“Atomistic modeling of Solid Phase Epitaxial Regrowth using Lattice Kinetic Monte Carlo: Facet formation and strain dependencies

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Junction Technology Group Meeting

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Outline

- The problem: introduction
- An atomistic solution: LKMC
- The model.
- Planar growth for different orientations.
- A look at time evolution
- Fin FETs
- SPER on rectangular shapes.
  - Why corners are different?
  - Introducing strain
  - Results
- Conclusions

Introduction

- Typicall ultra-shallow junctions produce substrate amorphization.
- Subsequent recrystallization, or Solid Phase Epitaxial Regrowth (SPER) can significantly modified the implanted profiles: SPER simulation is critical.
- SPER depends on the substrate orientation, with ratios 20:10:1 for (100), (110) and (111).

An atomistic solution: LKMC

- Existing non Lattice KMC models accurately predict the one-dimensional SPER.
- Unfortunately, such models do not have different speeds for different orientations, much less faceting.
- In this work, a Lattice KMC model is introduced to overcome these limitations.

The model (I)

- We introduce the silicon lattice in the amorphous/crystalline interface
- A flag “A”morphous or “C”rystalline is set for every of these lattice atoms.
- The transition of “A” atoms to “C” atoms is simulated following an Arrhenius rate
- We follow Drosd and Washburn ideas to define such a rate:
  - Activation energy is constant
  - Prefactor depends on the atom neighborhood.

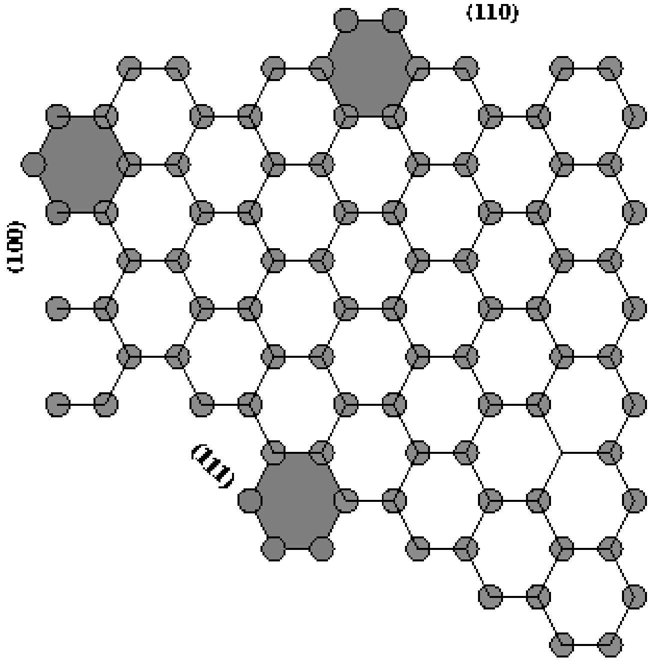
Drosd and Washburn, J. Appl. Phys. 53, 39 (1982)

The model (II)

- SPER rate is:

$$\upsilon = K(n) \times \exp(-(E + \lambda|\varepsilon_{xy}|)/K_B T)$$

- K(1), prefactor for atoms with two undistorted bonds.
- K(2), prefactor for atoms needing another one to join in a cluster
- K(3), prefactor for atoms needing two more to join in a cluster
- Model implemented in Sentaurus Process KMC



