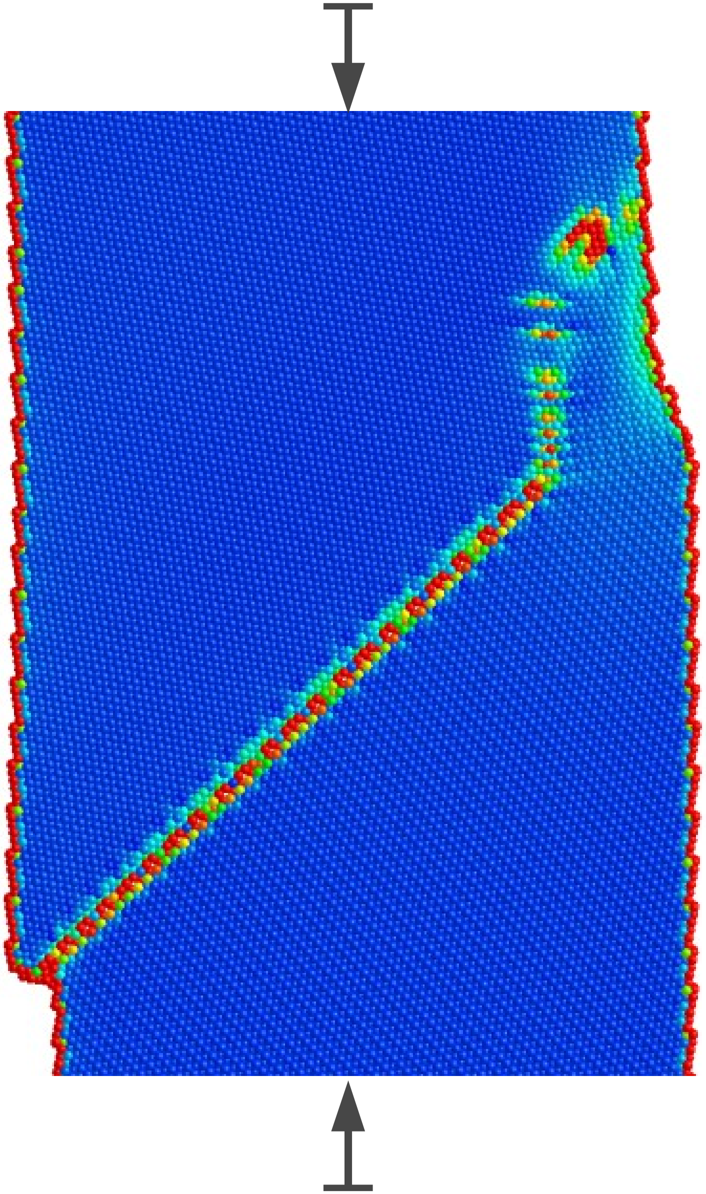


Nano-mechanical test: simulation

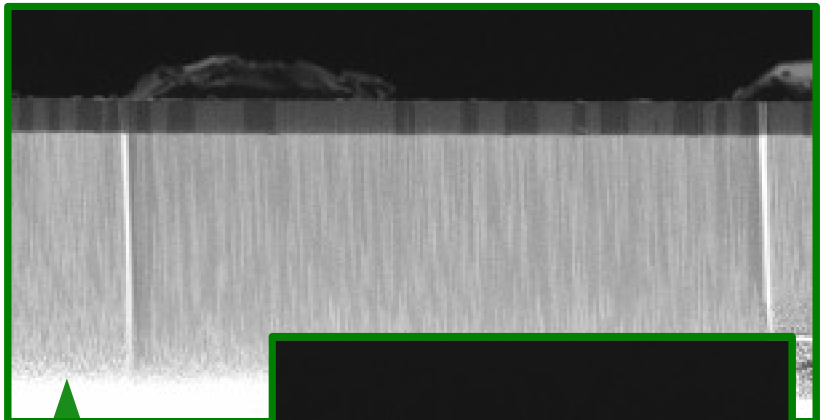
Strain: Δh = 3.2 nm







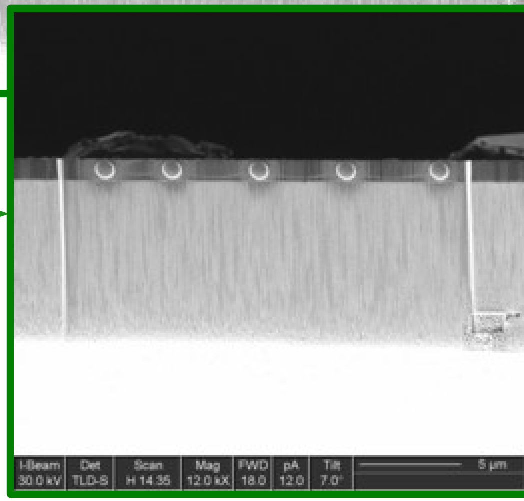
