



# Diffusive Molecular Dynamics for Mass Transport Applications

Michael Ortiz

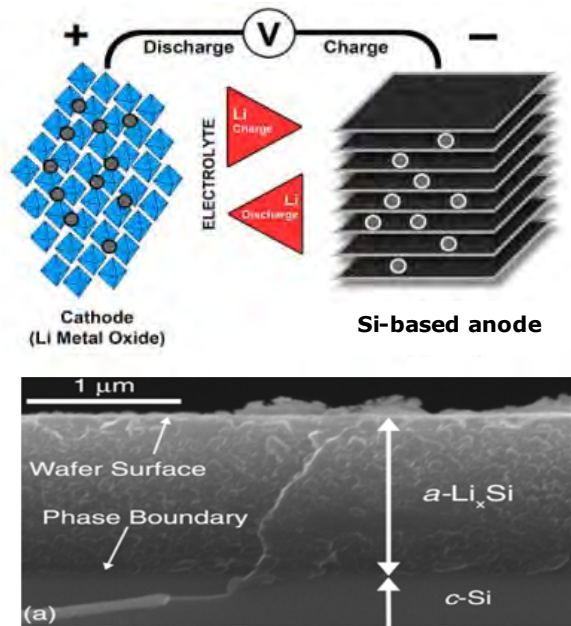
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40237 Düsseldorf, Germany  
December 14, 2018



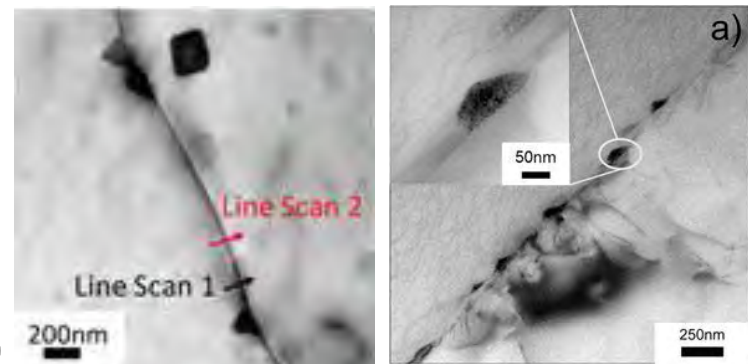
# Motivation – Diffusive time scale



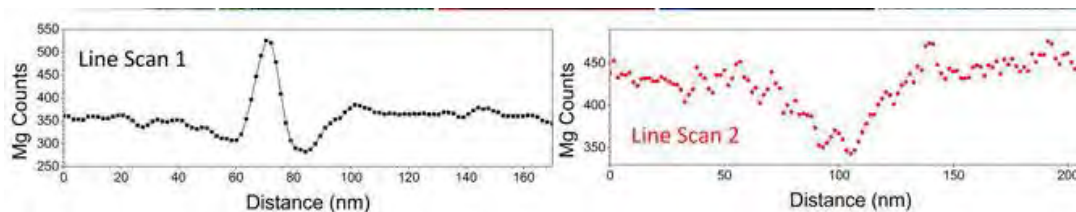
M. J. Chon *et al.*, *Phys. Rev. Lett.*, **107** (2011) 045503.

- Si-based anodes in Li-ion batteries
- Silicon loses crystalline structure upon lithiation and amorphizes
- Volume increase of 300%
- Loss of structure integrity and function after a few charge cycles

- Al-Mg 5xxxx series alloys
- Sensitization due to GBs
- Formation of  $\beta$  phase ( $\text{Mg}_2\text{Al}_3$ )
- Stress corrosion cracking



R. Zhang *et al.*, *Scientific Reports*, **7** (2017) 2961.



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# The spatial and temporal gaps

- The essential difficulty: *Multiple scales*
  - *Atomic level rate-limiting processes: Thermal activation, transport, defects, grain boundaries...*
  - *But macroscopic processes of interest:*
    - *Microstructure evolution in alloys*
    - *Long-term transport phenomena: Heat, mass...*
    - *Full chemistry: Corrosion, combustion...*
- *Time-scale gap*: From molecular dynamics (femtosecond) to macroscopic (seconds-years)
- *Spatial-scale gap*: From lattice defects (Angstroms) to macroscopic (mm-m)
- Problem intractable by brute force (even with exascale computing 😊), *ergo* must think...



# Diffusive Molecular Dynamics (DMD)

- **Objectives:** Thermodynamics without all the thermal vibrations; mass transport without all the hops; atomistics without all the atoms...
- Our approach<sup>1,2</sup> (max-ent+kinetics+QC):
  - *Treat atomic-level fluctuations statistically (away from equilibrium) through maximum-entropy principle*
  - *Append Onsager-like empirical atomic-level kinetic laws (heat and mass transport)*
  - *Quasicontinuum spatial coarse-graining*
- Implementation:
  - *Meanfield approximation of phase integrals*
  - *Quasistatic, forward integration of transport equations*

<sup>1</sup>Y. Kulkarni, J. Knap & MO, *J. Mech. Phys. Solids*, **56** (2008) 1417.

<sup>2</sup>G. Venturini, K. Wang, I. Romero, M.P. Ariza & MO,  
*J. Mech. Phys. Solids*, **73** (2014) 242-268.



# Max-Ent Non-Equilibrium SM

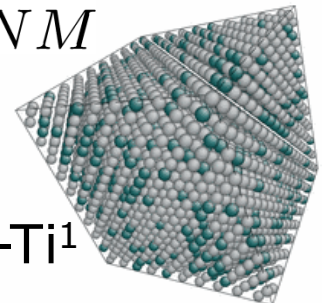
- Grand-canonical ensemble,  $N$  atoms,  $M$  species:

- State:  $(\{\mathbf{q}\}, \{\mathbf{p}\}, \{\mathbf{n}\}) \in \mathbb{R}^{3N} \times \mathbb{R}^{3N} \times \mathcal{O}_{NM}$

- Atomic positions:  $\{\mathbf{q}\} = \{\mathbf{q}_1, \dots, \mathbf{q}_N\}$

- Atomic momenta:  $\{\mathbf{p}\} = \{\mathbf{p}_1, \dots, \mathbf{p}_N\}$

Al-Ti<sup>1</sup>



- Occupancy:  $n_{ik} = \begin{cases} 1, & \text{site } i \text{ occupied by species } k, \\ 0, & \text{otherwise.} \end{cases}$

- Ensemble average of observable:  $\langle A \rangle =$

$$\sum_{\{\mathbf{n}\} \in \mathcal{O}_{NM}} \int A(\{\mathbf{q}\}, \{\mathbf{p}\}, \{\mathbf{n}\}) \underset{\substack{\uparrow \\ \text{grand-canonical pdf}}}{\rho(\{\mathbf{q}\}, \{\mathbf{p}\}, \{\mathbf{n}\})} d\mathbf{q} d\mathbf{p}$$



# Max-Ent Non-Equilibrium SM

- Assume  $H = \sum_{i=1}^N h_i$ , (e. g., EAM, TB...)
- Principle of max-ent<sup>1</sup>:  $\mathcal{S}[p] = -k_B \langle \log \rho \rangle \rightarrow \max!$   
 subject to:  $\langle \mathbf{q}_i \rangle = \bar{\mathbf{q}}_i, \quad \langle \mathbf{p}_i \rangle = \bar{\mathbf{p}}_i,$   
 $\langle h_i \rangle = e_i, \quad \langle n_{ik} \rangle = x_{ik}$  } local constraints!
- Lagrangian:      reciprocal temperatures      chemical potentials  

$$\mathcal{L}[p, \{\beta\}, \{\gamma\}] = \mathcal{S}[p] - k_B \overset{\downarrow}{\{\beta\}}^T \{\langle h \rangle\} - k_B \overset{\downarrow}{\{\gamma\}}^T \{\langle \mathbf{n} \rangle\}$$
- Gran-canonical pdf:  $\rho = \frac{1}{\Xi} e^{-\{\beta\}^T \{h\} - \{\gamma\}^T \{\mathbf{n}\}},$

on affine subspace  $\left\{ \langle \{\mathbf{q}\} \rangle = \{\bar{\mathbf{q}}\}, \langle \{\mathbf{p}\} \rangle = \{\bar{\mathbf{p}}\} \right\}$



<sup>1</sup>E.T. Jaynes, *Physical Review Series II*, **106**(4) (1957) 620–630; **108**(2) (1957) 171–190.

# Max-Ent Non-Equilibrium SM

- Gran-canonical free entropy:

$$\Phi(\{\bar{\mathbf{q}}\}, \{\bar{\mathbf{p}}\}, \{\beta\}, \{\gamma\}) = \underline{k_B \log \Xi}$$

- Local equilibrium relations:

$$e_i = -\frac{1}{k_B} \frac{\partial \Phi}{\partial \beta_i}, \quad x_{ik} = \frac{1}{k_B} \frac{\partial \Phi}{\partial \gamma_{ik}}$$

- Mesoscopic dynamics:

$$\beta_i \frac{d\bar{\mathbf{q}}_i}{dt} = \frac{1}{k_B} \frac{\partial \Phi}{\partial \bar{\mathbf{p}}_i}, \quad \beta_i \frac{d\bar{\mathbf{p}}_i}{dt} + \boxed{\frac{1}{k_B} \frac{\partial \Phi}{\partial \bar{\mathbf{q}}_i}} = 0$$

quasistatic!

- Equilibrium SM recovered when  $\beta_i = \beta$ ,  $\gamma_{ik} = \gamma_k$

- $\Phi \rightarrow \Phi_{\text{MF}}$  meanfield approximation!



# Non-equilibrium SM – Meanfield theory

- Space of trial *local Hamiltonians*:  $\mathcal{H}_0$
- Free-entropy inequality: For all  $\{h_0\} \in \mathcal{H}_0$ ,
  - i)  $\Phi \geq \Phi_0 - k_B \{\beta\}^T \{\langle h - h_0 \rangle_0\} \equiv \mathcal{S}[\{h_0\}]$
  - ii)  $\Phi = \mathcal{S}[\{h_0\}] \Leftrightarrow \{h_0\} = \{h\}$
- Best approximation:  $\Phi_{\text{MF}} = \max_{\{h_0\} \in \mathcal{H}_0} \mathcal{S}[\{h_0\}]$
- Meanfield local equilibrium relations:

$$e_i = -\frac{1}{k_B} \frac{\partial \Phi_{\text{MF}}}{\partial \beta_i}, \quad x_{ik} = \frac{1}{k_B} \frac{\partial \Phi_{\text{MF}}}{\partial \gamma_{ik}}$$

- Meanfield mesoscopic dynamics:

$$\beta_i \frac{d\bar{q}_i}{dt} = \frac{1}{k_B} \frac{\partial \Phi_{\text{MF}}}{\partial \bar{p}_i}, \quad \beta_i \frac{d\bar{p}_i}{dt} = -\frac{1}{k_B} \frac{\partial \Phi_{\text{MF}}}{\partial \bar{q}_i}$$



# Non-equilibrium SM – Meanfield theory

- Example:  $\mathcal{H}_0 \equiv$  local harmonic oscillators,

$$h_{0i} = \frac{1}{2m(\mathbf{n}_i)} |\mathbf{p}_i - \bar{\mathbf{p}}_i|^2 + \frac{m(\mathbf{n}_i)\omega_i^2}{2} |\mathbf{q}_i - \bar{\mathbf{q}}_i|^2$$

- Entropy function (parameterized by  $\{\omega\}$ ):

$$\Phi_{\text{MF}} = \sum_{i=1}^N k_B \left( \frac{\beta_i}{2m_i} |\bar{\mathbf{p}}_i|^2 + \beta_i \langle V_i \rangle_0 + 3 \log(\hbar \beta_i \omega_i) - 3 \right)$$

← Gaussian integrals!

- Meanfield mesoscopic dynamics: Hermite quadrature!

$$\dot{\bar{\mathbf{q}}}_i = \frac{\bar{\mathbf{p}}_i}{m_i}, \quad \dot{\bar{\mathbf{p}}}_i = -\frac{\partial}{\partial \bar{\mathbf{q}}_i} \sum_{j=1}^N \langle V_j \rangle_0,$$

- Meanfield optimality:  $\frac{\partial}{\partial \omega_i} \sum_{j=1}^N \beta_j \langle V_j \rangle_0 + \frac{3}{\omega_i} = 0$



# Non-equilibrium SM – Kinetics

- Need equations of evolution for  $\{\beta\}$  and  $\{\gamma\}$

- Local conservation equations:  $j \bullet \longrightarrow \bullet i$

$$\underbrace{\dot{e}_i = \dot{w}_i + \mu_i^T \dot{x}_i + \sum_{j \neq i} R_{ij}}_{\text{energy}}, \quad \underbrace{\dot{x}_i = \sum_{j \neq i} J_{ij}}_{\text{mass}}$$

- Local dissipation inequality:

$$\Sigma_{ij} = k_B(\beta_i - \beta_j)R_{ij} + k_B(\gamma_i - \gamma_j) \cdot J_{ij} \geq 0$$

- General kinetic relations: calibrate from exp. data!

$$\underbrace{R_{ij} = f(\beta_i - \beta_j)}_{\text{Discrete Fourier law}}, \quad \underbrace{J_{ij} = g(\gamma_i - \gamma_j)}_{\text{Discrete Fick's law}}$$



# Non-equilibrium SM – Sample potentials

- Structure of typical multispecies EAM potential:

$$V = \sum_{i=1}^N \left[ n_i F_i(\rho_i) + \frac{1}{2} \sum_{j \neq i} n_i n_j S_{ij}(n_i, n_j) \phi_{ij}(r_{ij}) \right]$$

- Meanfield equilibrium:  $\mu_i = \frac{k_B T}{2} \log \frac{x_i}{1 - x_i}$

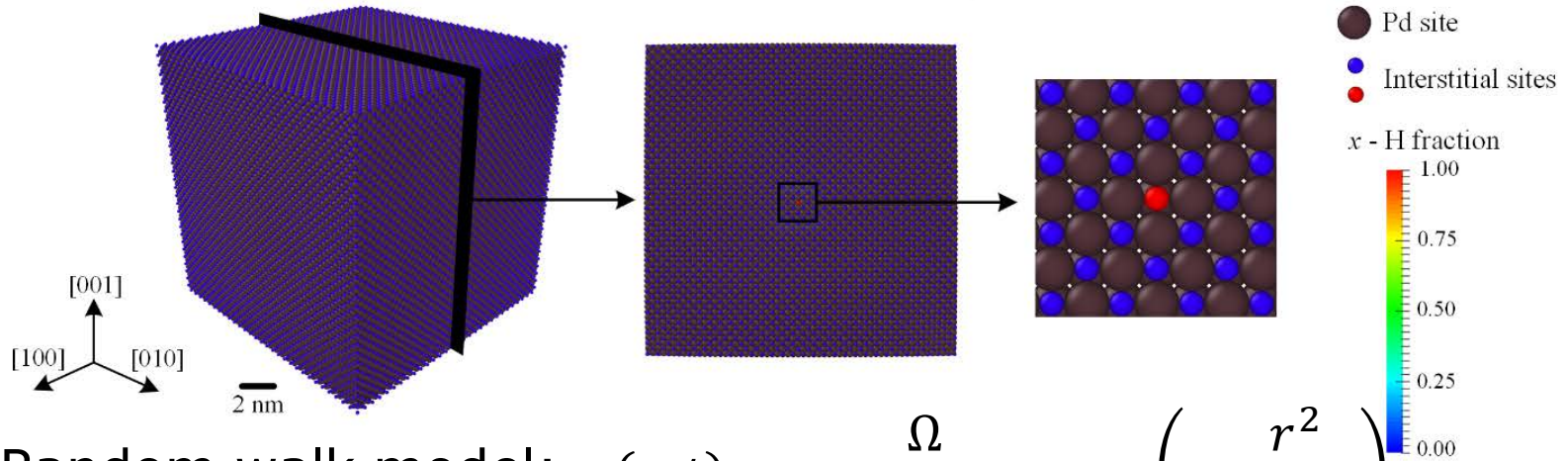
- Master equation:  $\frac{\partial x_i}{\partial t} = \sum_{\langle i, j \rangle} (\psi_{j \rightarrow i} - \psi_{i \rightarrow j})$

- Transition probabilities:

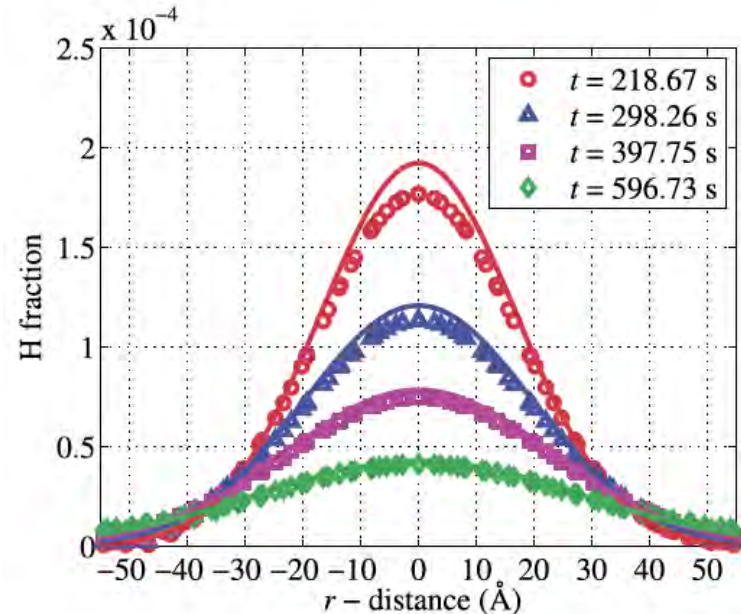
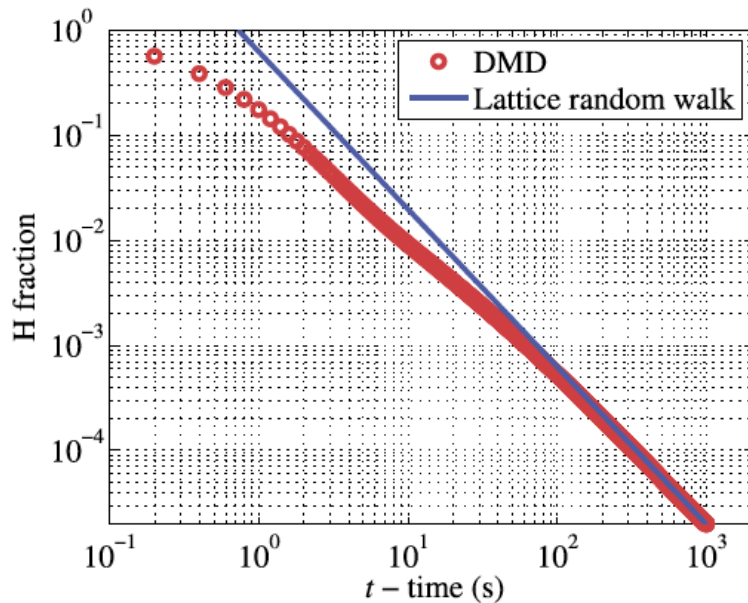
$$\psi_{i \rightarrow j} = \underbrace{\nu_i}_{\text{attempt frequency}} x_j (1 - x_i) e^{-\beta \left( \underbrace{E_{i \rightarrow j}}_{\text{energy barrier}} + (\mu_i - \mu_j)/2 \right)}$$