Idea: Two undistorted bonds needed

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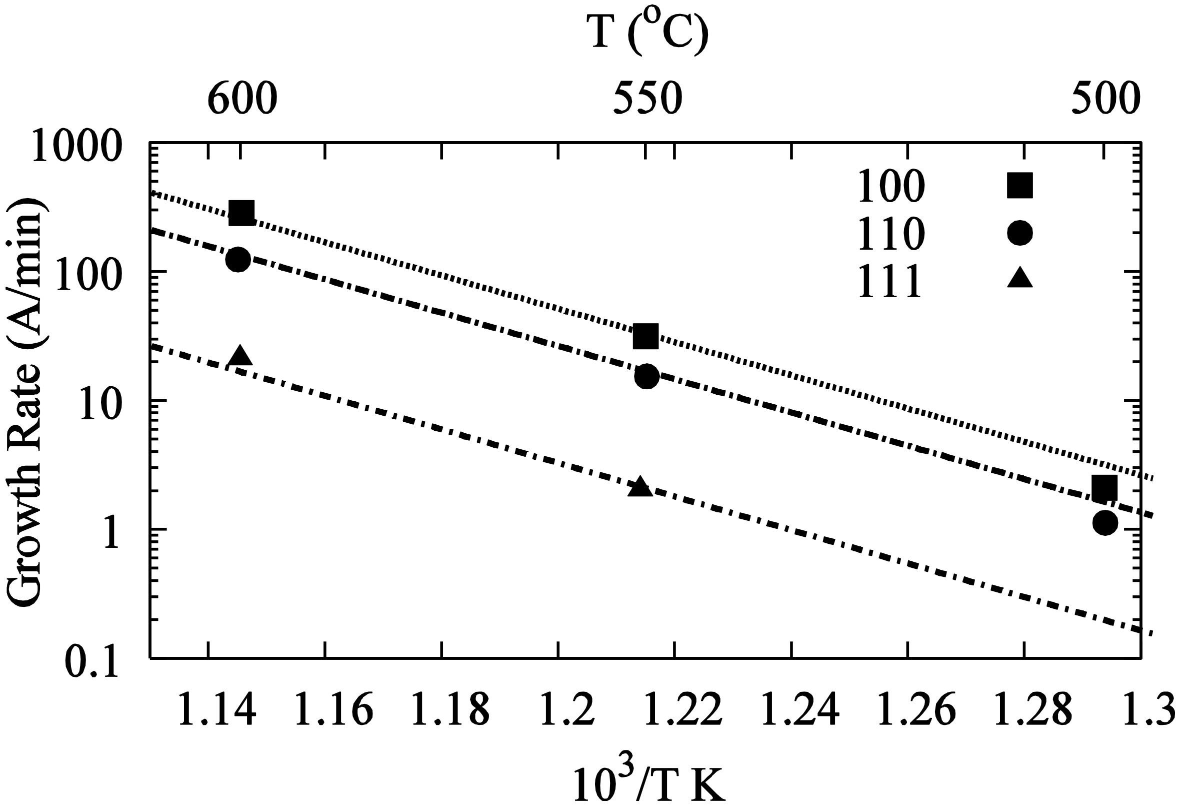
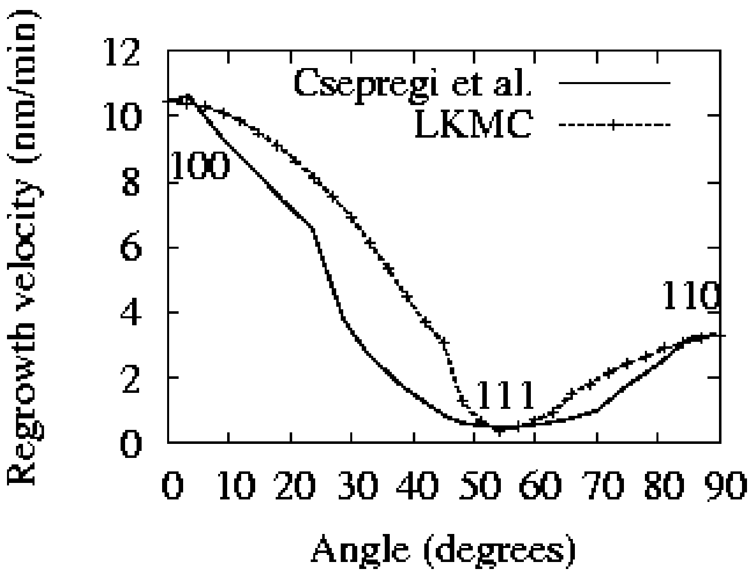
Planar growth for different orientations (I)



Lines, our work: Appl. Phys. Lett. 95, 123123 (2009)
Symbols: G.L. Olson and J. A. Roth. Mater. Sci. Rep. 3 1 (1988)