Using FIB: gold nano-pillars: ~ 1 µm × Ø 200 nm (NCEM - Berkeley)

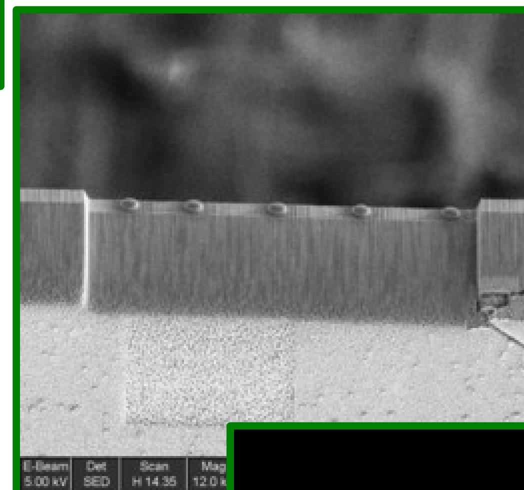


Au (h = 1µm)

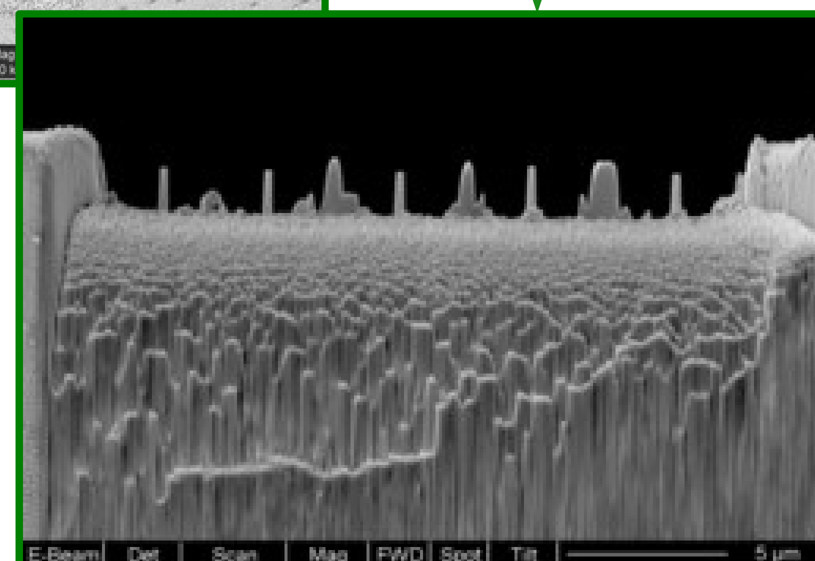
Ge (h = 6µm)