# MD vs. DMD in pictures



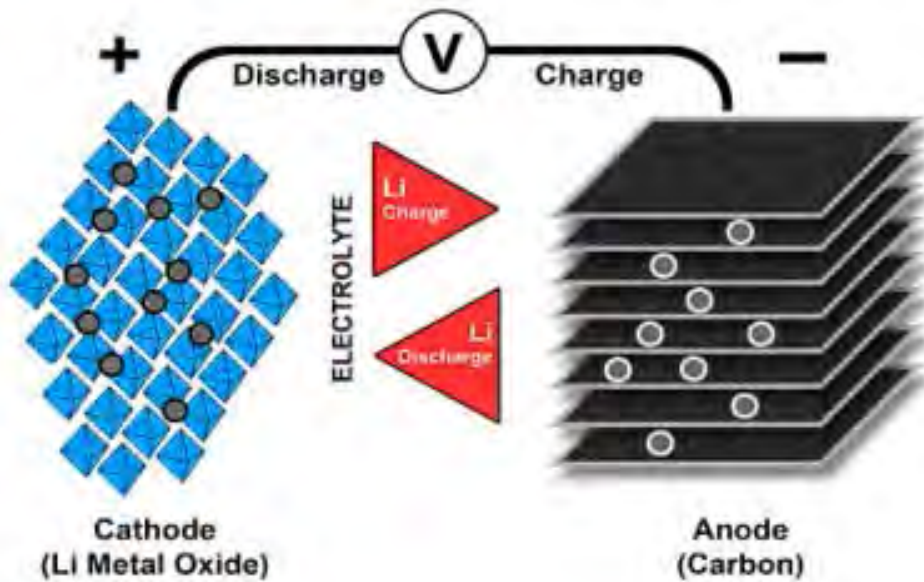
Random walk model: 
$$x(r, t) = \frac{\Omega}{(4\pi D_H t)^{3/2}} \exp\left(-\frac{r^2}{4\pi D_H t}\right)$$



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X. Sun, M. P. Ariza, M. Ortiz, K. G. Wang, J Comput Phys, **350**:470-492, 2017. MPIE 2018

# Application: Lithium-ion batteries



Nano-Micro Lett. (2014) 6(4):347–358

| Element | Gravimetric capacity (mAh g <sup>-1</sup> ) | Volumetric capacity (mAh cm <sup>-3</sup> ) | Cost | Toxicity | Safety |
|---------|---------------------------------------------|---------------------------------------------|------|----------|--------|
| Si      | <u>4,200</u>                                | 2,400                                       | Low  | No       | High   |
| C       | 372                                         | 890                                         | Low  | No       | Low    |
| Ge      | 1,568                                       | 2,300                                       | High | High     | High   |
| Sn      | 990                                         | 2,020                                       | Low  | No       | High   |
| P       | 2,600                                       | 2,250                                       | Low  | High     | Low    |
| Sb      | 660                                         | 1,890                                       | Low  | High     | Low    |
| Pb      | 549                                         | 1,790                                       | Low  | High     | Low    |

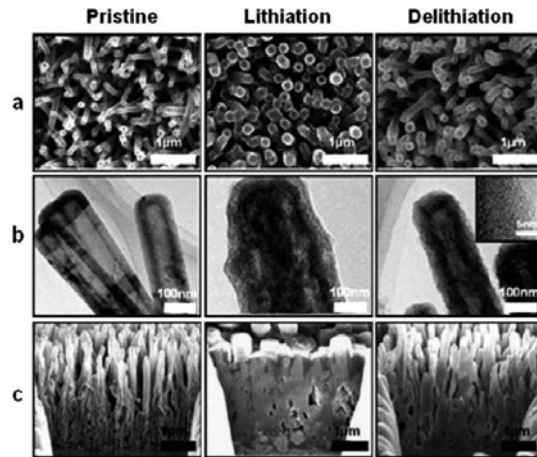
[http://batteryuniversity.com/learn/article/lithium\\_based\\_batteries](http://batteryuniversity.com/learn/article/lithium_based_batteries)

- Si-based anodes offer the highest specific capacity (ten time the specific capacity of graphite)
- But: 300% expansion during charging (lithiation)
- Si undergoes amorphization upon lithiation
- Mechanical failure (pulverization) after a few cycles...

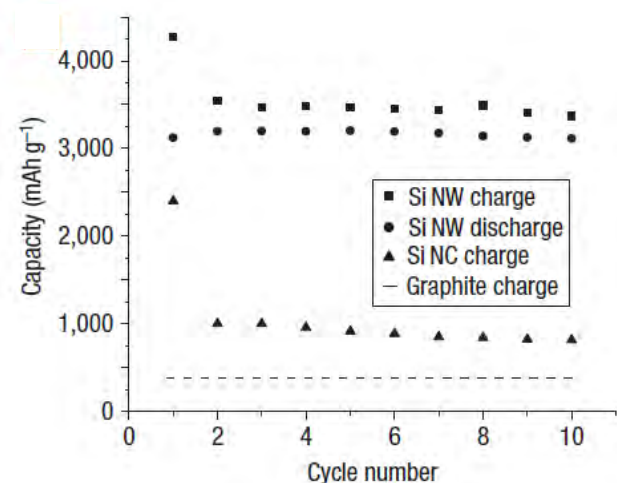


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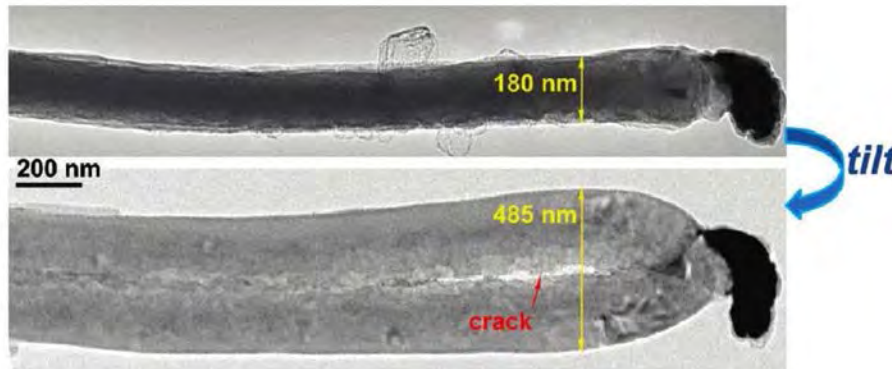
# Nano-engineered Si anodes



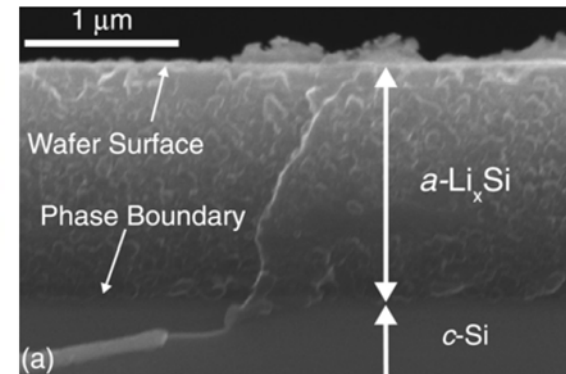
Si-nanowire anodes,  
lithiation-delithiation<sup>1</sup>



Si-nanowire anodes,  
capacity vs. #cycles<sup>2</sup>



Lithiation of Si nanowire<sup>3</sup>



Lithiation of Si nanowire<sup>4</sup>



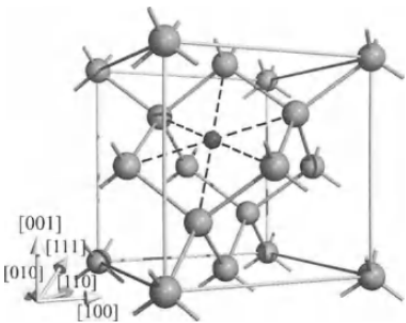
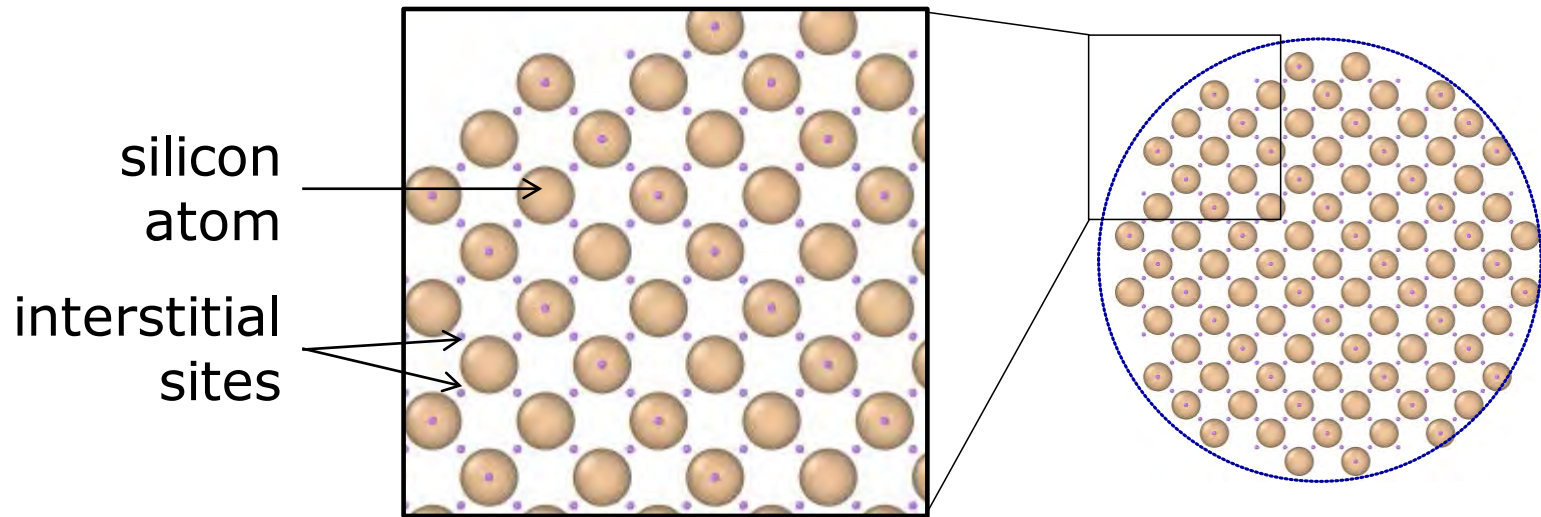
<sup>1</sup>T. Song *et al.*, *Nano Letters*, **10**(5) (2010) 1710–1716.

<sup>2</sup>C.K. Chan *et al.*, *Nature Nanotech.*, **3** (2008) 31–35.

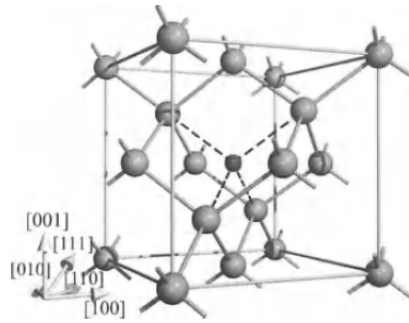
<sup>3</sup>X.H. Liu and H. Zheng, *Nano Letters*, **11**(8) (2011) 3312–3318.

<sup>4</sup>M.J. Chon *et al.*, *Phys. Rev. Lett.*, **107**(4) (2011) 045503.

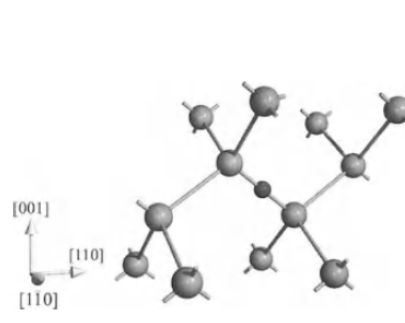
# Si lithiation model



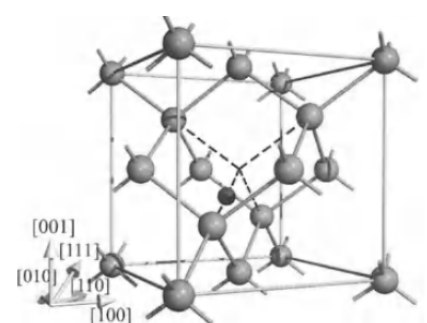
Hexagonal interstitial:  
*2 interst./Si atom*



Tetrahedral interstitial:  
*1 interst./Si atom*



Bond-centered interstitial:  
*2 interst./Si atom*



Anti-bond interstitial:  
*4 interst./Si atom*

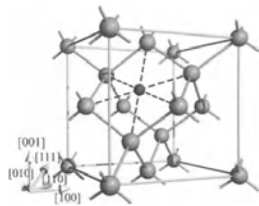
## Interstitial sites of diamond Si



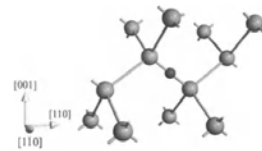
# Si nanowire lithiation simulations

- Si nanowire @ Li saturation on outer boundary

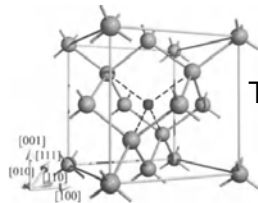
- 2NN MEAM for Si-Li<sup>1</sup>
- $T = 300K$
- Master transport equation<sup>2</sup>
- Diffusion parameters:
  - $\nu = 1013 \text{ 1/s}$
  - $\Delta E = 0.55 \text{ eV}$
- 5 interstitials/atom



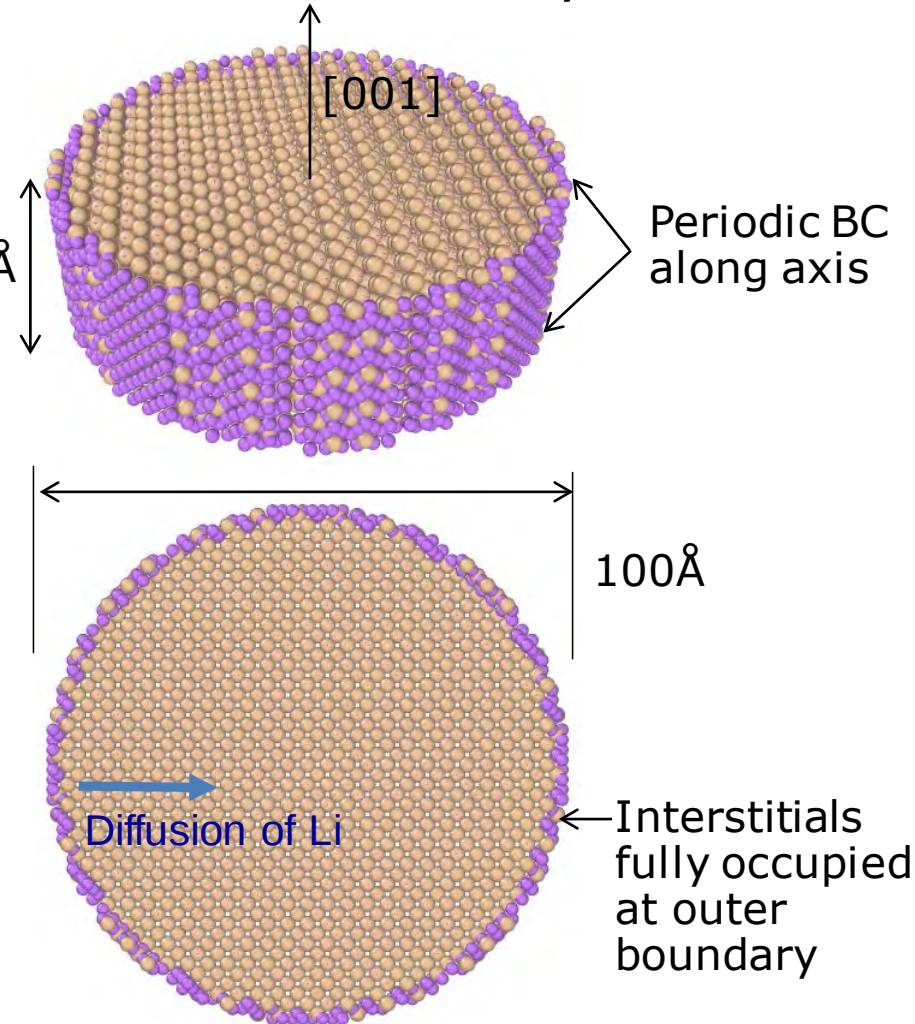
Hexagonal interstitial:  
2 interst./Si atom



Bond-centered interstitial:  
2 interst./Si atom



Tetrahedral interstitial:  
1 interst./Si atom



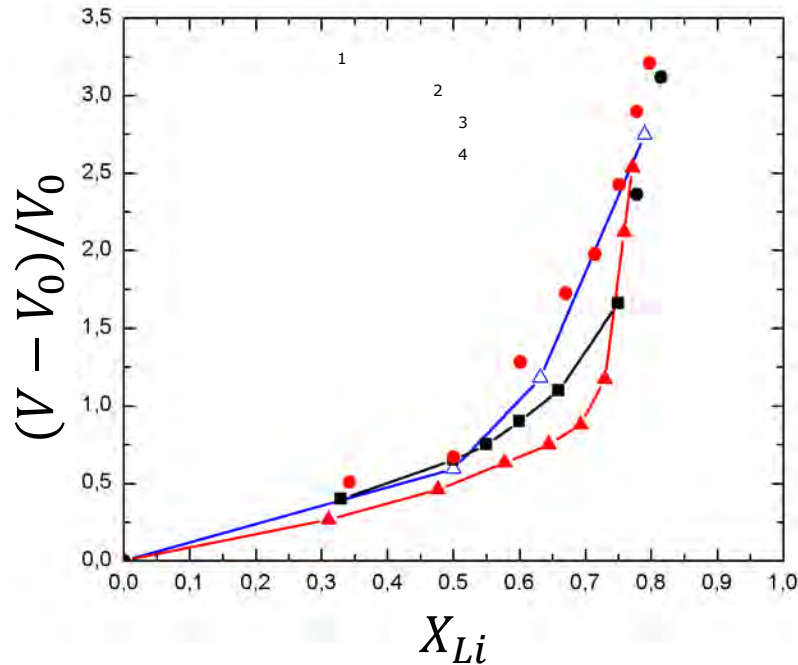
<sup>1</sup>Z. Cui et al., *J. Power Sources*, **207** (2012) 150–159.