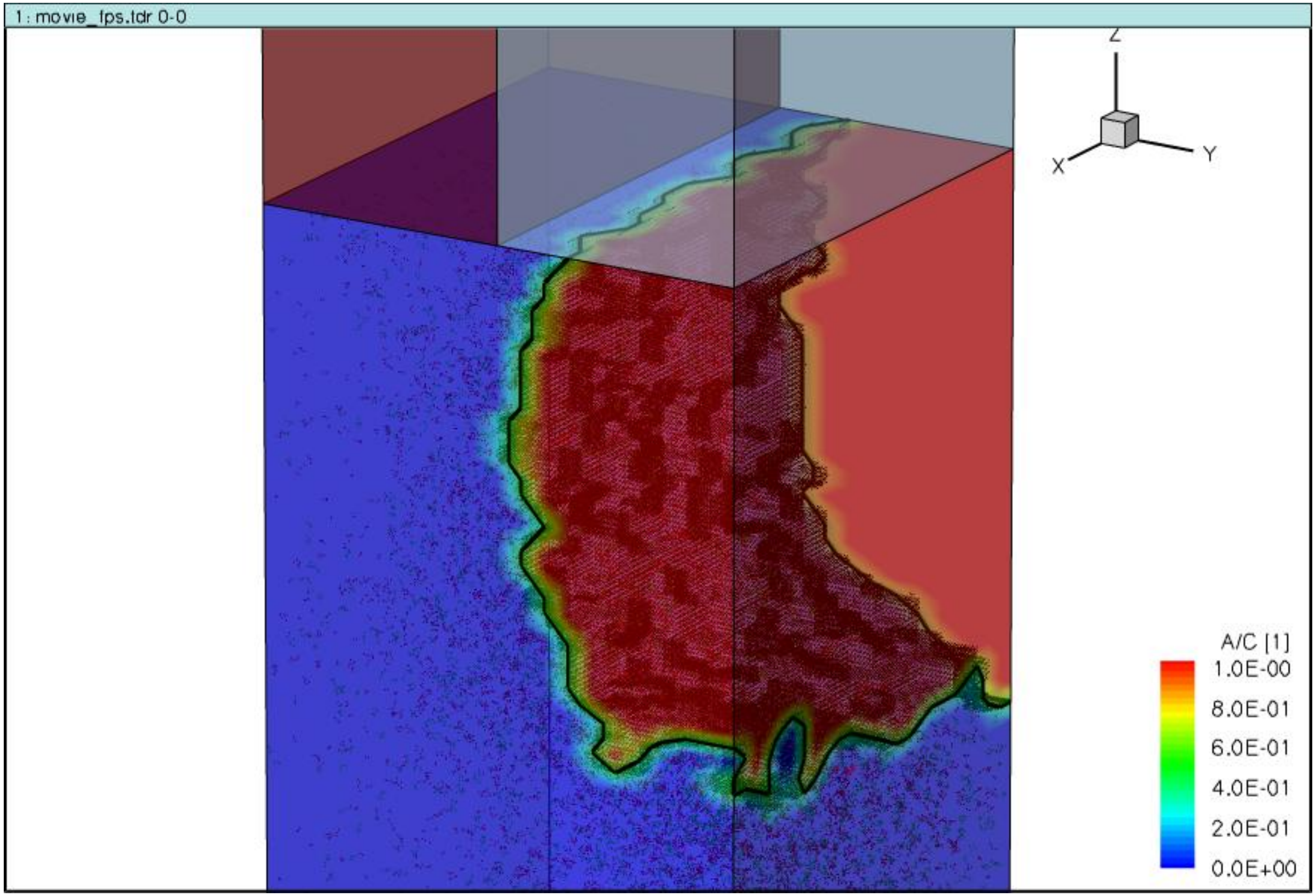
Planar growth for different orientations (II)