Ion beam image

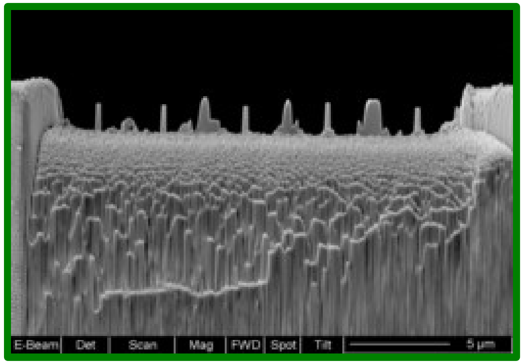


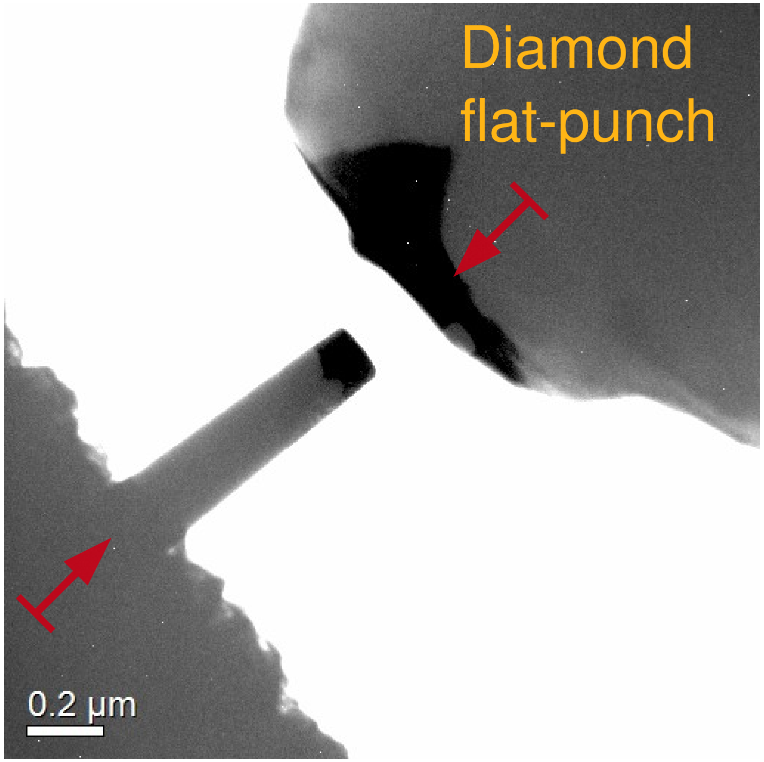


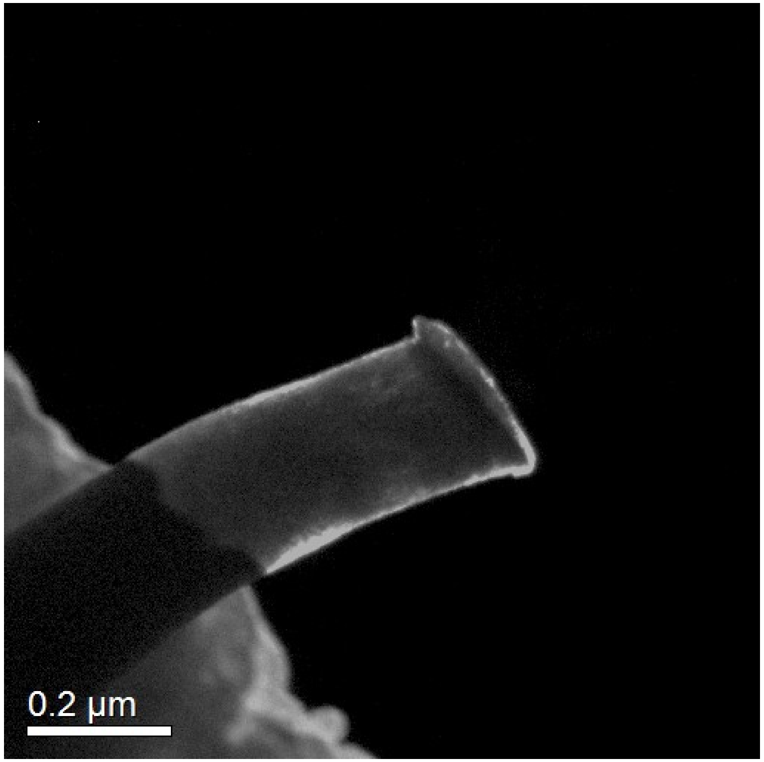
e⁻ beam image



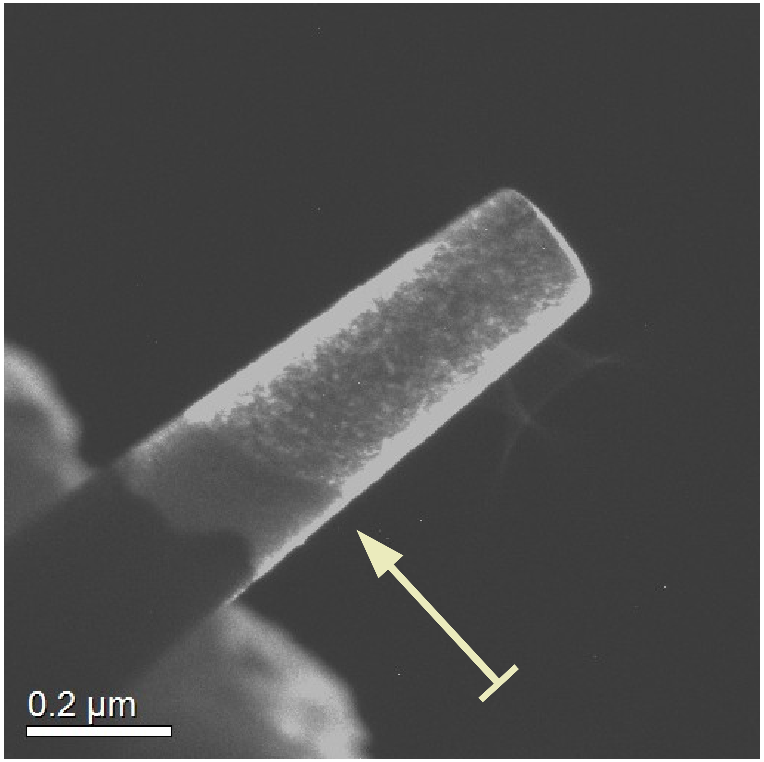