<sup>2</sup>F. Zhang and W. A. Curtin, *MSMSE* 16, 055006 (2008).

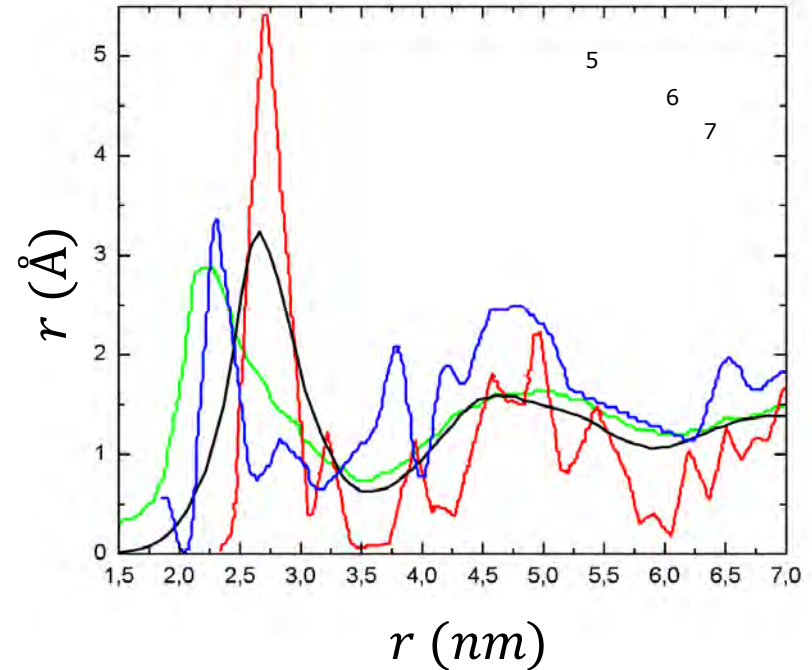
10,126 Si atoms,  
50,565 interstitials

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# Si lithiation model - Validation



Volume expansion  
vs. Li molar fraction



Radial distribution function  
at full lithiation

<sup>1</sup>P. Johari *et al.*, *Nano Lett.*, **11**(12) (2011) 5494–5500.

<sup>2</sup>H.S. Lee and B.J. Lee, *Met. Mater. Int.*, **20**(6) (2014), 1003-1009.

<sup>3</sup>L.Y. Beaulieu *et al.*, *Electrochem. Solid-State Lett.*, **4**(9) (2001) A137-A140.

<sup>4</sup>L.Y. Beaulieu *et al.*, *J. Electrochem. Soc.*, **150**(11) (2003) A1457-64.

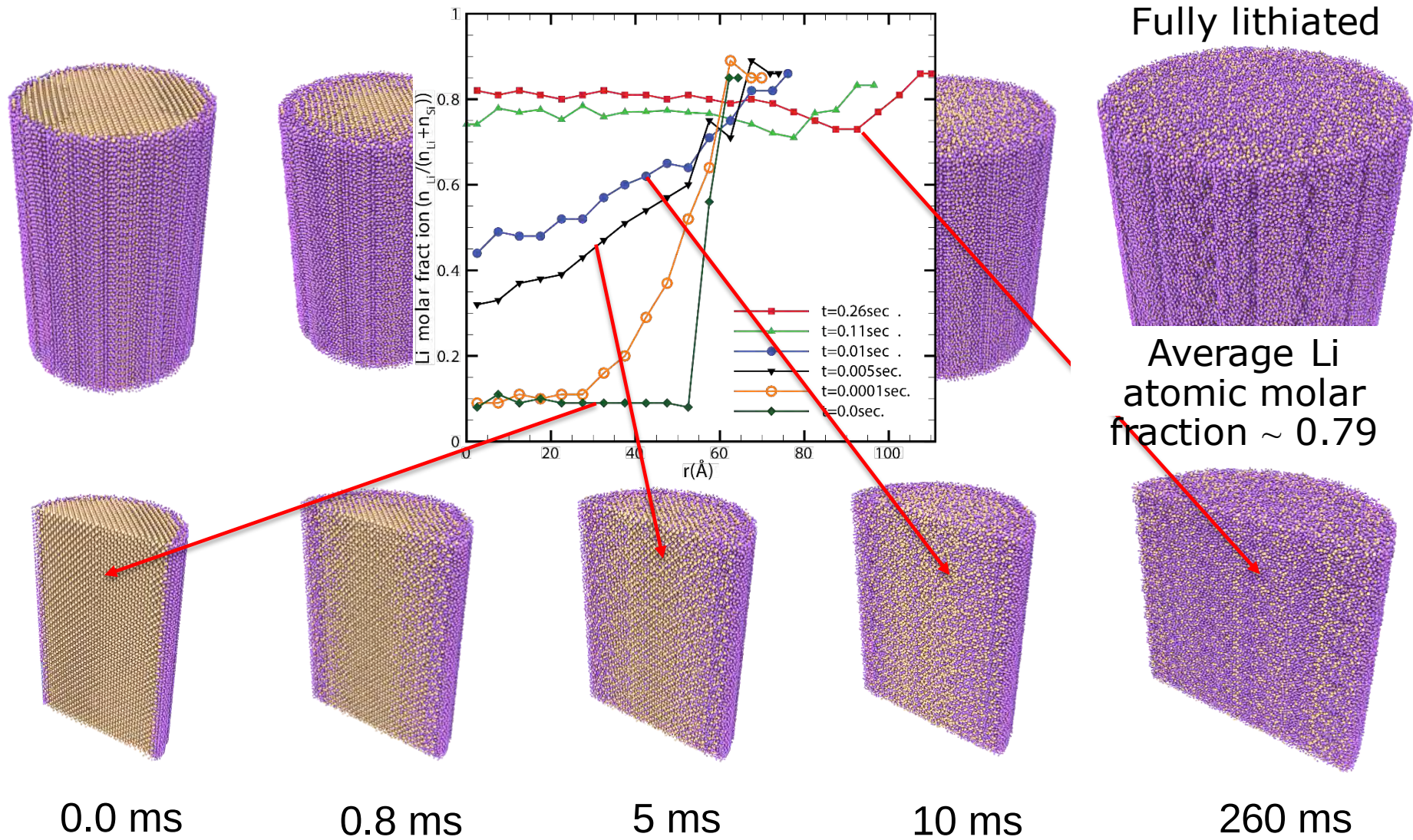
F. Fan *et al.*, *Modelling Simul. Mater. Sci. Eng.*, **21** (2013) 074002.

V.L. Chevrier and J.R. Dahn, *J. Electrochem. Soc.*, **156**(6) (2009) A454-A458.

B. Key *et al.*, *J. Am. Chem. Soc.*, **133** (2010) 503-512.



# Si nanopillar lithiation – Atomic fractions

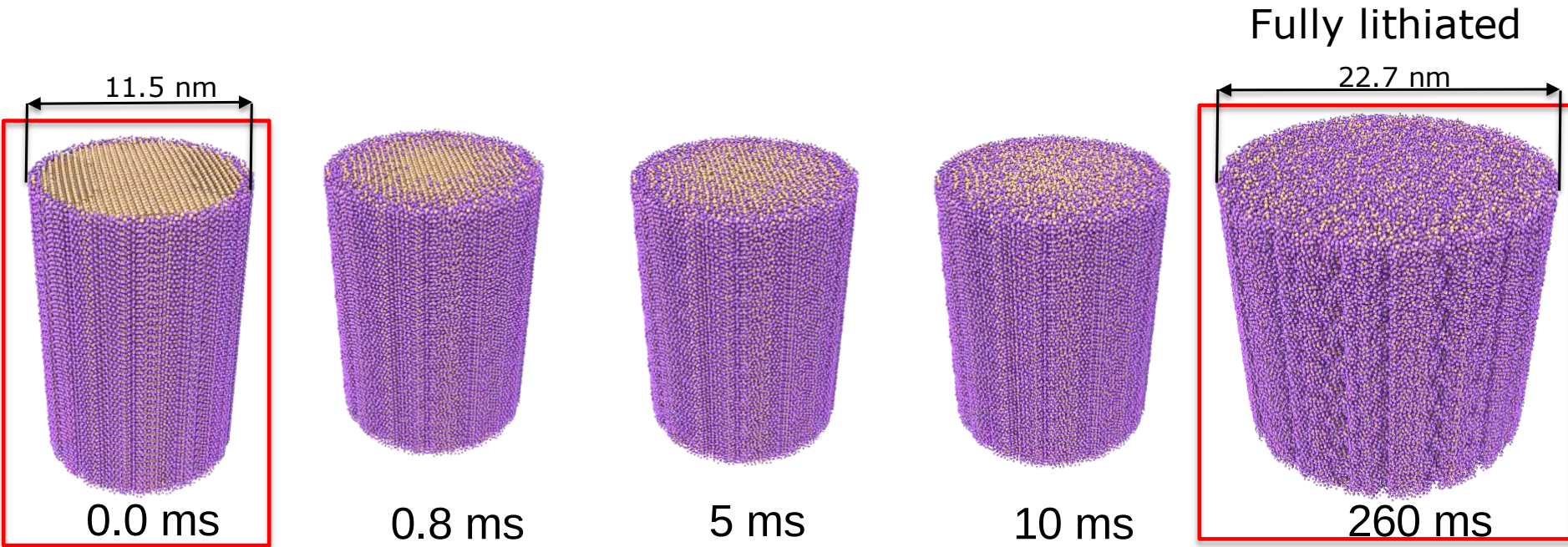


Si atoms  
Li atoms

J.P. Mendez, M. Ponga, M. Ortiz,  
*JMPS*, **115** (2018) 123-141.

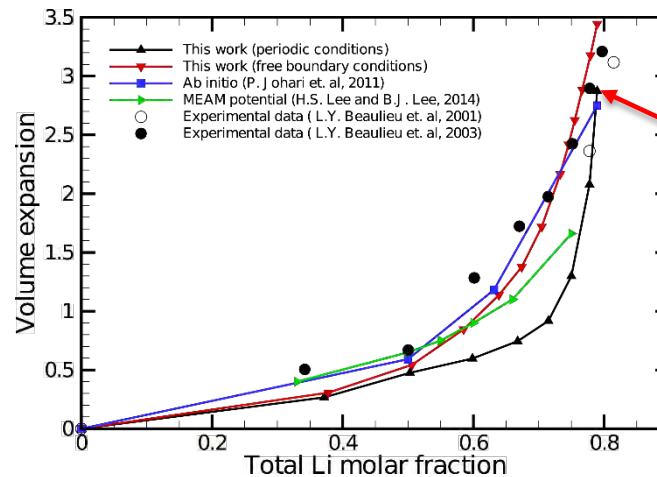
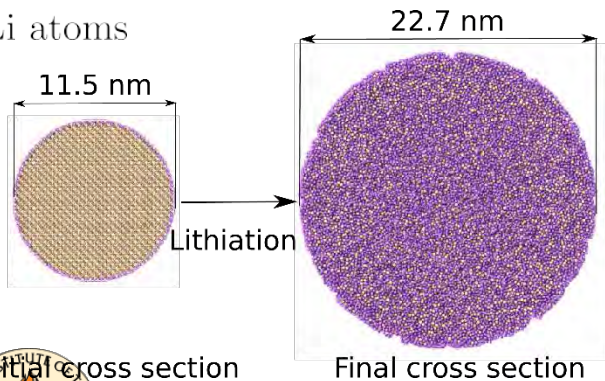
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# Si nanopillar lithiation – Volume



Si atoms

Li atoms

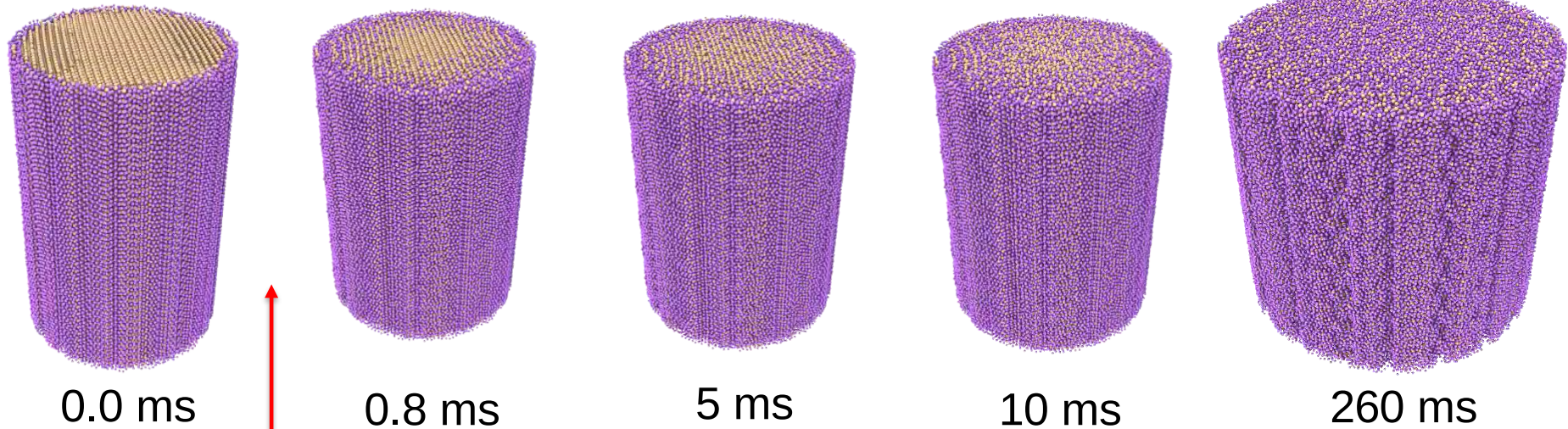


Volume expansion of 287%



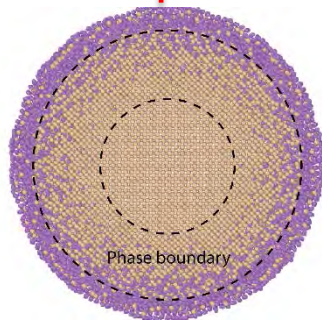
# Si nanopillar lithiation – Interface

Fully lithiated

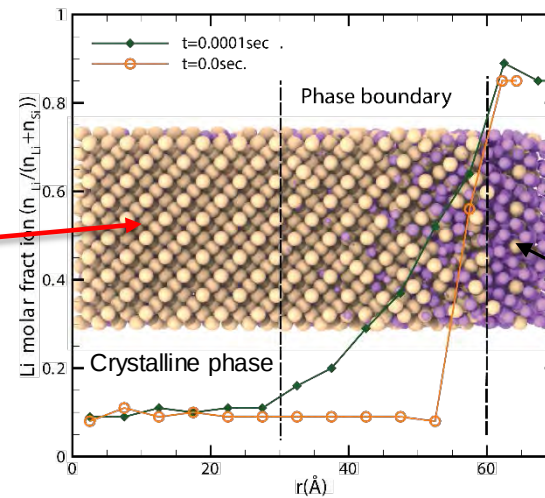
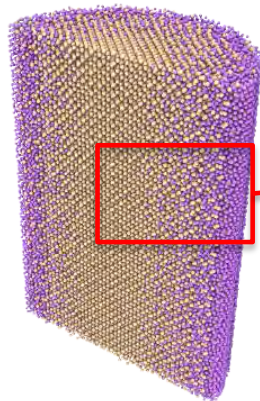


Si atoms

Li atoms



0.1 ms

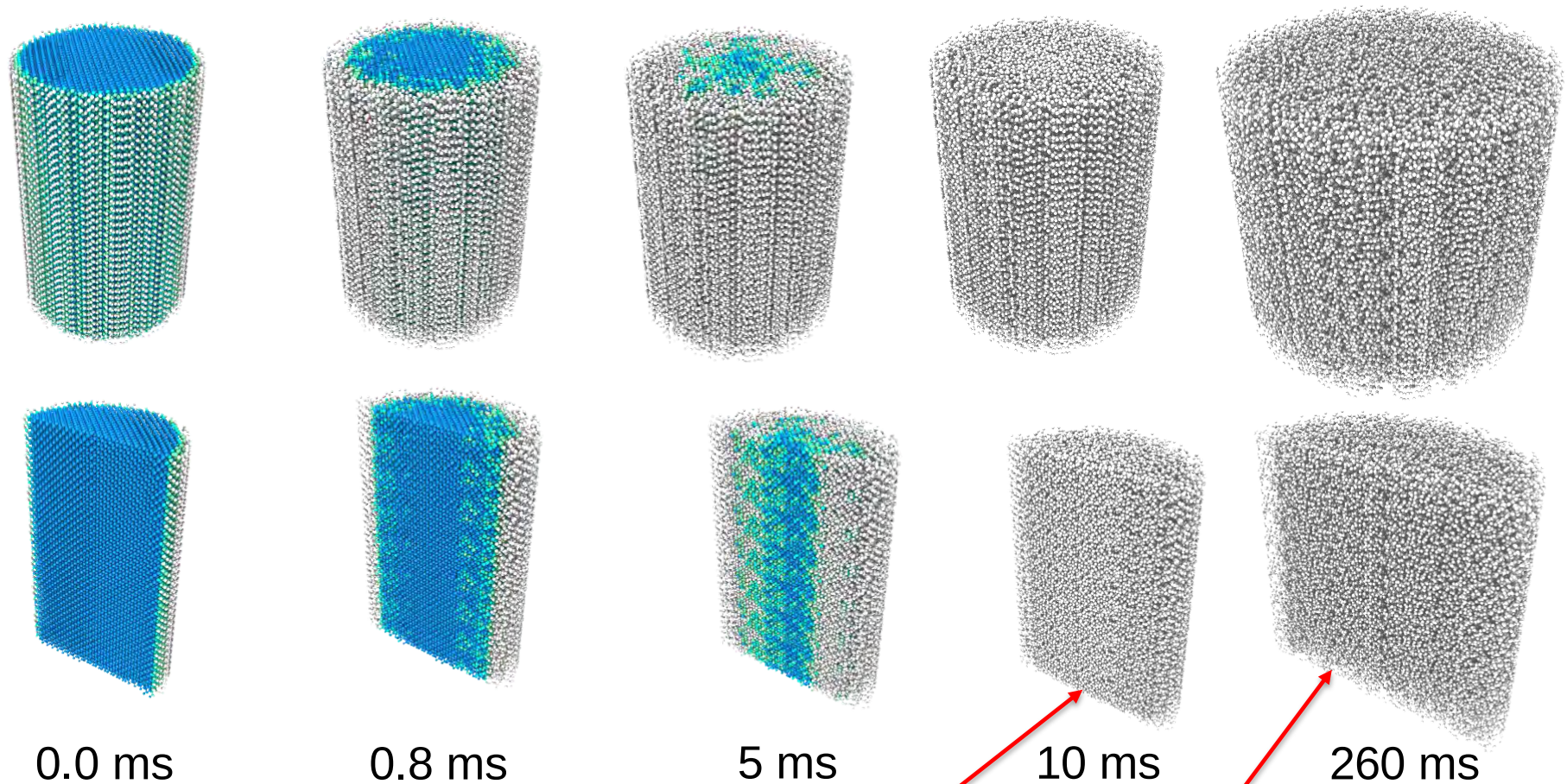


Phase boundary  
 $\sim 20 \text{\AA}$

Amorphous phase



# Si nanopillar lithiation – Amorphization



Amorphous  
Cubic diamond  
Cubic diamond (1st neighbor)  
Cubic diamond (2nd neighbor)