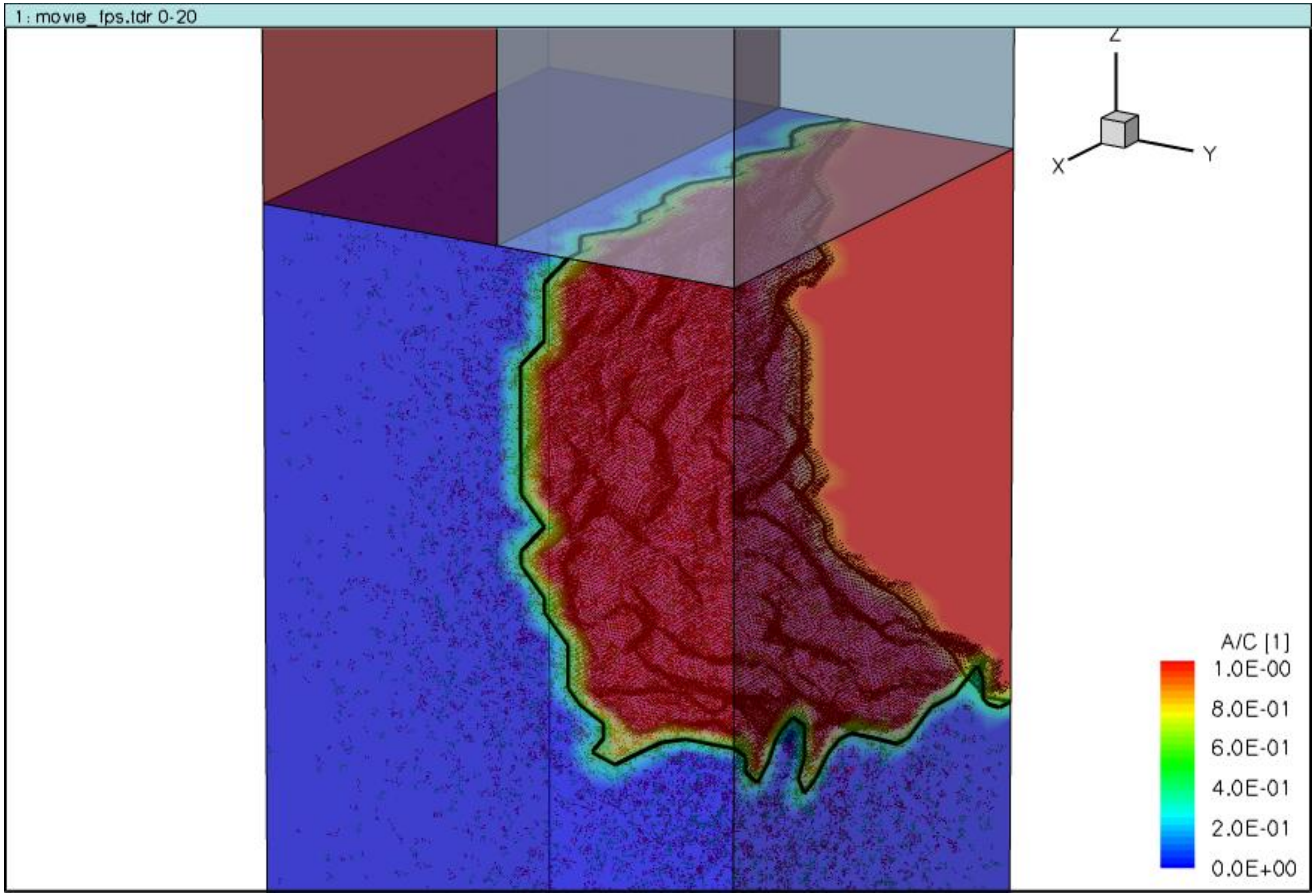
- E = 2.7 eV
- K(1) = 9.0×10^{16} atoms/s
- K(2) = 2.3×10^{15} atoms/s
- K(3) = 1.1×10^{11} atoms/s
- K(1), K(2), K(3) related with the microscopical growth of (100), (110) and (111)

Experimental results from Csepregi et al. J. Appl. Phys. 49, 3906 (1978)