Nano-mechanical test: in the microscope (*in situ*)







First successful mechanical test in the microscope



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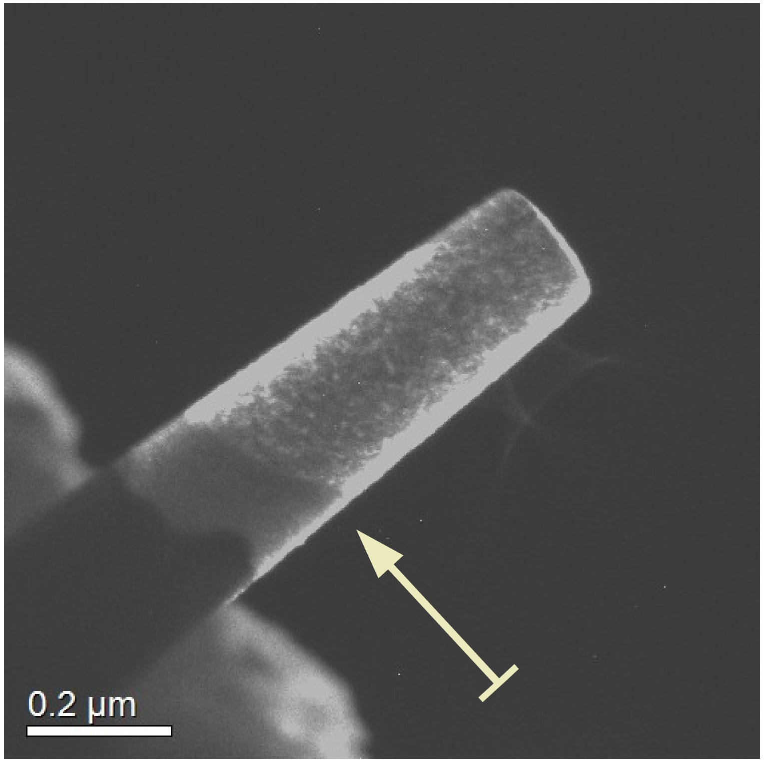