Full amorphization

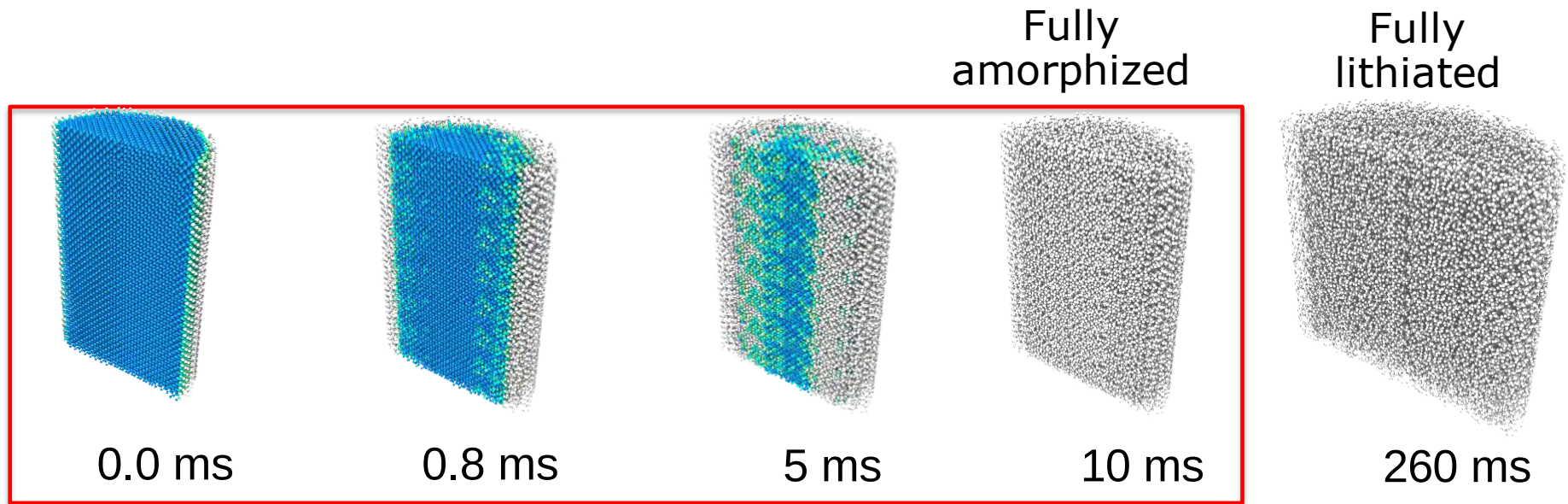
Lithiated phase

J.P. Mendez, M. Ponga, M. Ortiz,  
*JMPS*, **115** (2018) 123-141.

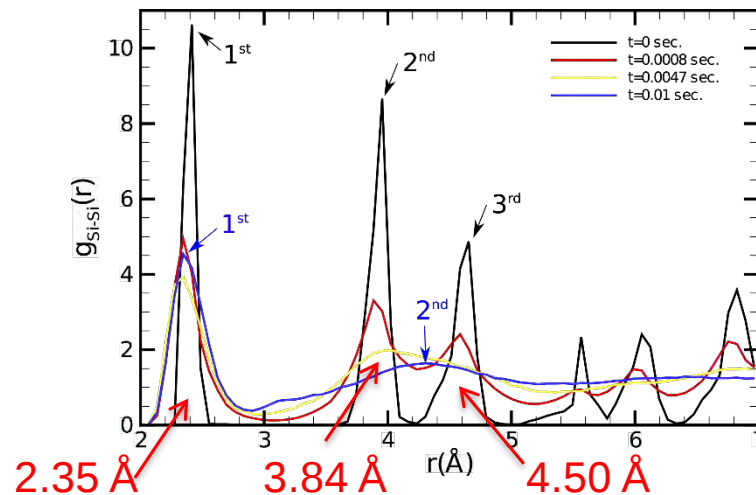
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# Si nanopillar lithiation – Amorphization



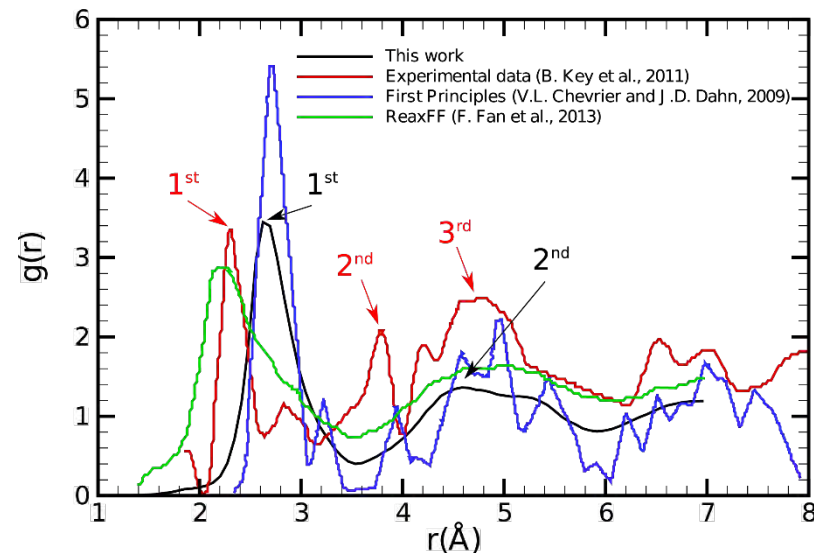
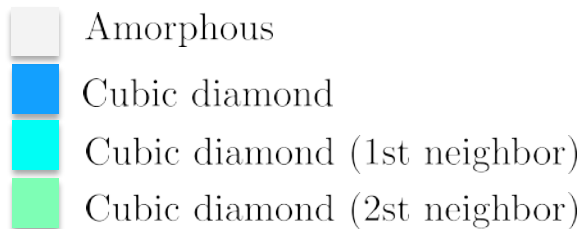
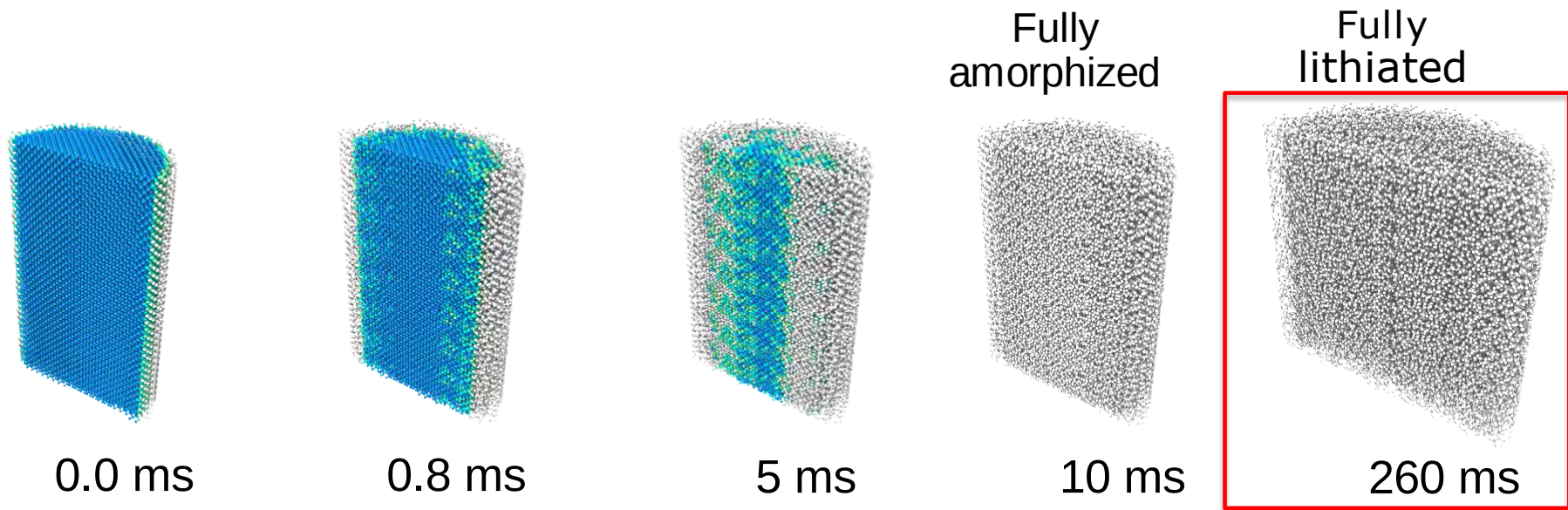
Amorphous  
Cubic diamond  
Cubic diamond (1st neighbor)  
Cubic diamond (2nd neighbor)



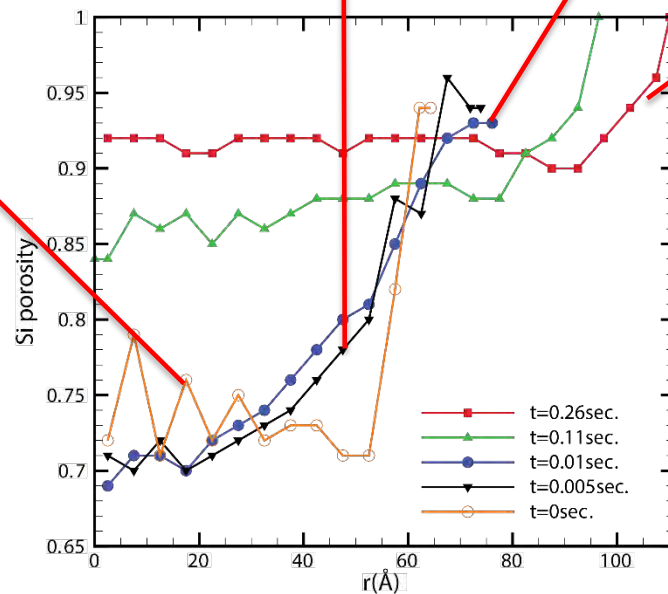
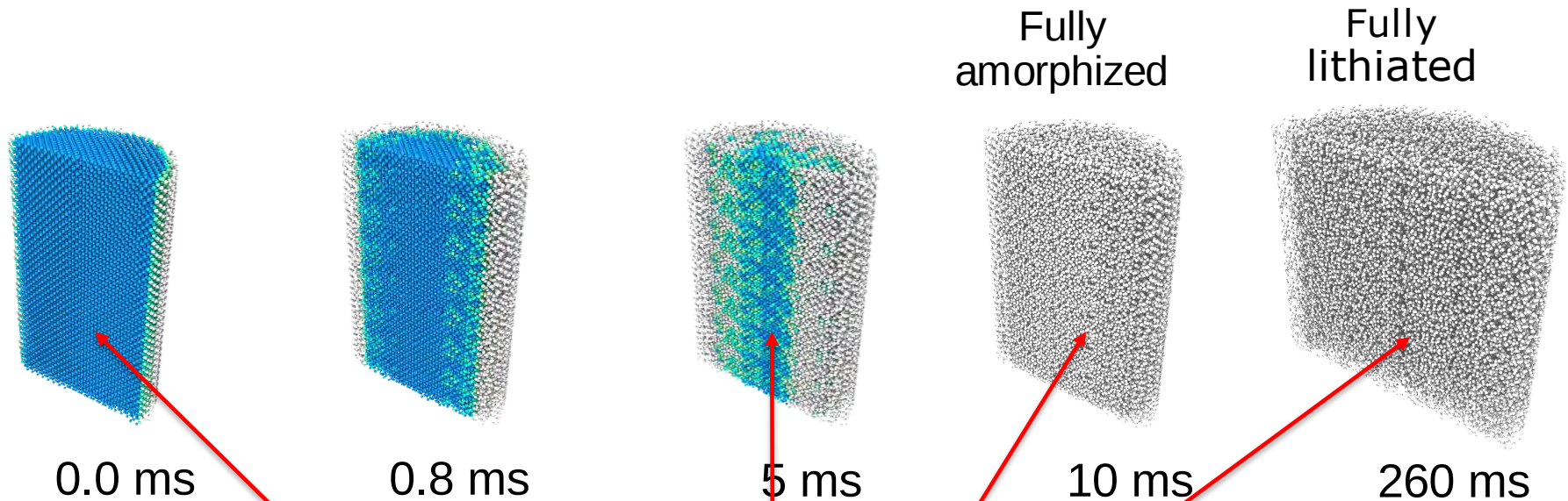
radial  
distribution  
function



# Si nanopillar lithiation – Amorphization



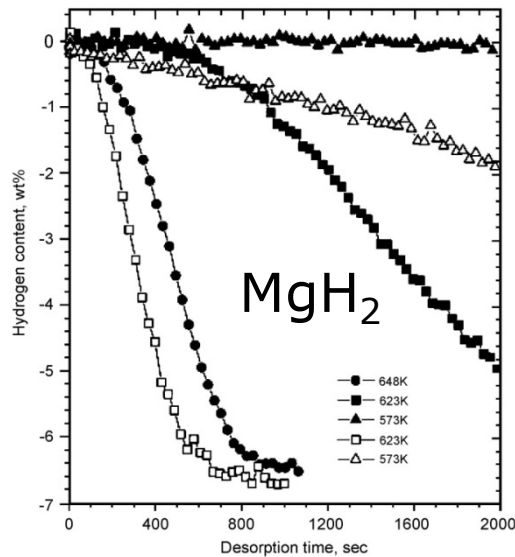
# Si nanopillar lithiation – Porosity



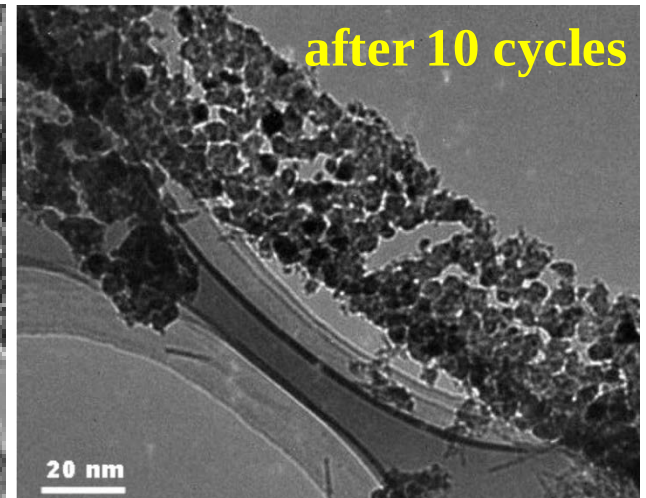
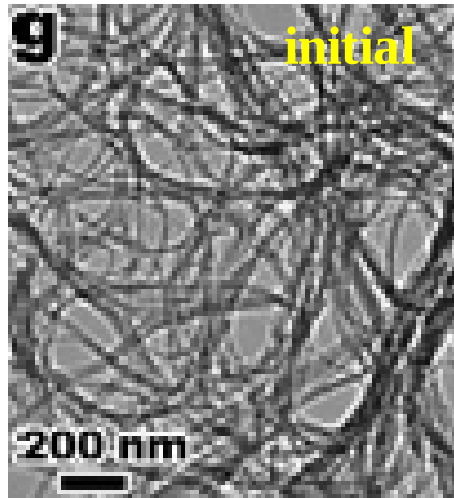
Amorphous  
Cubic diamond  
Cubic diamond (1st neighbor)  
Cubic diamond (2nd neighbor)



# Application: Hydrogen storage in Pd



- Hydrogen storage is a key element of the hydrogen economy...
- Typical absorption/desorption times are temperature/pressure dependent and in hour range<sup>1</sup>
- Outlook: Store hydrogen in nanostructured metals (particles, nanowires)
- But: Structural effects,
  - Volume expansion
  - Pulverization
- Mg disintegrates after 10 hydration cycles<sup>2</sup>
- Predictive capability:
  - Atomistic realism
  - Long-time behavior...



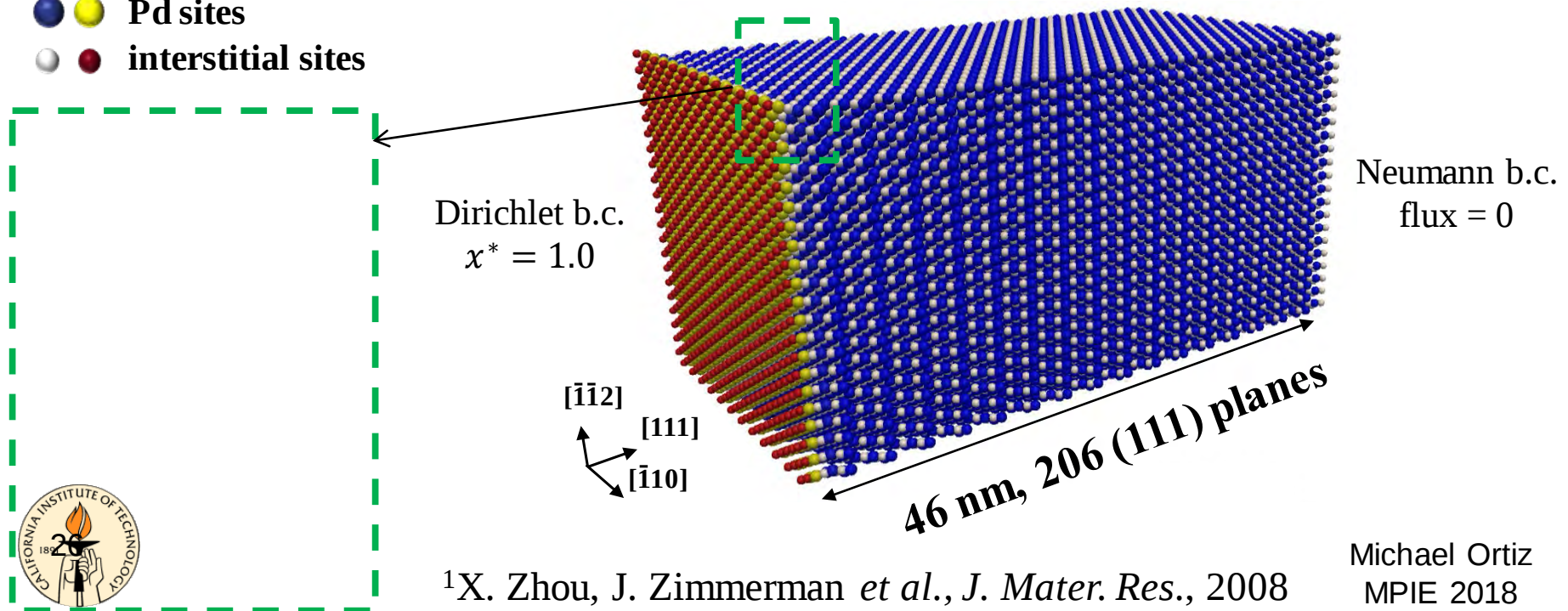
<sup>1</sup>B. Sakintuna, F. Darkrim and M. Hirscher, *Int.J. Hydrogen Energy*, **32** (2007) 1121– 1140.