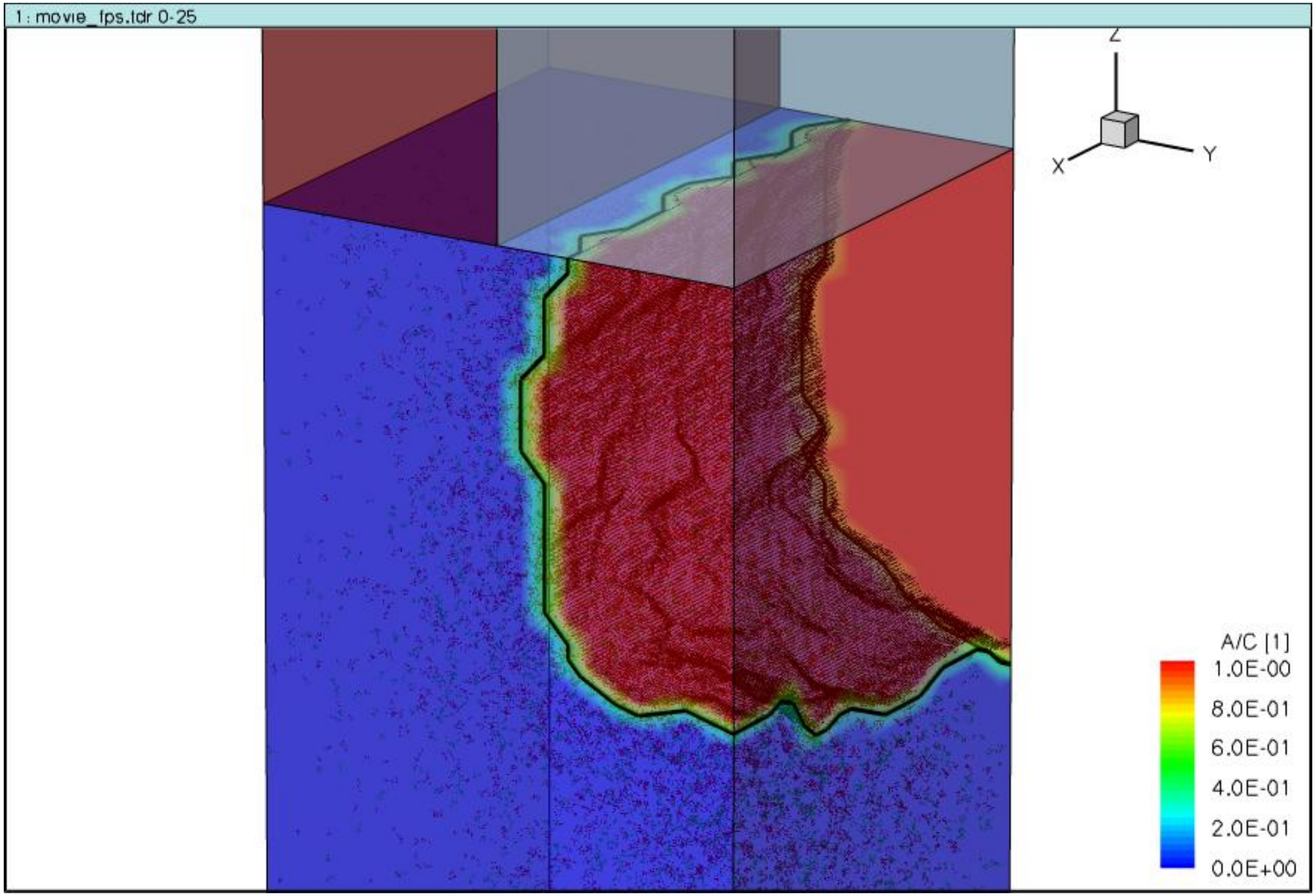
A look at time evolution.