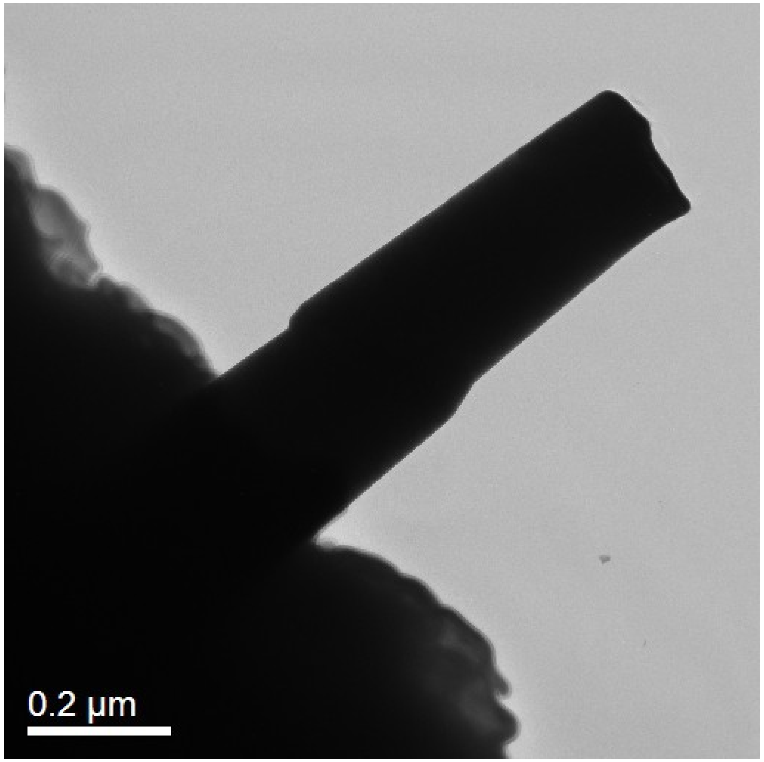

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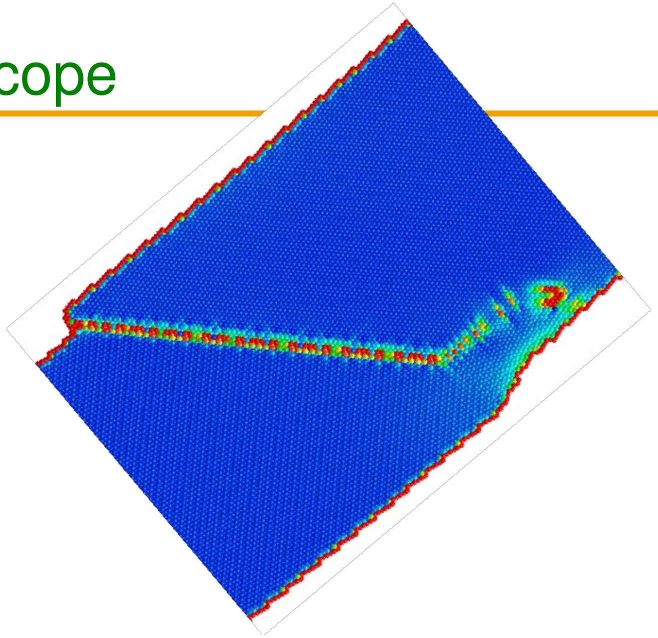