<sup>2</sup>W. Li, C. Li et al., *J. Am. Chem. Soc.*, 2007

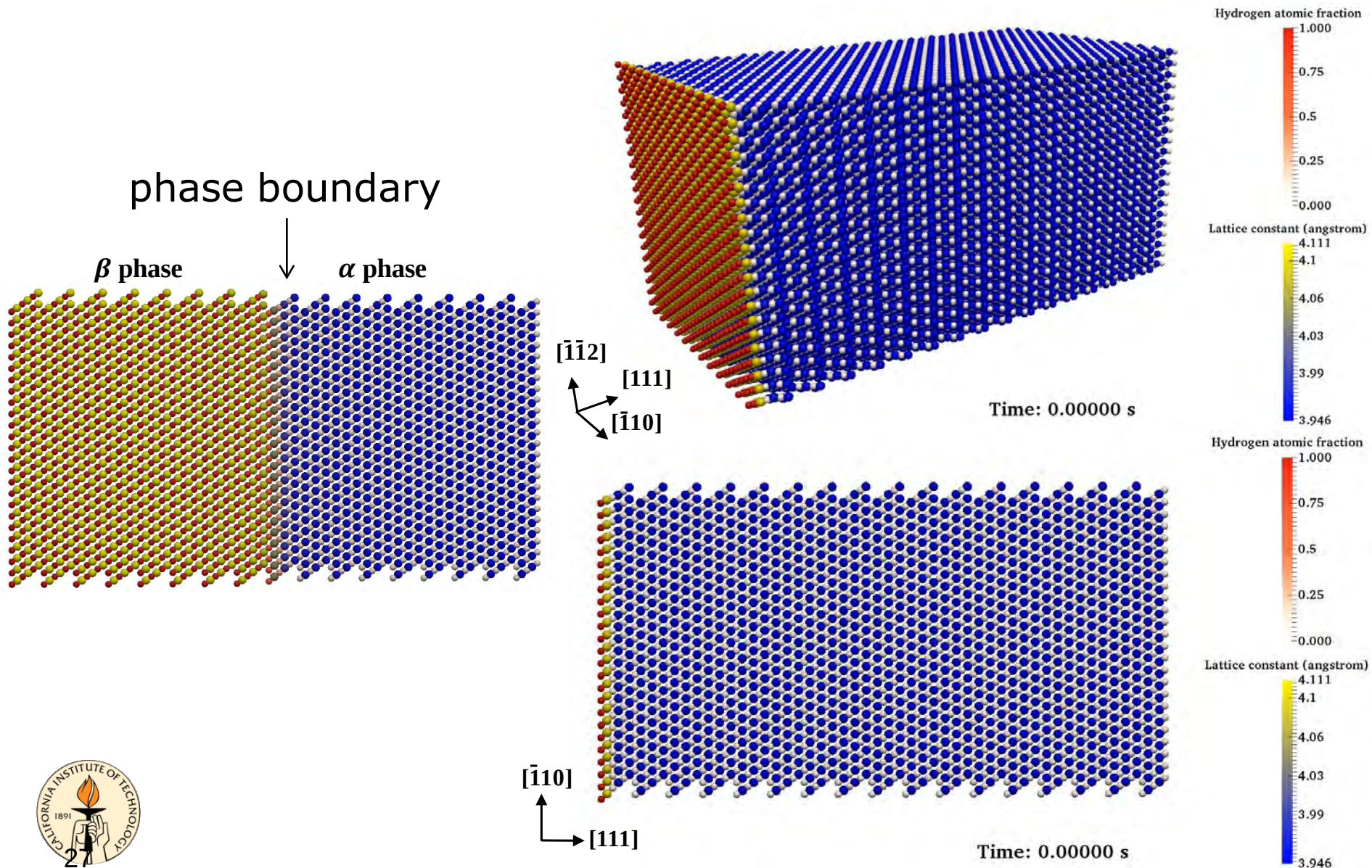
# H storage in Pd NW – $\alpha$ – $\beta$ interface

- $\text{PdH}_x$  exists in two phases at room temperature:
  - $\alpha$  phase:  $0 < x \leq 0.03$     •  $\beta$  phase:  $0.608 \leq x \leq 1$
- In both phases: H occupies octahedral sites of FCC Pd lattice
- Phase transition ( $\alpha \rightarrow \beta$ ): 10.4% volume expansion
- Computational setup: EAM potential<sup>1</sup>, NN transport kinetics

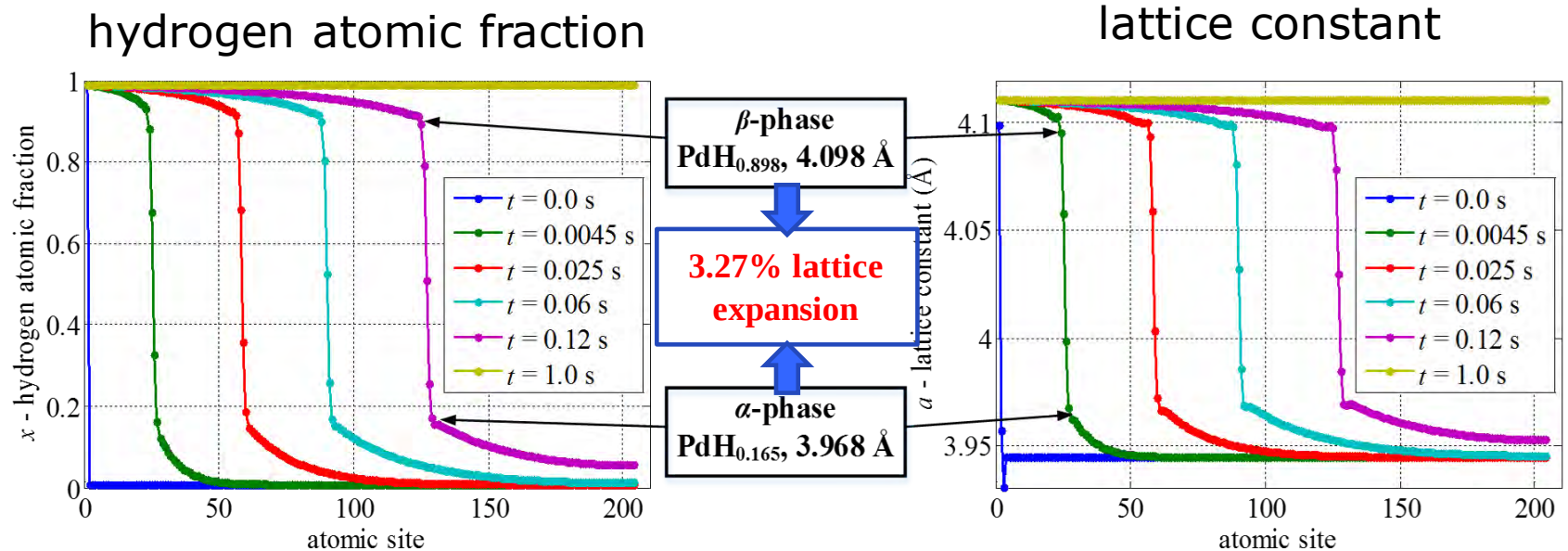
● ● Pd sites  
● ● interstitial sites



# H storage in Pd NW – $\alpha$ - $\beta$ interface



# H storage in Pd NW – $\alpha$ – $\beta$ interface



- Phase transition predicted (3.27% vs. 3.35%)
- Phase boundary motion, velocity, predicted ( $\sim 100$  nm/s)
- In progress:  $\text{MgH}_2$  (hcp  $\alpha$ -phase, rutile  $\beta$ -phase)



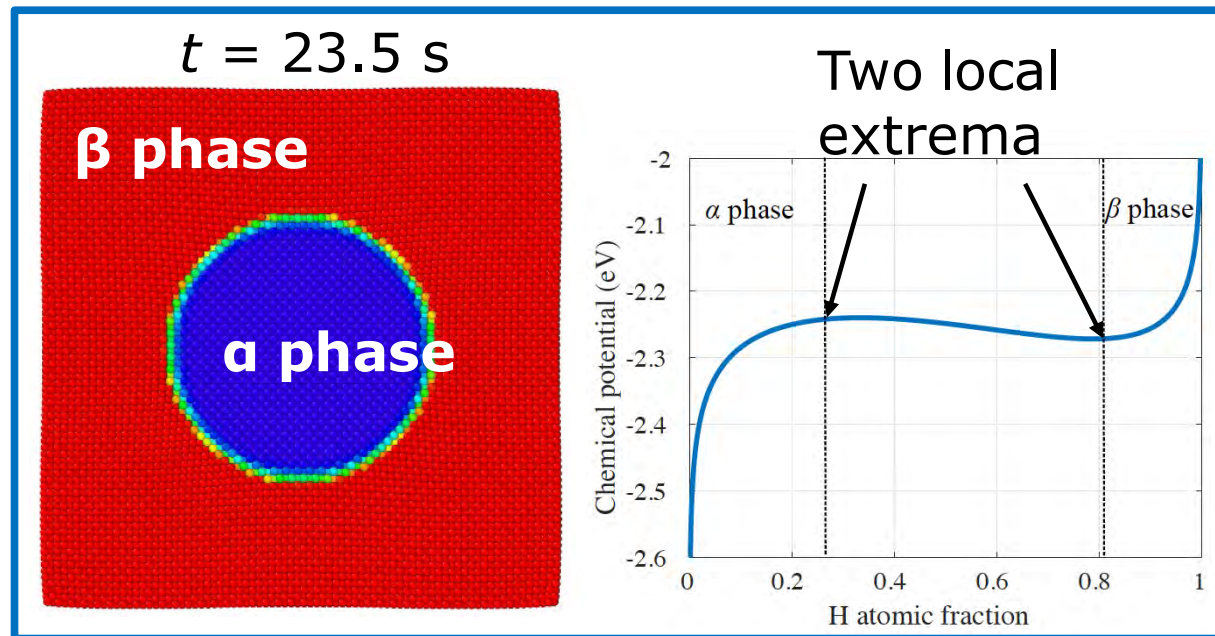
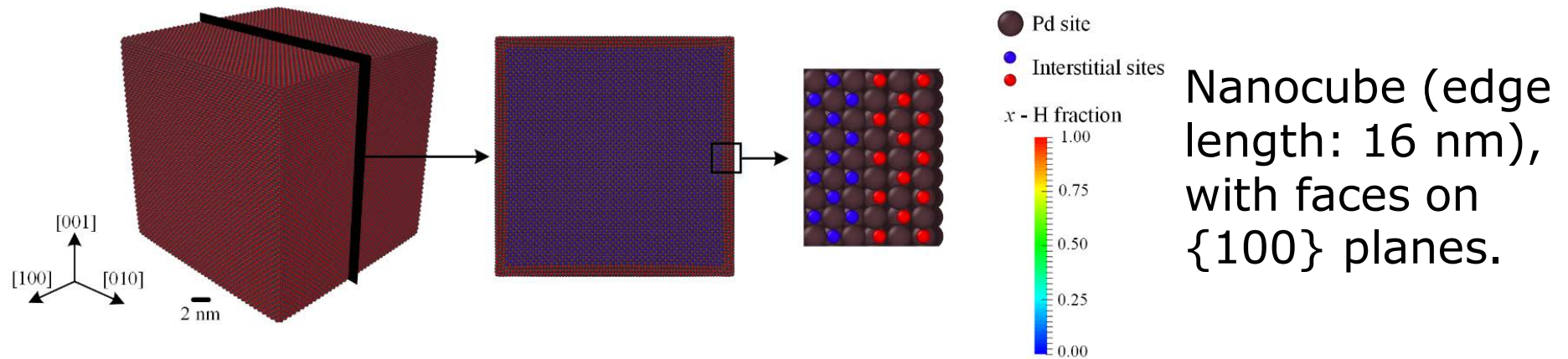
# Application: H storage in Pd nanoparticles



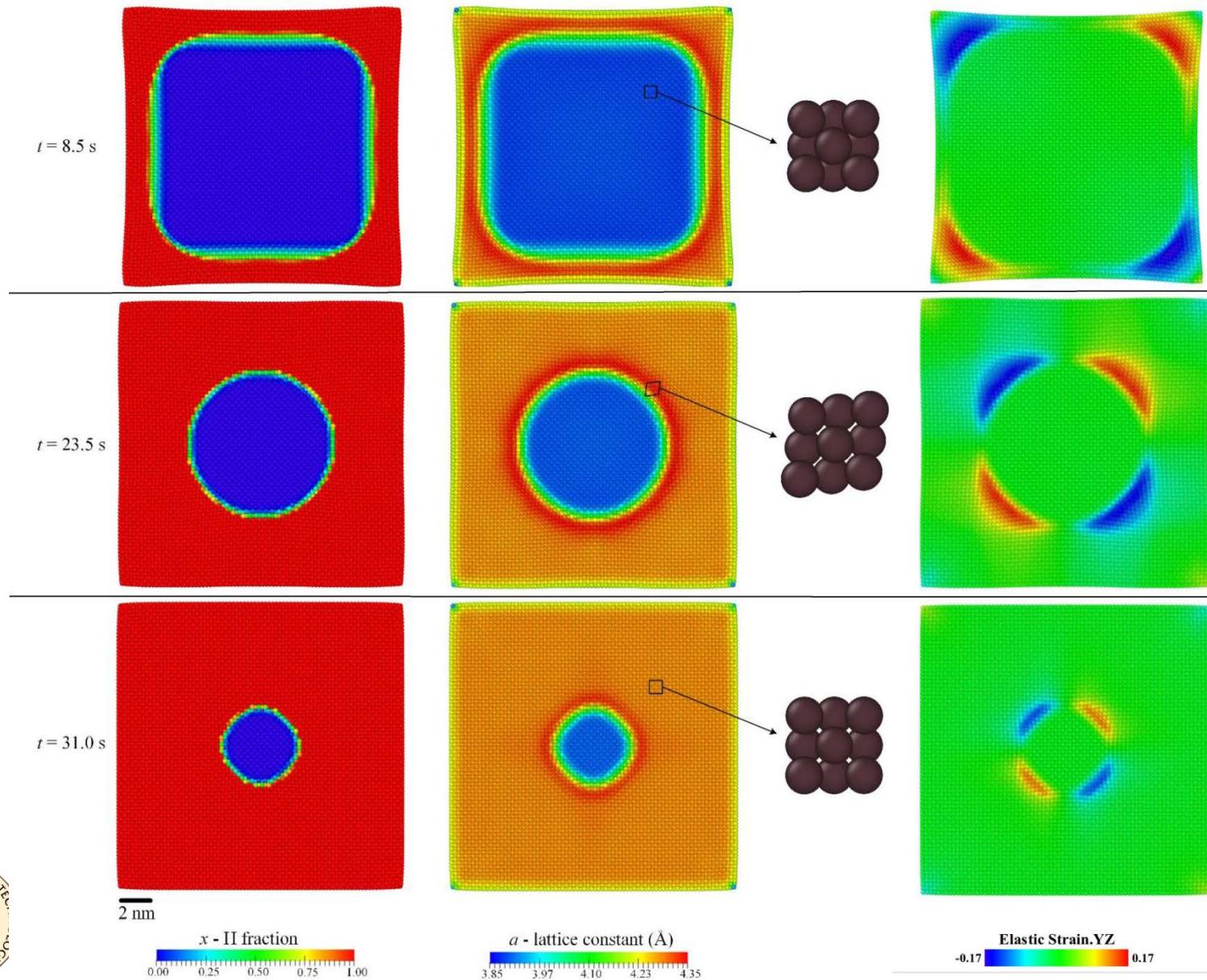
STEM frames showing  $\alpha$  to  $\beta$  phase evolution



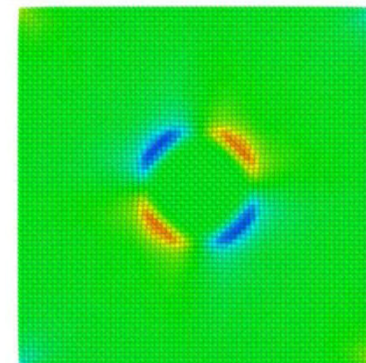
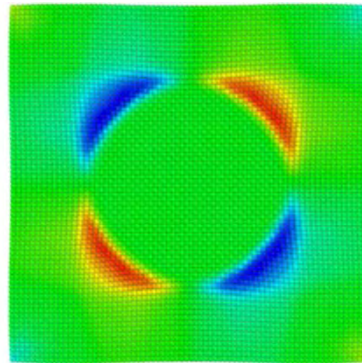
# H storage in Pd NP – Problem setup



# H storage in Pd NP – Interfacial strain

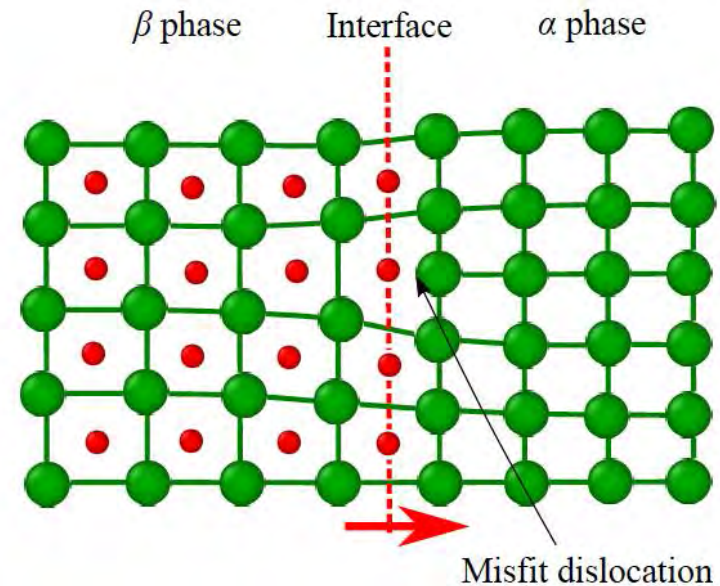
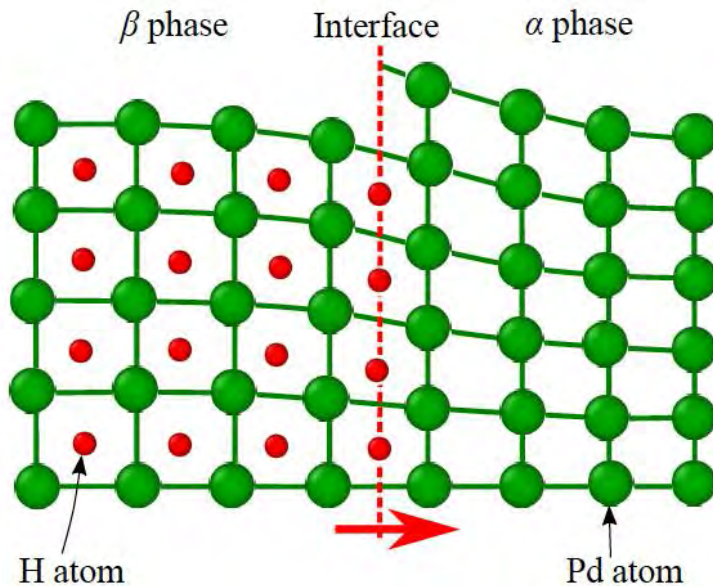