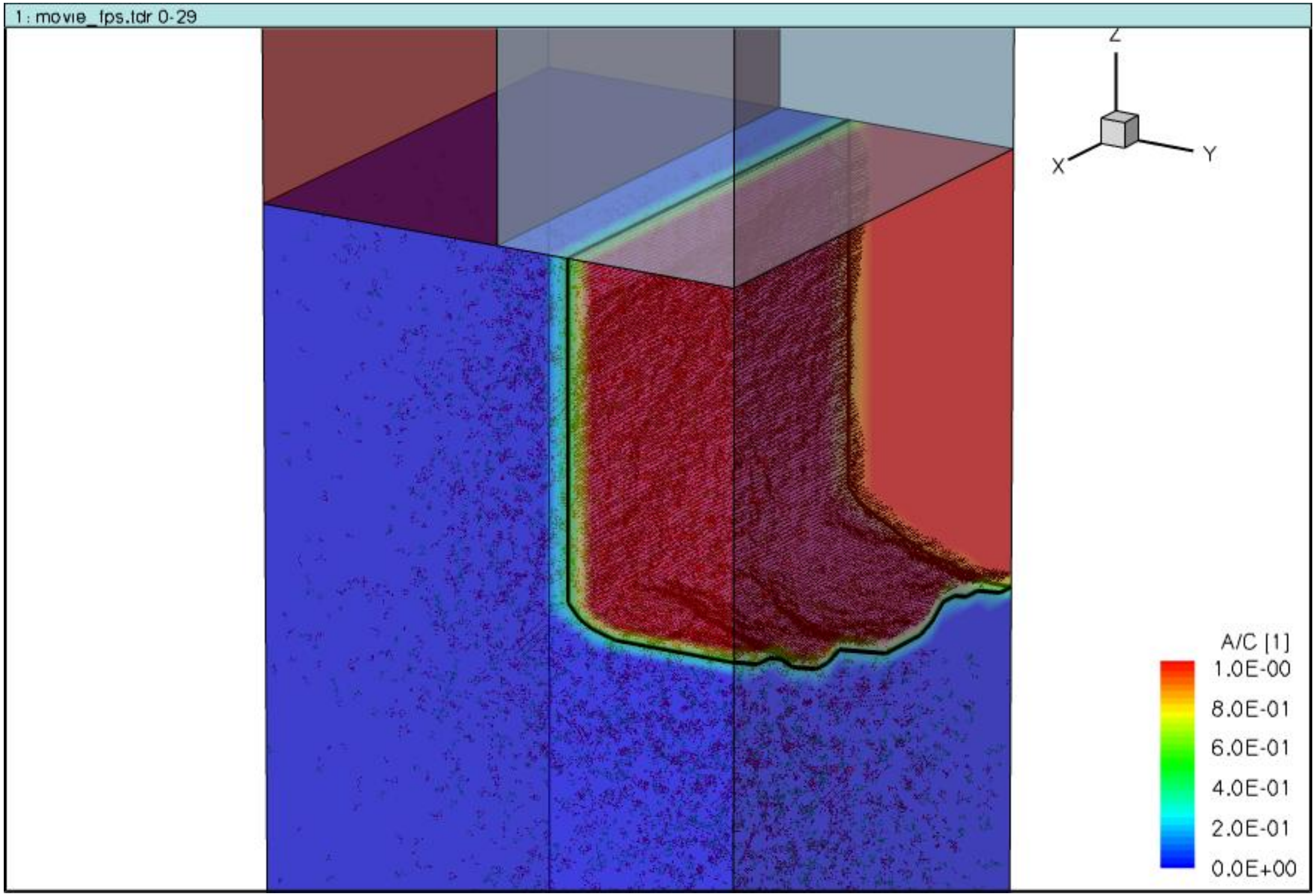
A look at time evolution. |



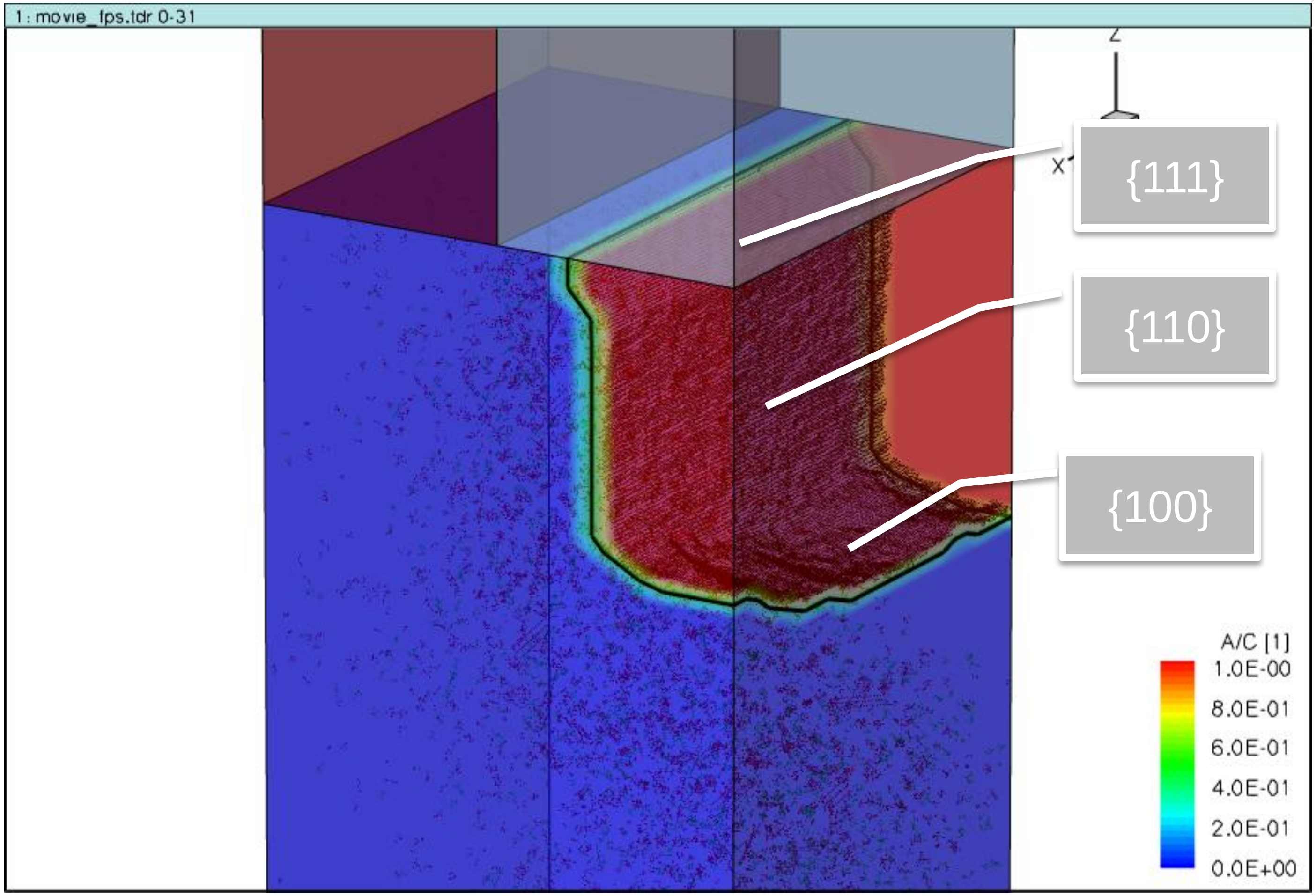