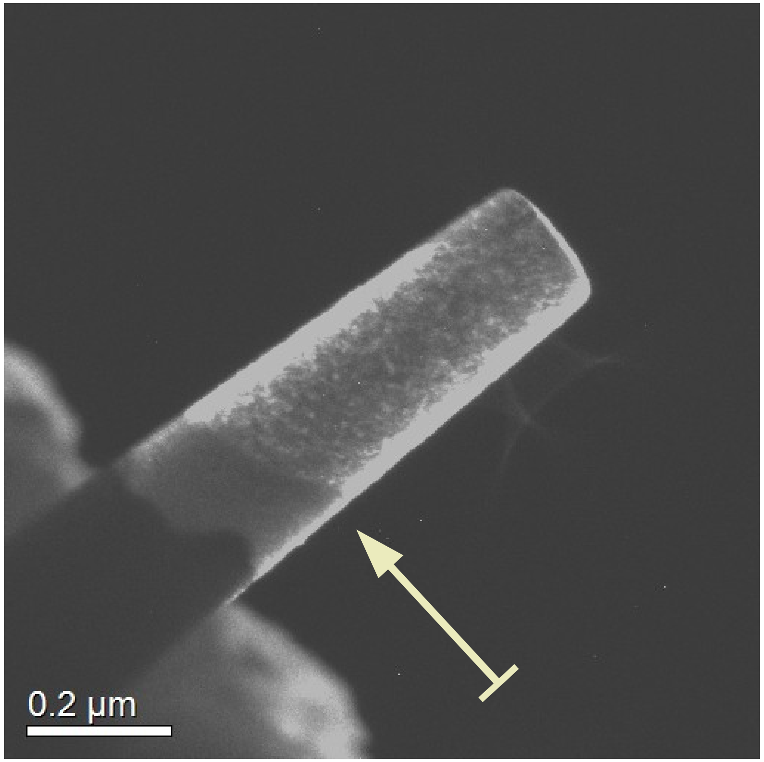

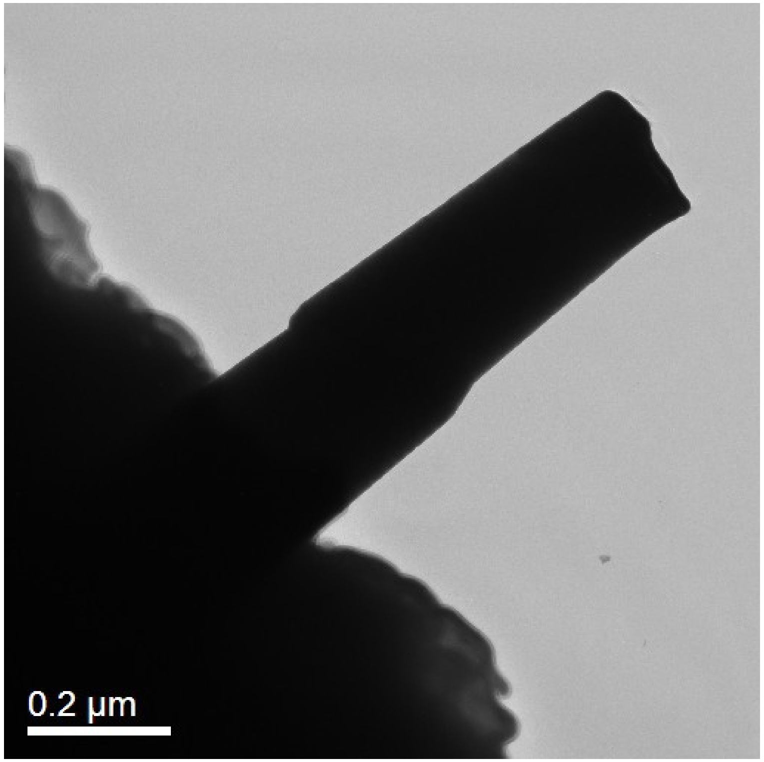