# Interfacial dislocations



misfit  
strain  
evolution

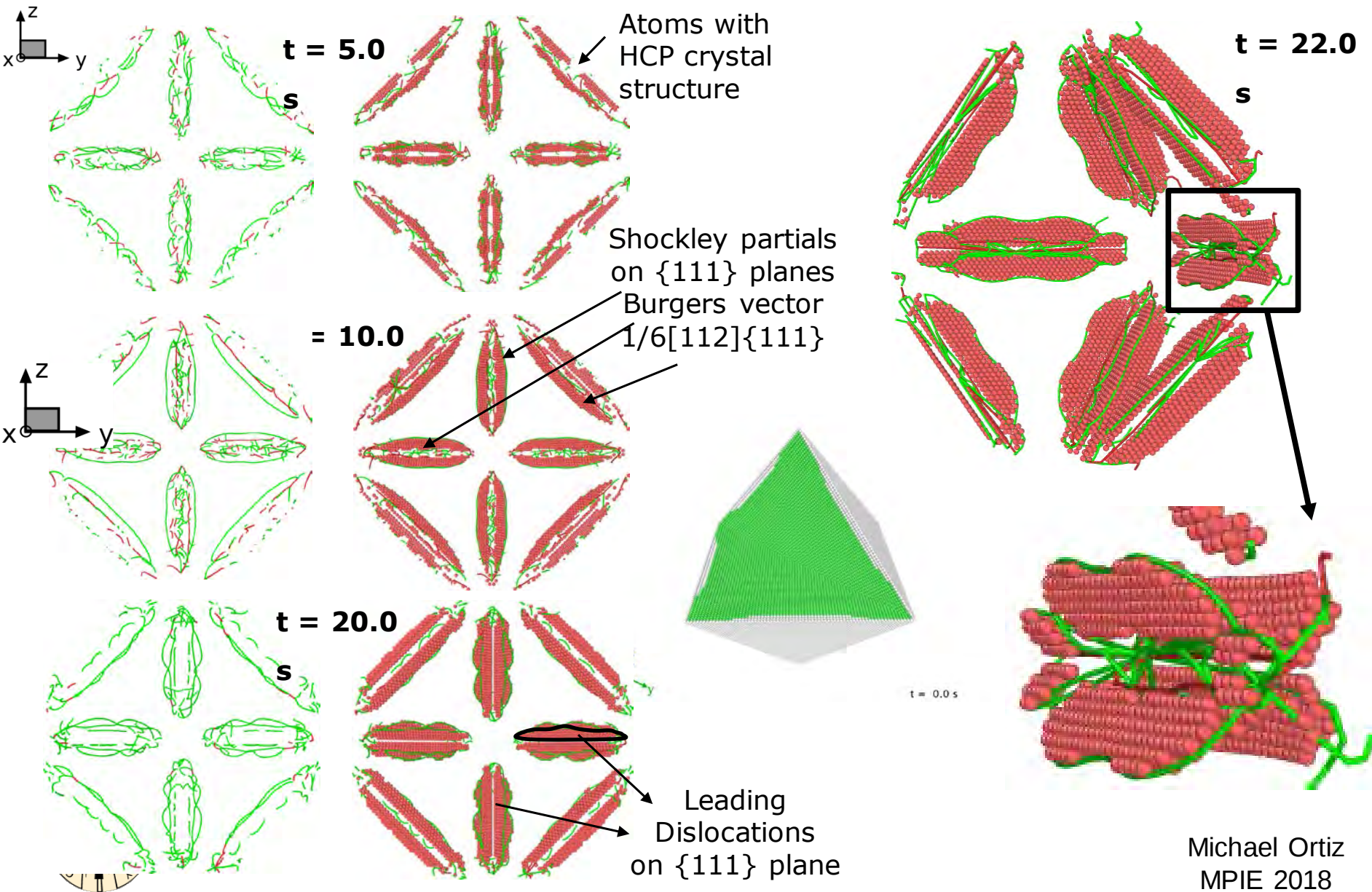
Elastic Strain.YZ  
-0.17 0.17



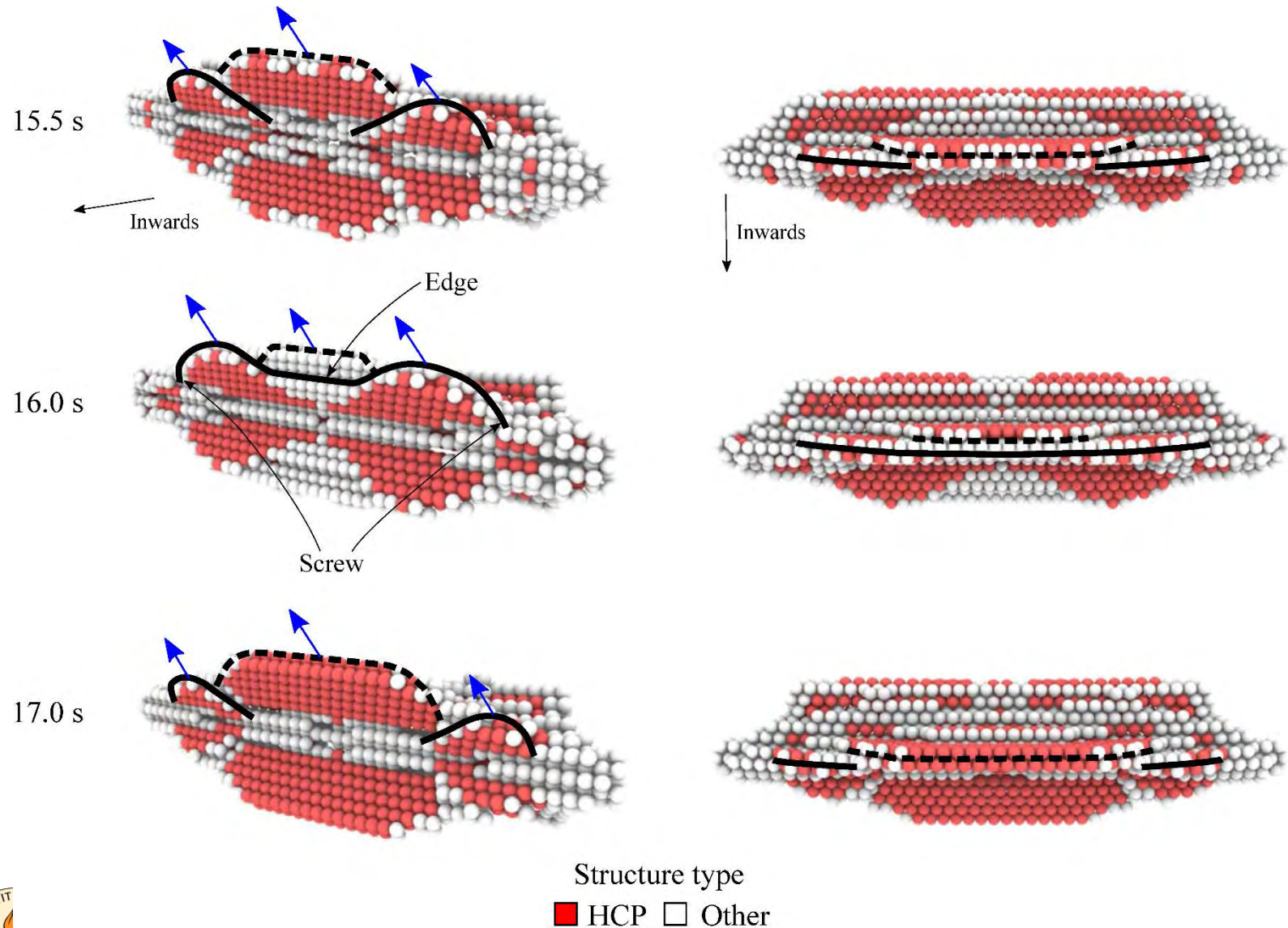
Misfit strain is relieved by misfit dislocations



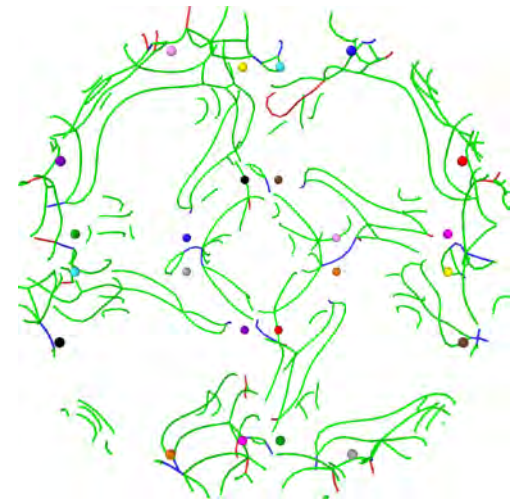
# PdH: Interfacial misfit dislocations



# PdH: Interfacial misfit dislocations



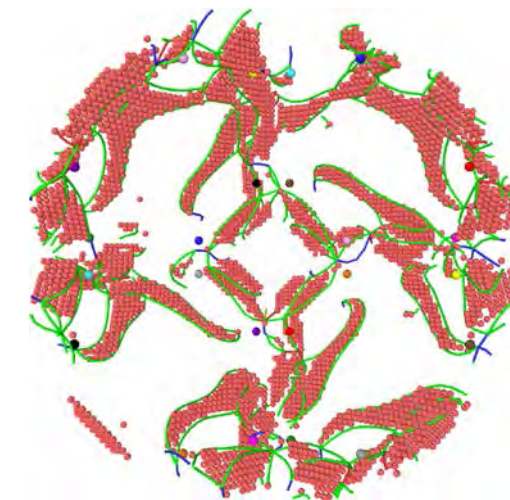
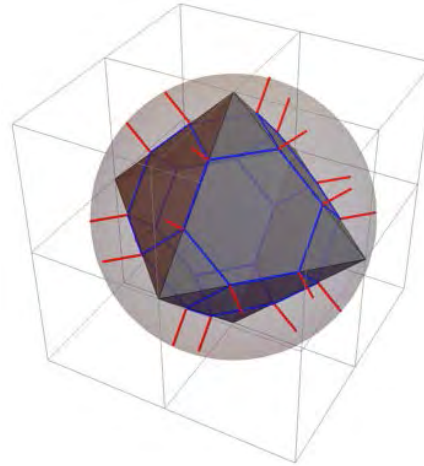
# PdH: Interfacial misfit dislocations



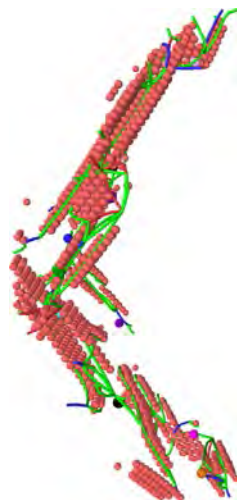
(100) plane



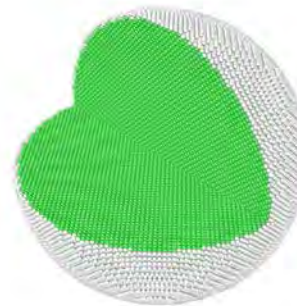
(111) direction



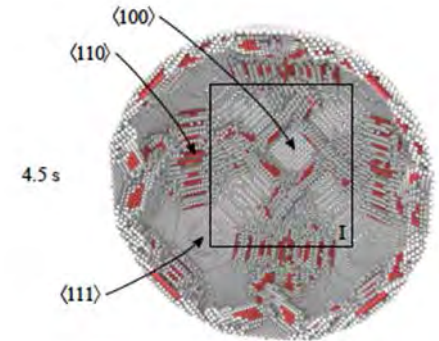
(100) plane



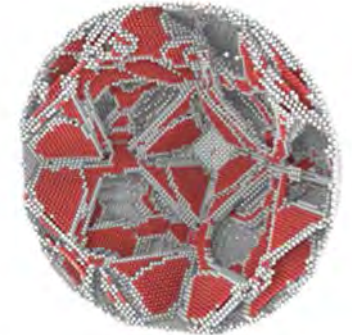
(111) direction



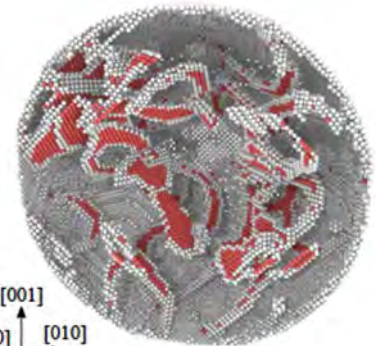
$t = 0.0 \text{ s}$



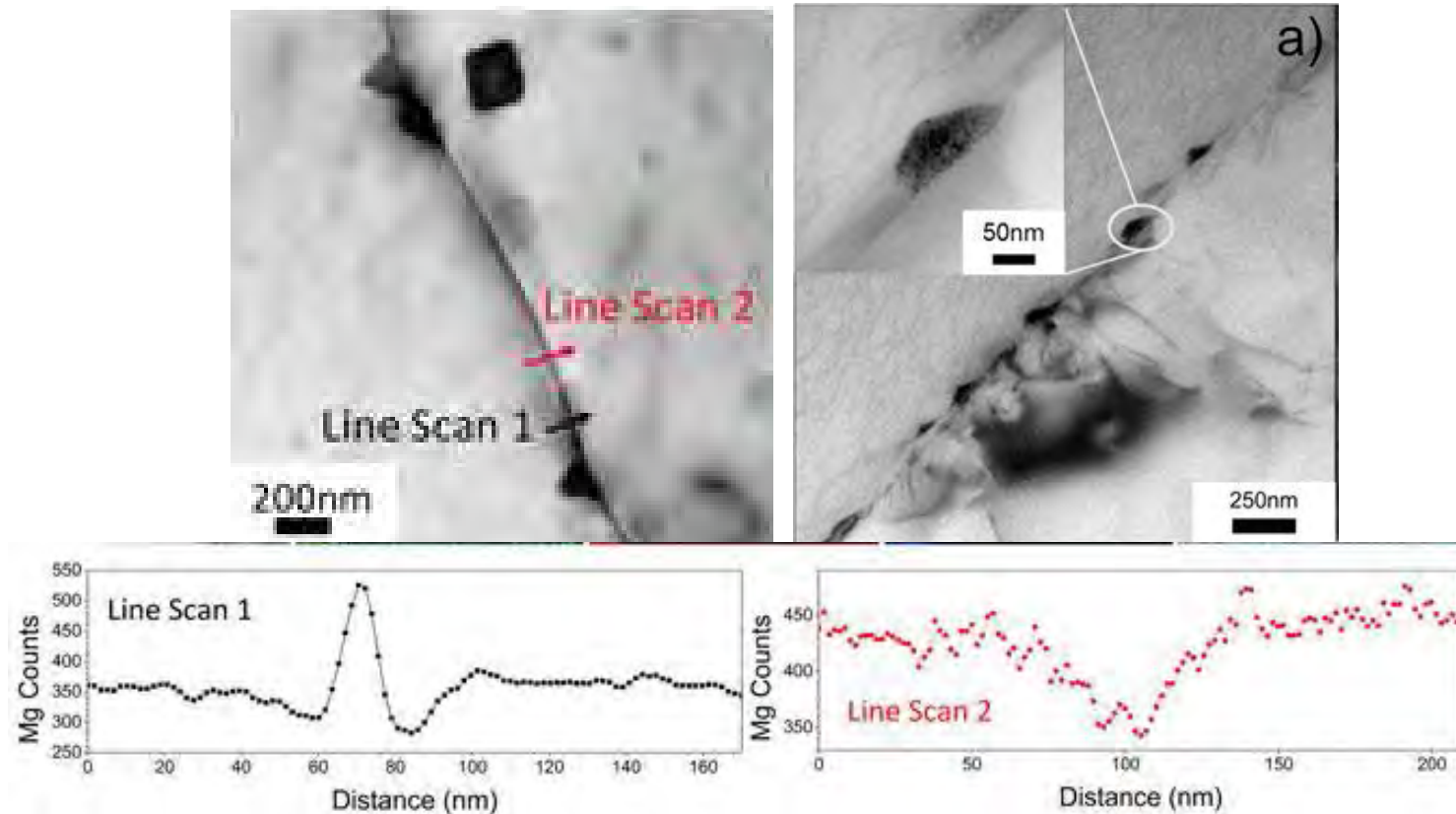
17.5 s



41.5 s



# Work in progress: Mg–Al alloys



- Al-Mg 5xxxx series alloys
  - Sensitization due to GBs
  - Formation of  $\beta$  phase ( $\text{Mg}_2\text{Al}_3$ )
  - Stress corrosion cracking
- Time scale:  $\sim$  days!  
Not accessible to MD



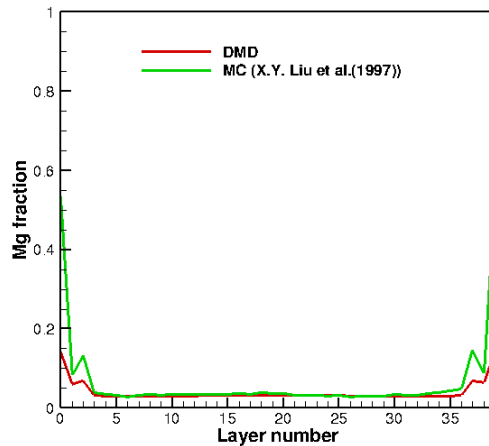
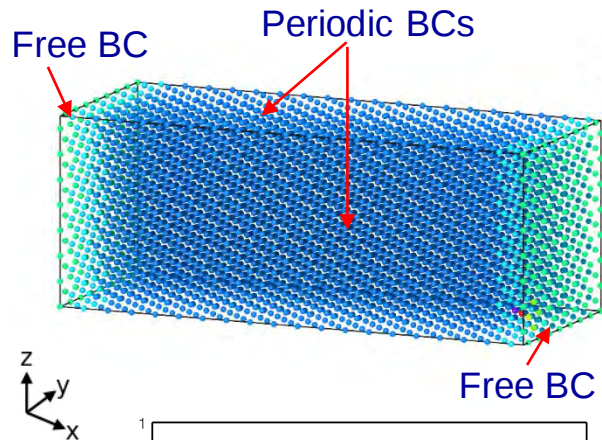
R. Zhang *et al.*, *Scientific Reports*, 7 (2017) 2961