A look at time evolution. -



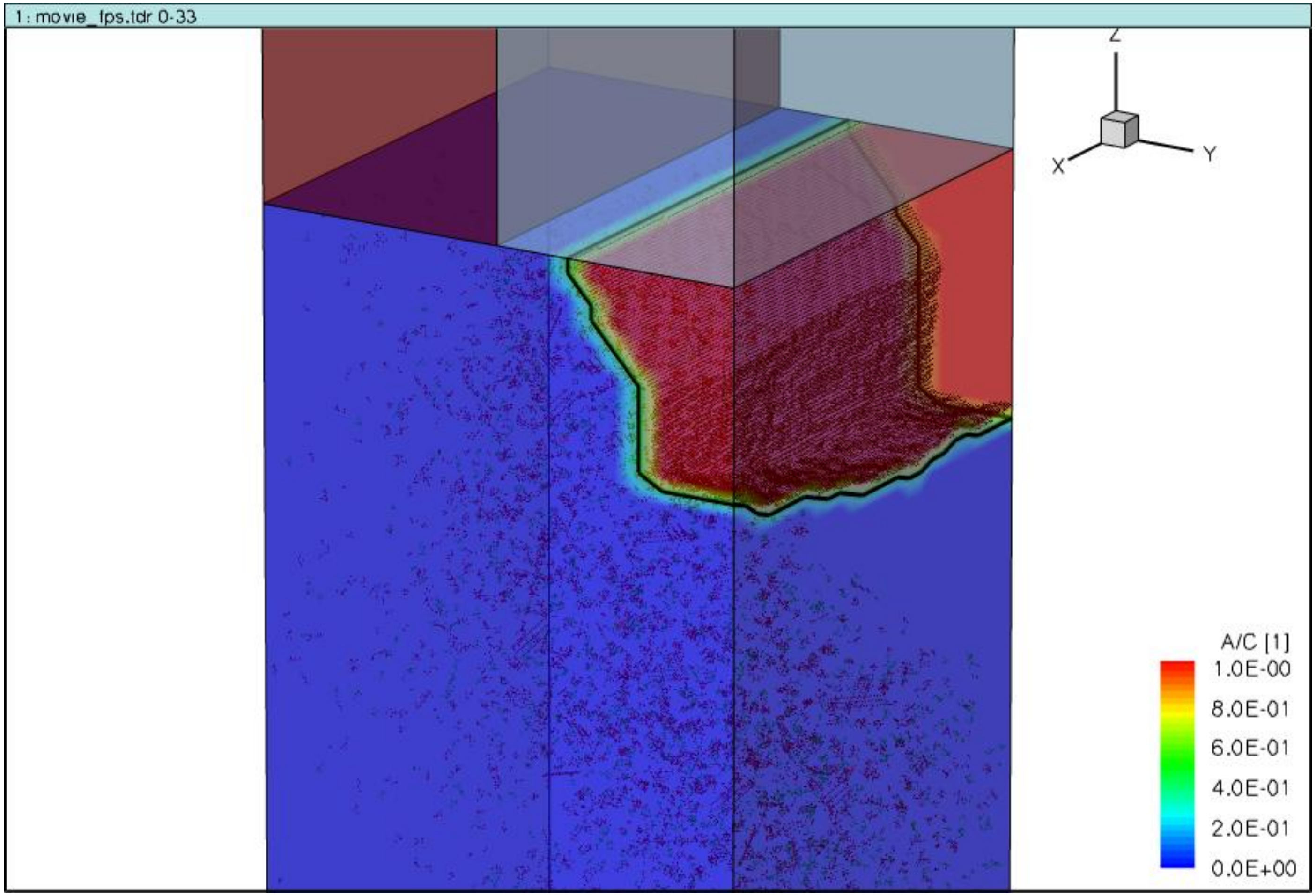
A look at time evolution. |



A look at time evolution. -