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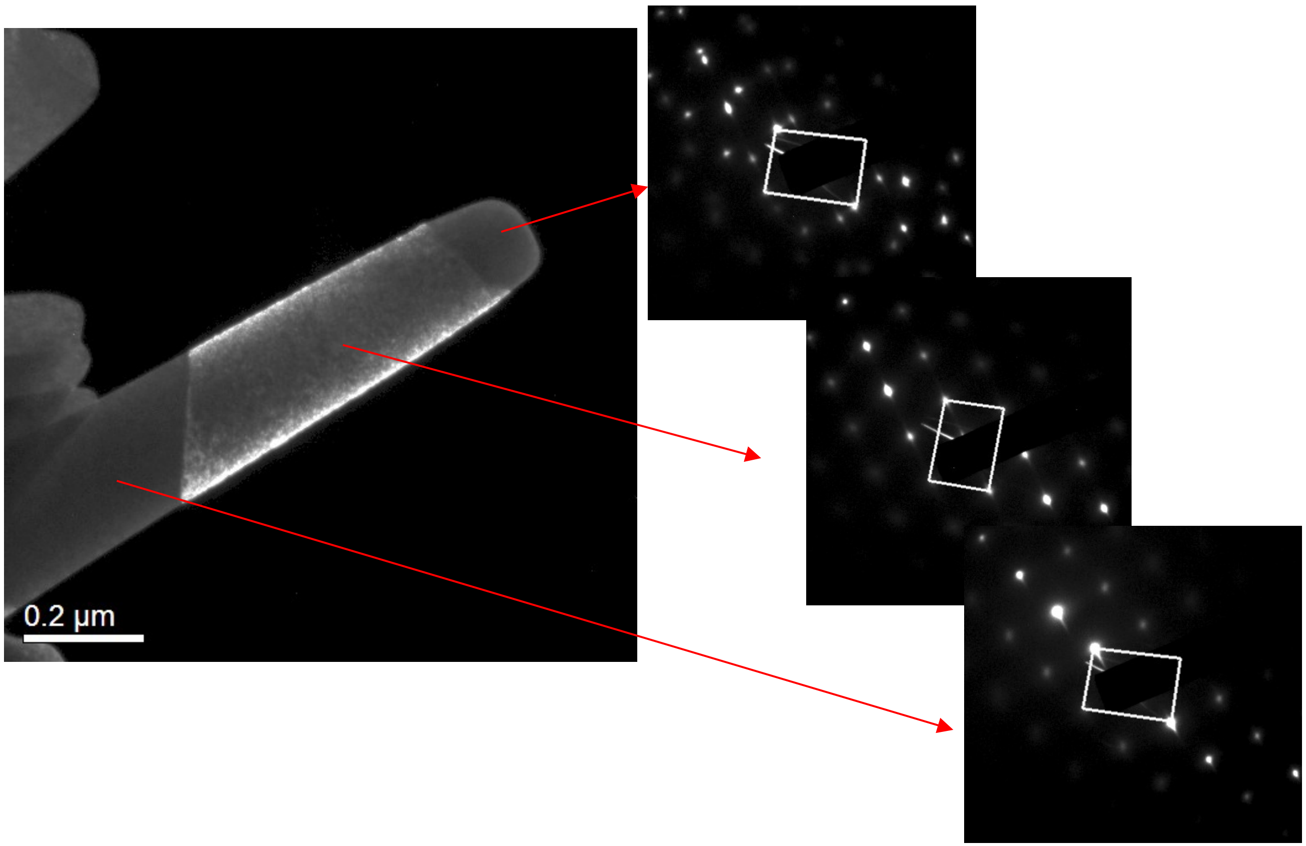