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# DMD validation – Surface segregation

Al-4%Mg alloy at 600K

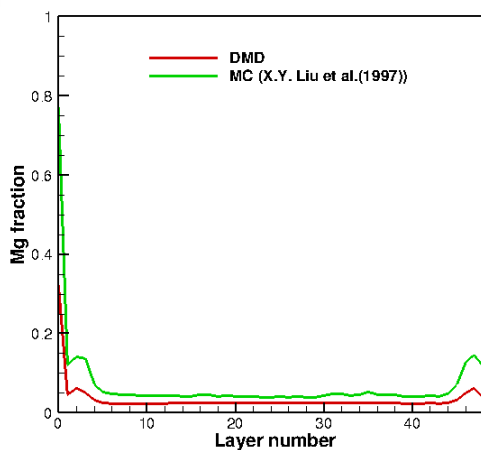
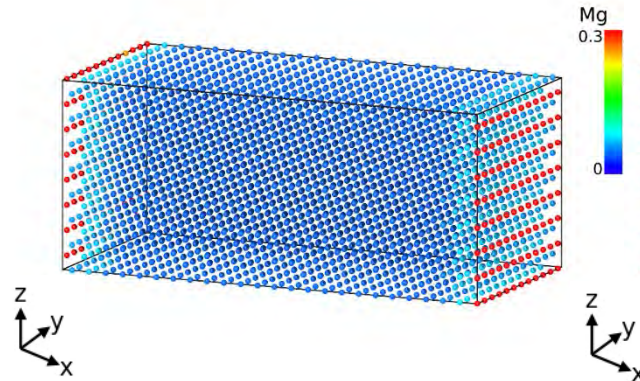
(100) surface



After 71 ms

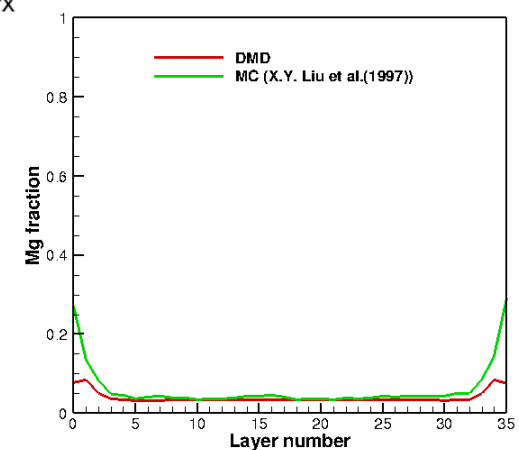
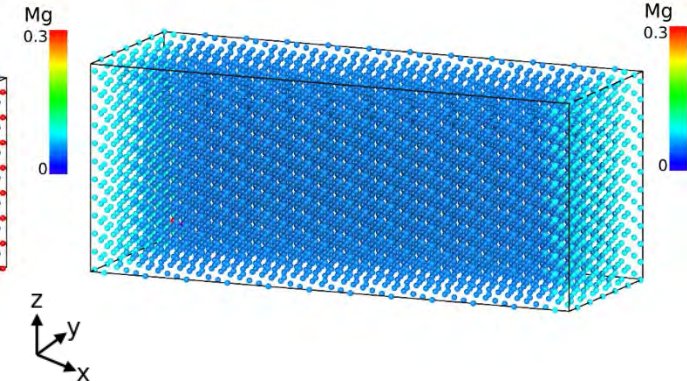
(110) surface

$D(T=600K) = 5.4914 \cdot 10^{-16} \text{m}^2/\text{s}$



After 82 ms

(111) surface

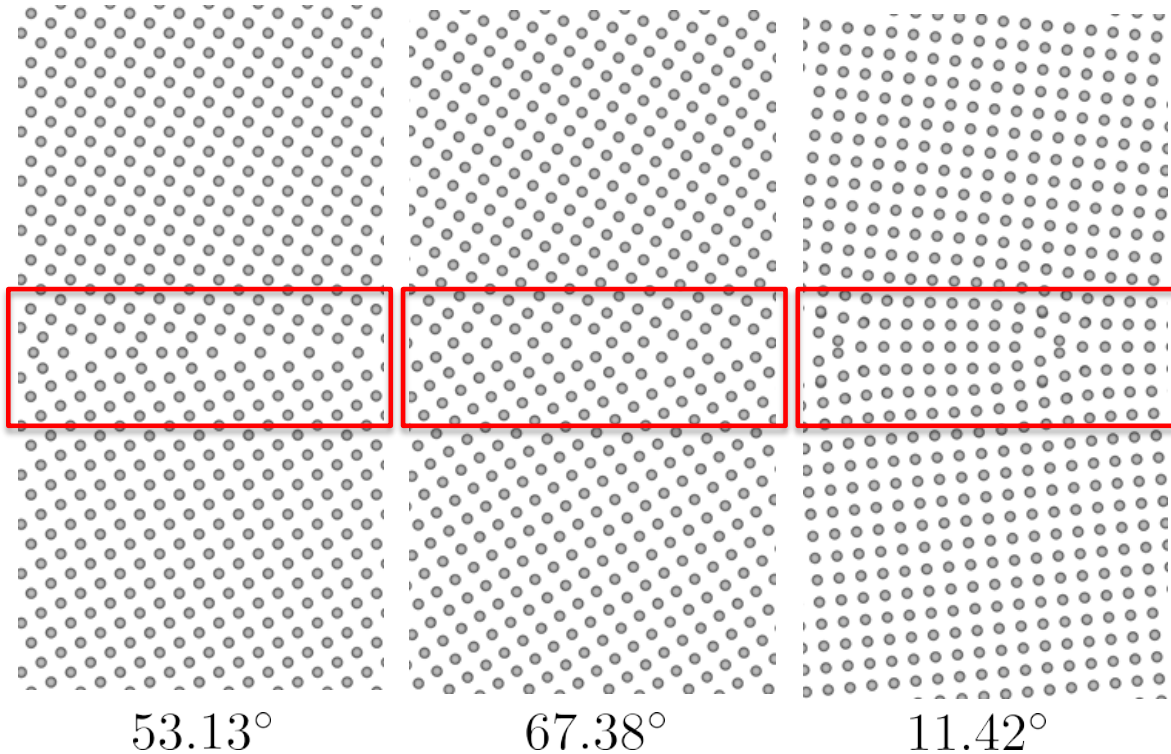


After 142 ms

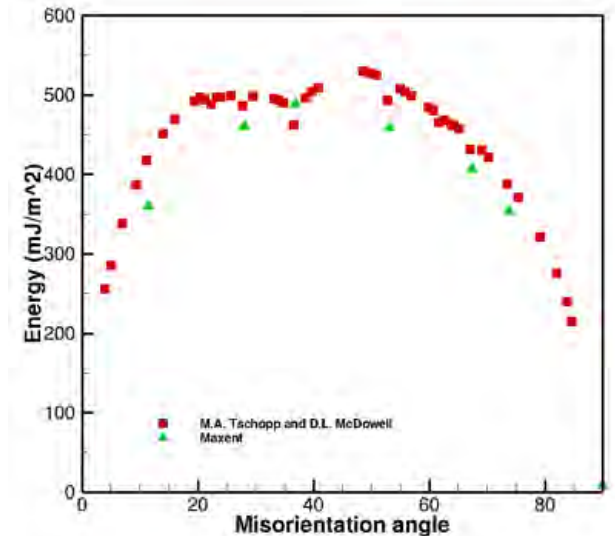


# DMD validation – GB segregation

Al-4%Mg alloy at 600K



Symmetric grain boundary energies



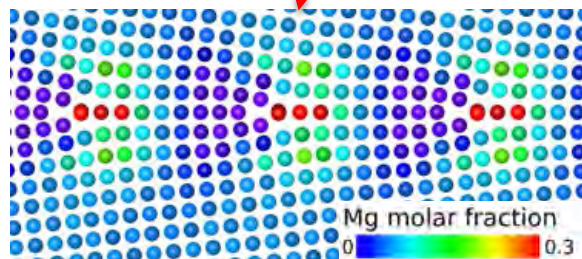
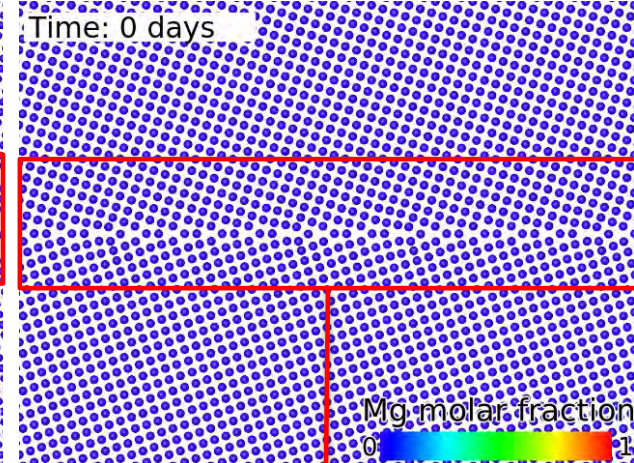
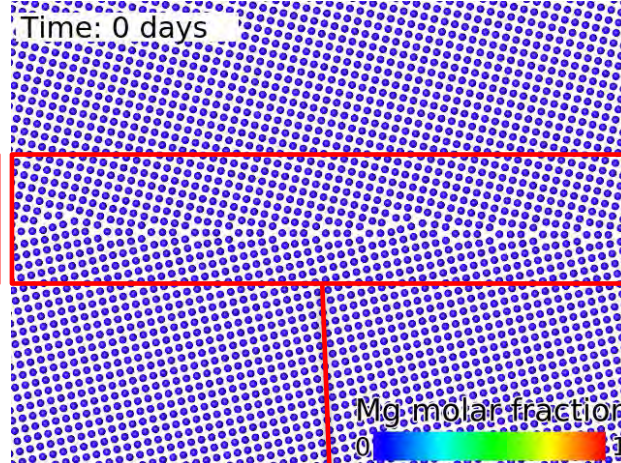
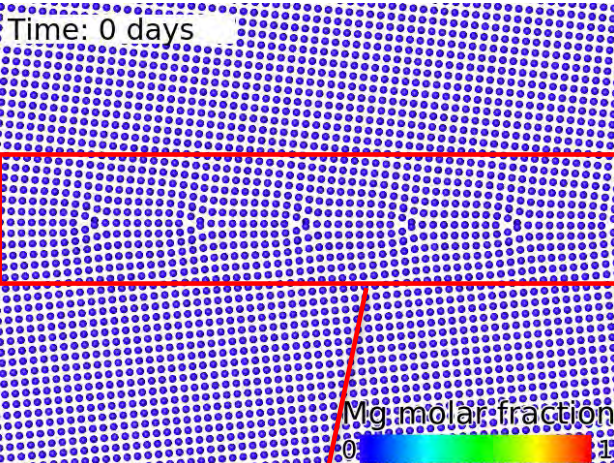
# DMD validation – GB segregation

Al-4%Mg alloy at 300K

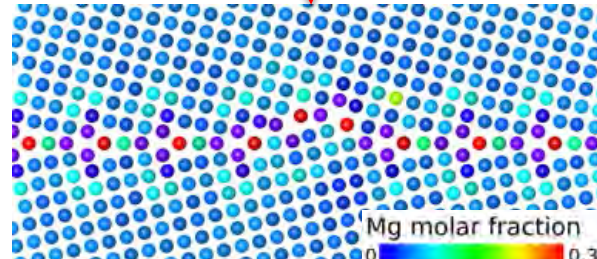
11.42°

28.07°

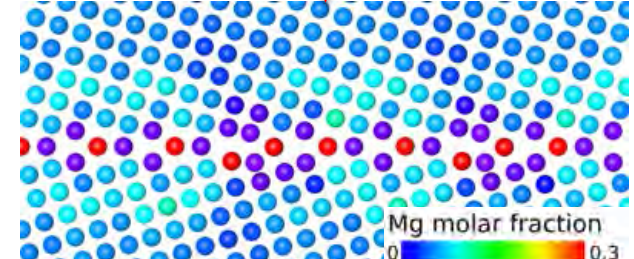
36.87°



After 377 days



After 97 days



After 245 days



Z. Li, et al., *Scientific Reports*, **6** (2016) 29973.

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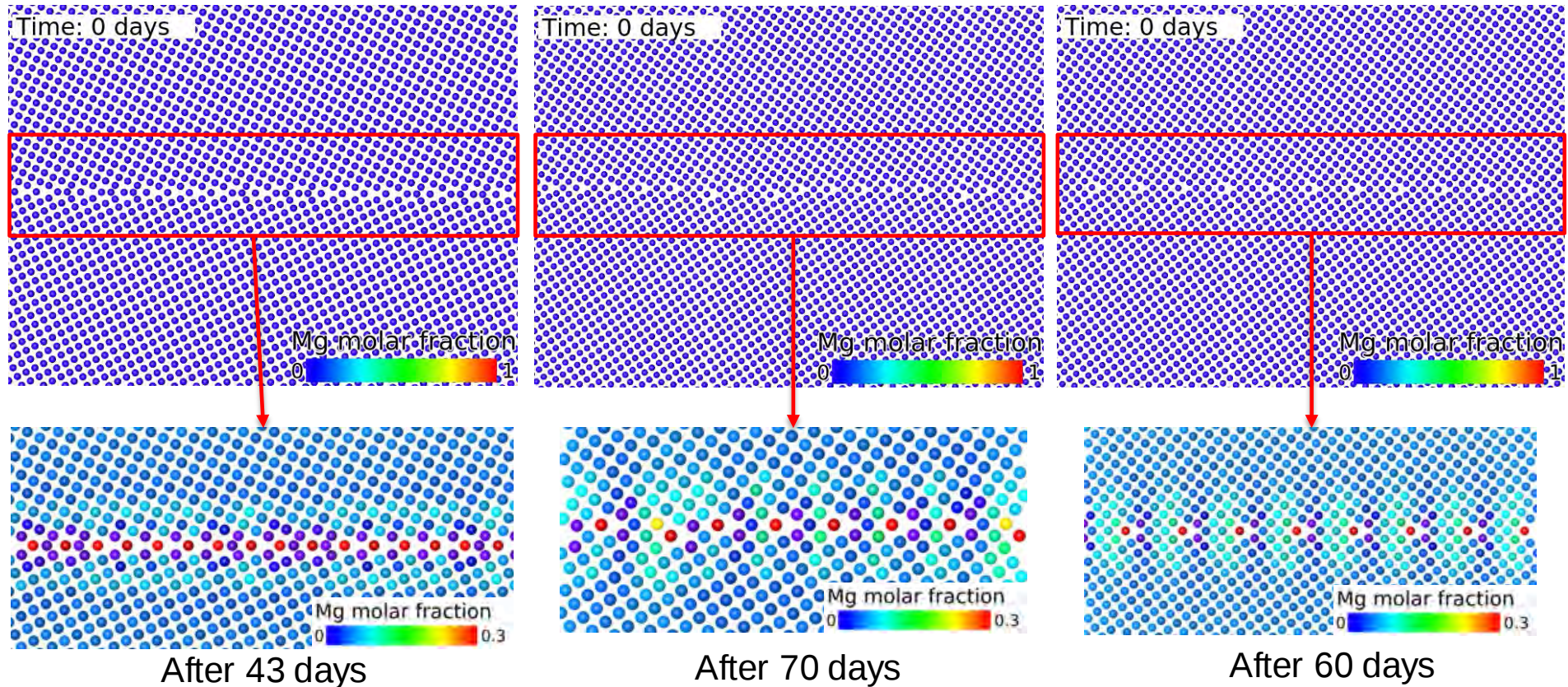
# DMD validation – GB segregation

Al-4%Mg alloy at 300K

53.13°

67.38°

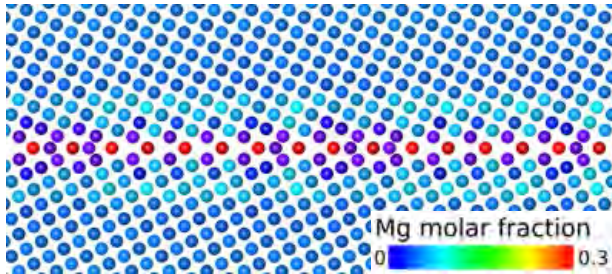
73.74°



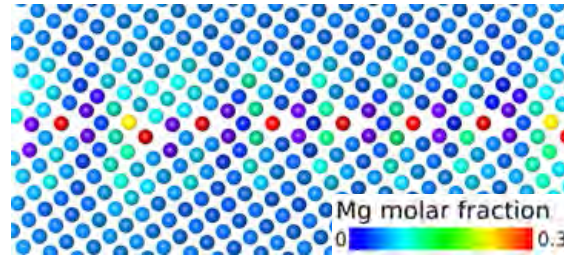
Z. Li, *et al.*, *Scientific Reports*, **6** (2016) 29973.

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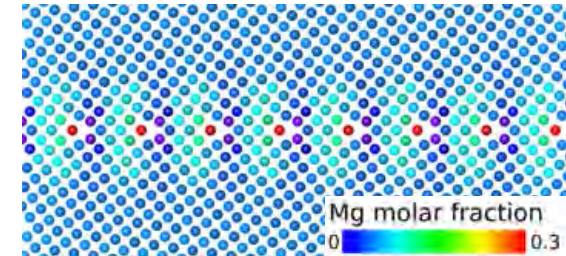
# DMD validation – GB segregation



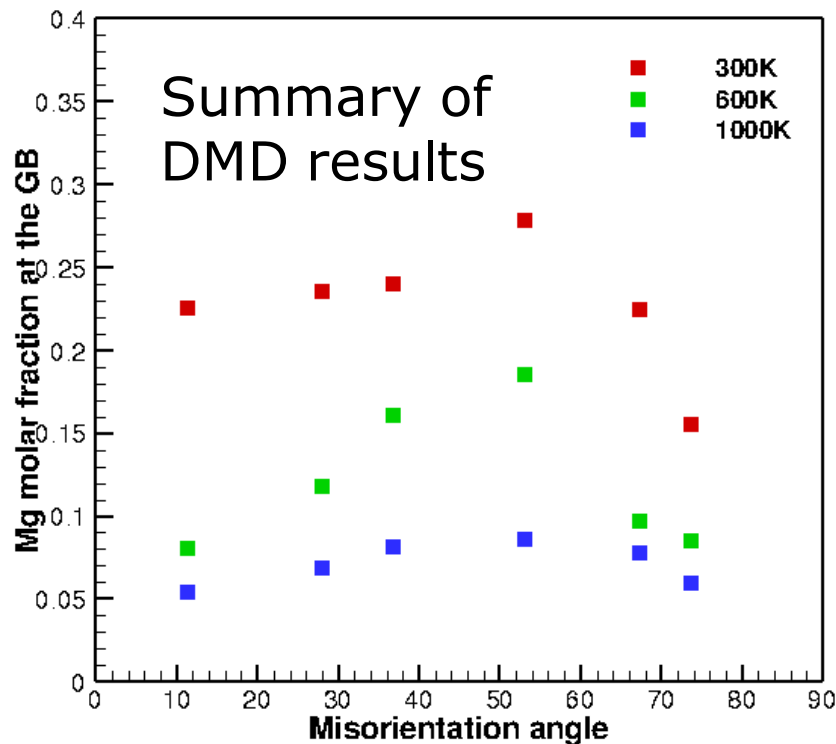
After 43 days



After 70 days



After 60 days

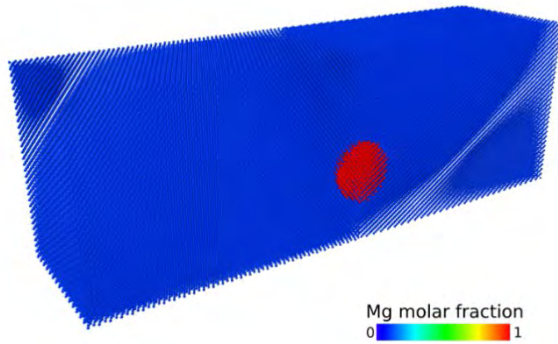


- Mg segregation to Al GBs takes place on time scale of days or months.
- Mg segregation to Al GBs depends on misorientation angle
- Mg segregation to Al GBs depends on temperature.
- An increase in temperature reduces segregation

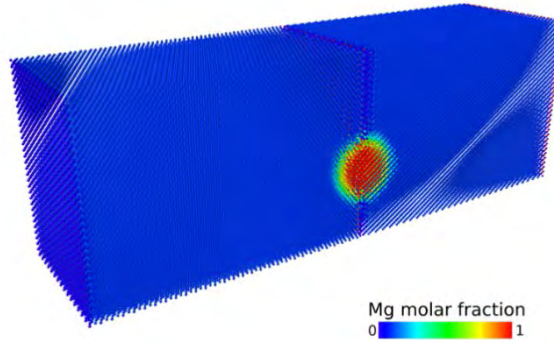


# DMD validation – GB segregation

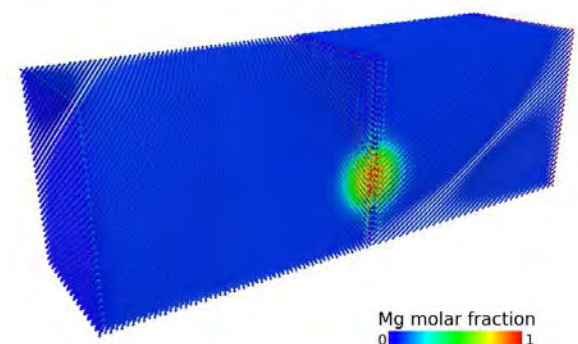
Al-4%Mg alloy at 300K  
Dissolution of Mg precipitate



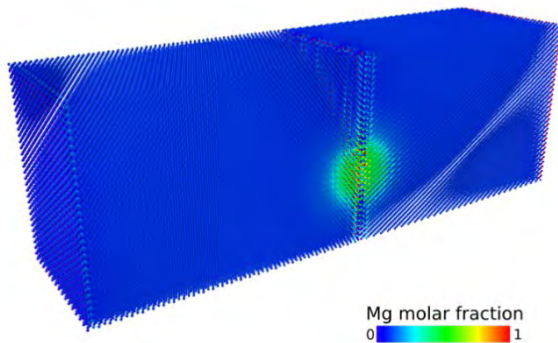
After 0 days



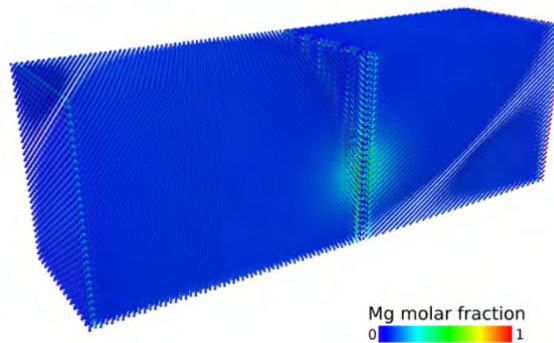
After 1 days



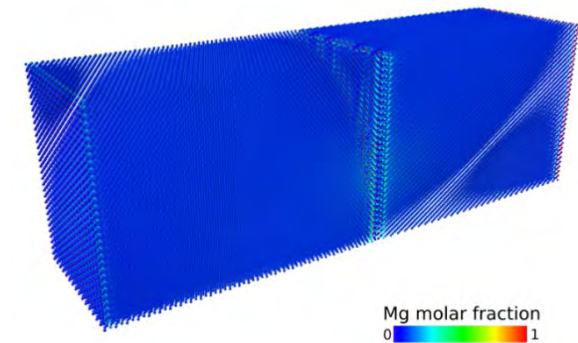
After 2 days



After 12 days



After 20 days



After 69 days

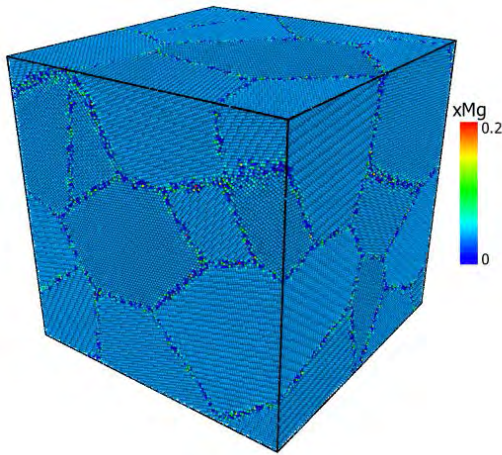


Z. Li, *et al.*, *Scientific Reports*, **6** (2016) 29973.

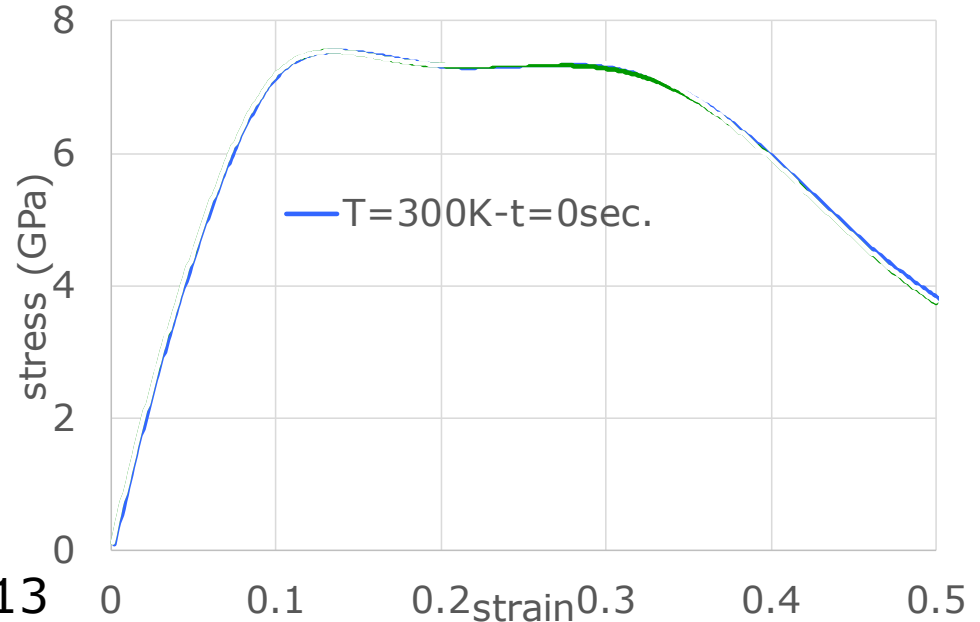
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# Al-4%Mg Polyxals – Mechanical testing

After 84 hours



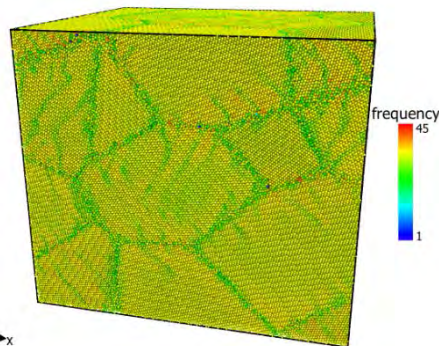
Uniaxial test - strain rate: 1e10 1/sec



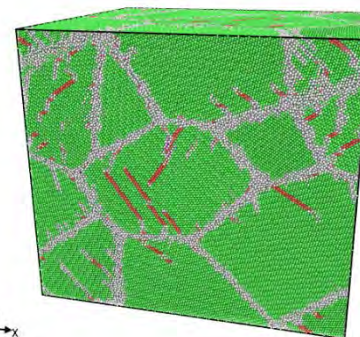
$D(T=300\text{K}) = 3.3364 \cdot 10^{-26} \text{ m}^2/\text{s}$   
 Hopping frequency (1/s) =  $1.0 \cdot 10^{13}$   
 Barrier energy (eV) = 1.1542

Frequency

$\epsilon = 0.15$



Dislocation analysis



| Color             | Structure         | Count   | Fraction |
|-------------------|-------------------|---------|----------|
| Other             | Other             | 426934  | 19.7%    |
| FCC               | FCC               | 1675814 | 77.4%    |
| HCP               | HCP               | 61698   | 2.9%     |
| BCC               | BCC               | 0       | 0.0%     |
| Cubic diamond     | Cubic diamond     | 0       | 0.0%     |
| Hexagonal diamond | Hexagonal diamond | 0       | 0.0%     |



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# Concluding remarks

- *Diffusive Molecular Dynamics* (DMD) provides a useful paradigm for describing slow/long term diffusion/transport phenomena with atomistic realism
- Non-equilibrium thermodynamics without all the thermal vibrations; mass transport without all the hops; atomistics without all the atoms...
- Work in progress: Microstructure evolution in alloys (work in collaboration with SINTEF/ Norway, NTNU, HZG...)



A word cloud featuring the phrase "thank you" in various languages and scripts. The central text "thank you" is the largest and most prominent. Surrounding it are numerous other expressions of gratitude, including:

- English:** thank you, gracias, merci, obrigado, bedankt, dank u, dank je, dank, thanks, thank you very much, thank you so much, thank you for, thank you for everything, thank you for your help, thank you for your support, thank you for your contribution, thank you for your time, thank you for your attention, thank you for your interest, thank you for your participation, thank you for your presence, thank you for your input, thank you for your feedback, thank you for your suggestions, thank you for your comments, thank you for your questions, thank you for your answers, thank you for your assistance, thank you for your cooperation, thank you for your collaboration, thank you for your partnership, thank you for your friendship, thank you for your love, thank you for your life, thank you for your family, thank you for your friends, thank you for your community, thank you for your country, thank you for your world, thank you for your universe, thank you for your existence, thank you for your journey, thank you for your adventure, thank you for your discovery, thank you for your knowledge, thank you for your wisdom, thank you for your courage, thank you for your strength, thank you for your resilience, thank you for your perseverance, thank you for your determination, thank you for your commitment, thank you for your dedication, thank you for your passion, thank you for your enthusiasm, thank you for your energy, thank you for your positivity, thank you for your optimism, thank you for your hope, thank you for your faith, thank you for your belief, thank you for your trust, thank you for your confidence, thank you for your respect, thank you for your honor, thank you for your dignity, thank you for your integrity, thank you for your honesty, thank you for your transparency, thank you for your accountability, thank you for your responsibility, thank you for your leadership, thank you for your guidance, thank you for your mentorship, thank you for your coaching, thank you for your training, thank you for your education, thank you for your learning, thank you for your growth, thank you for your development, thank you for your progress, thank you for your achievement, thank you for your success, thank you for your accomplishment, thank you for your triumph, thank you for your victory, thank you for your conquest, thank you for your triumph over adversity, thank you for your triumph over challenges, thank you for your triumph over obstacles, thank you for your triumph over difficulties, thank you for your triumph over setbacks, thank you for your triumph over failure, thank you for your triumph over doubt, thank you for your triumph over fear, thank you for your triumph over uncertainty, thank you for your triumph over adversity, thank you for your triumph over challenges, thank you for your triumph over obstacles, thank you for your triumph over difficulties, thank you for your triumph over setbacks, thank you for your triumph over failure, thank you for your triumph over doubt, thank you for your triumph over fear, thank you for your triumph over uncertainty.
- Other Languages:**
  - Spanish: gracias, gracias mucho, muchas gracias, un millón de gracias, gracias de todo corazón, gracias por todo, gracias por todo lo que has hecho por mí, gracias por todo lo que has hecho por nosotros, gracias por todo lo que has hecho por el mundo.
  - French: merci, merci beaucoup, merci infiniment, merci de tout cœur, merci pour tout, merci pour tout ce que vous avez fait pour moi, merci pour tout ce que vous avez fait pour nous, merci pour tout ce que vous avez fait pour le monde.
  - German: danke, danke sehr, danke sehr sehr, danke von ganzem Herzen, danke für alles, danke für alles was Sie für mich getan haben, danke für alles was Sie für uns getan haben, danke für alles was Sie für die Welt getan haben.
  - Portuguese: obrigado, obrigado muito, obrigado demais, obrigado de todo o coração, obrigado por tudo, obrigado por tudo o que você fez por mim, obrigado por tudo o que você fez por nós, obrigado por tudo o que você fez pelo mundo.
  - Italian: grazie, grazie mille, grazie infinite, grazie di tutto il cuore, grazie per tutto, grazie per tutto ciò che ha fatto per me, grazie per tutto ciò che ha fatto per noi, grazie per tutto ciò che ha fatto per il mondo.
  - Japanese: ありがとう (arigatou), ありがとうございます (arigatou gozaimasu), 誠にありがとうございます (makoto ni arigatou gozaimasu), 心からありがとうございます (kokoro kara arigatou gozaimasu), 感謝しています (kankan shiteimasu), 感謝しております (kankan shite orimasu).
  - Chinese: 谢谢 (xie xie), 非常感谢 (fēn fēn xiè xie), 万分感谢 (wàn fēn xiè xie), 衷心感谢 (zhōng xīn xiè xie), 感谢一切 (gǎn xiè yī qiè), 感谢您所做的一切 (gǎn xiè nín suǒ zuò de yī qiè), 感谢您所做的一切 (gǎn xiè nín suǒ zuò de yī qiè), 感谢您所做的一切 (gǎn xiè nín suǒ zuò de yī qiè).
  - Russian: спасибо (spasibo), спасибо большое (spasibo bol'shoye), спасибо очень (spasibo ochen'), спасибо от всего сердца (spasibo ot vsego serdtsa), спасибо за всё (spasibo za vsyo), спасибо за всё что вы сделали для меня, спасибо за всё что вы сделали для нас, спасибо за всё что вы сделали для мира.
  - Polish: dziękuję, dziękuję bardzo, dziękuję serdecznie, dziękuję z całego serca, dziękuję za wszystko, dziękuję za wszystko co Pan/Pani dla mnie zrobił/zrobiła, dziękuję za wszystko co Pan/Pani dla nas zrobił/zrobiła, dziękuję za wszystko co Pan/Pani dla świata zrobił/zrobiła.
  - Ukrainian: дякую (dyakuyu), дякую дуже (dyakuyu duzhe), дякую від усього серця (dyakuyu vid usogo serca), дякую за все (dyakuyu za vse), дякую за все що ви зробили для мене, дякую за все що ви зробили для нас, дякую за все що ви зробили для світу.
  - Hebrew: תודה (todah), תודה רבה (todah rabah), תודה מכל הלב (todah mikol ha'lev), תודה על הכל (todah al ha'kol), תודה על כל מה שאתה/את/אתם עושה/עושה/עושים בשבילי/שבילך/שבילכם, תודה על כל מה שאתה/את/אתם עושה/עושה/עושים בשבילנו, תודה על כל מה שאתה/את/אתם עושה/עושה/עושים בשביל העולם.
  - Arabic: شكرا (shukra), شكرا جزيلا (shukra jazila), شكرا كثيرا (shukra kithira), شكرا من كل القلب (shukra min kul al-qalb), شكرا على كل شيء (shukra ala kul shayn), شكرا على كل ما فعلته/فعلتي/فعلتم من مني/منك/منكم, شكرا على كل ما فعلته/فعلتي/فعلتم من مني/منك/منكم, شكرا على كل ما فعلته/فعلتي/فعلتم من مني/منك/منكم.
  - Yiddish: דאנק (dank), דאנק ווייניג (dank veynig), דאנק זייער (dank zeyer), דאנק פון גאנצן הערצן (dank fun ganzn hartsn), דאנק פאר אלעס (dank far aleks), דאנק פאר אלעס וואסוויילסטו/וואסוויילסטו/וואסוויילסטו פאר מיין, דאנק פאר אלעס וואסוויילסטו/וואסוויילסטו/וואסוויילסטו פאר מיין, דאנק פאר אלעס וואסוויילסטו/וואסוויילסטו/וואסוויילסטו פאר מיין.
  - Yiddish: דאנק (dank), דאנק ווייניג (dank veynig), דאנק זייער (dank zeyer), דאנק פון גאנצן הערצן (dank fun ganzn hartsn), דאנק פאר אלעס (dank far aleks), דאנק פאר אלעס וואסוויילסטו/וואסוויילסטו/וואסוויילסטו פאר מיין, דאנק פאר אלעס וואסוויילסטו/וואסוויילסטו/וואסוויילסטו פאר מיין, דאנק פאר אלעס וואסוויילסטו/וואסוויילסטו/וואסוויילסטו פאר מיין.
  - Yiddish: דאנק (dank), דאנק ווייניג (dank veynig), דאנק זייער (dank zeyer), דאנק פון גאנצן הערצן (dank fun ganzn hartsn), דאנק פאר אלעס (dank far aleks), דאנק פאר אלעס וואסוויילסטו/וואסוויילסטו/וואסוויילסטו פאר מיין, דאנק פאר אלעס וואסוויילסטו/וואסוויילסטו/וואסוויילסטו פאר מיין, דאנק פאר אלעס וואסוויילסטו/וואסוויילסטו/וואסוויילסטו פאר מיין.