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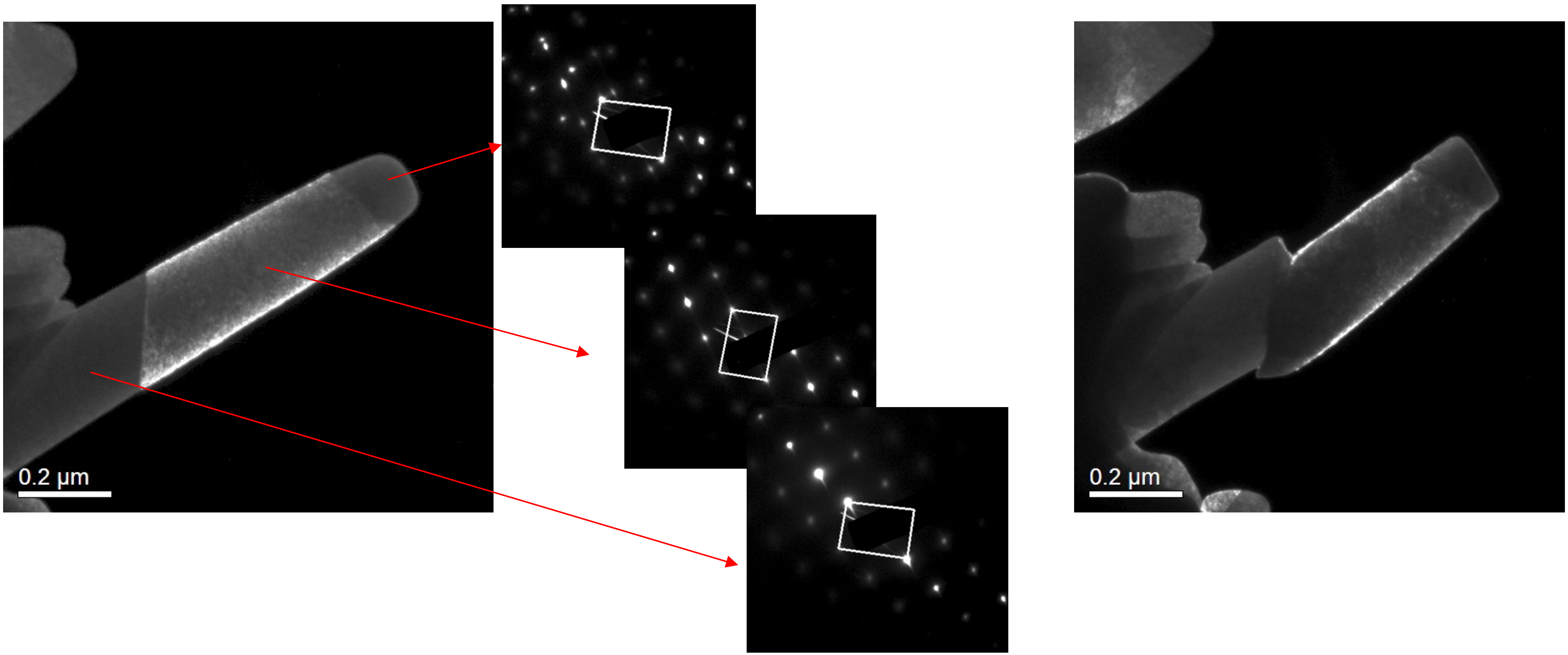

Grain boundaries: interplay between modeling and high resolution electron microscopy

Frédéric Lançon, Damien Caliste, Jean-Luc Rouvière ; **Grenoble**, France
J. Ye, A. Minor, A. Gautam, C. Ophus, Ulrich Dahmen ; **Berkeley**, USA

— Fruitful cross-talk between experiment, simulation and theory:

electron microscopy ↔ computer experiment ↔ theoretical prediction ↔ nanomechanical test