A look at time evolution. |



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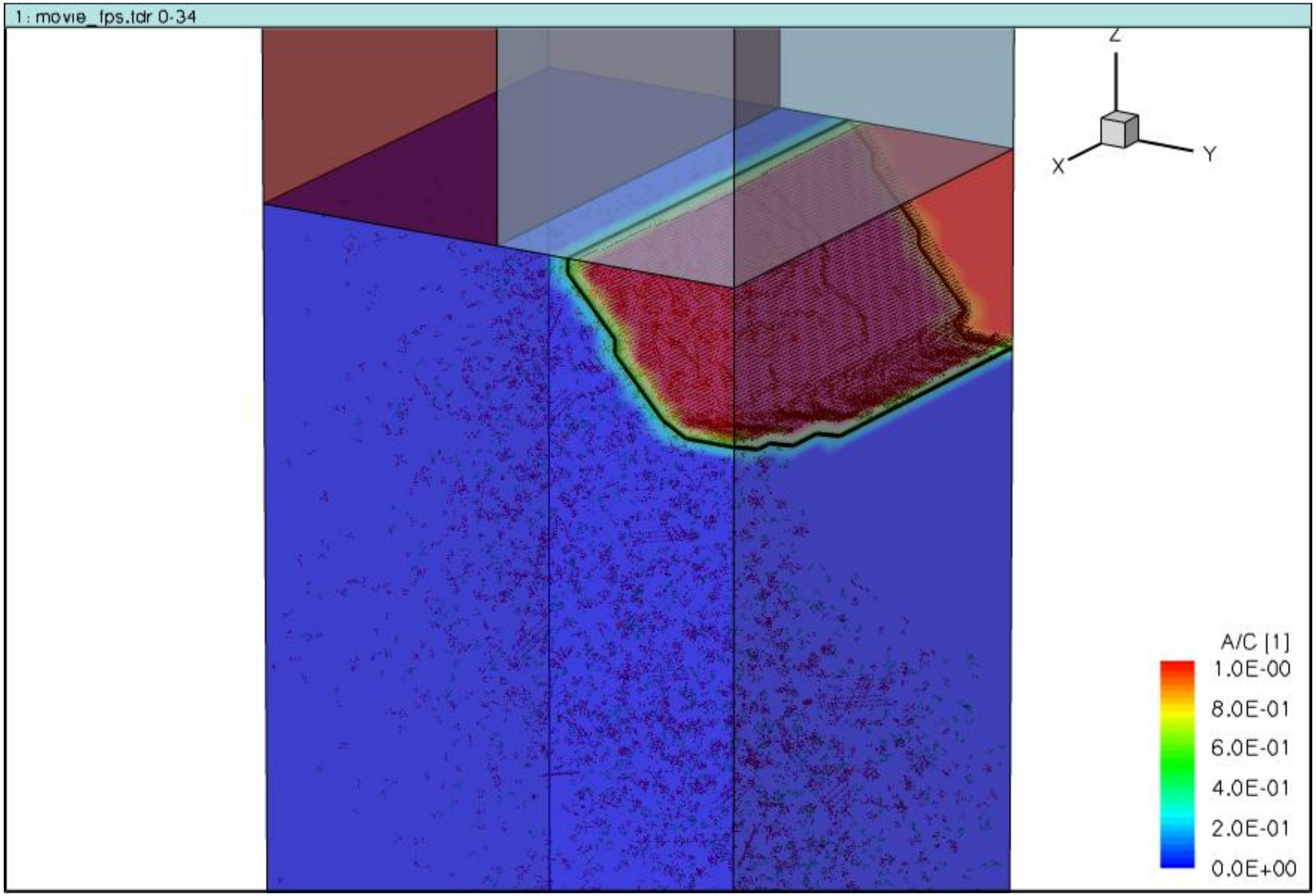
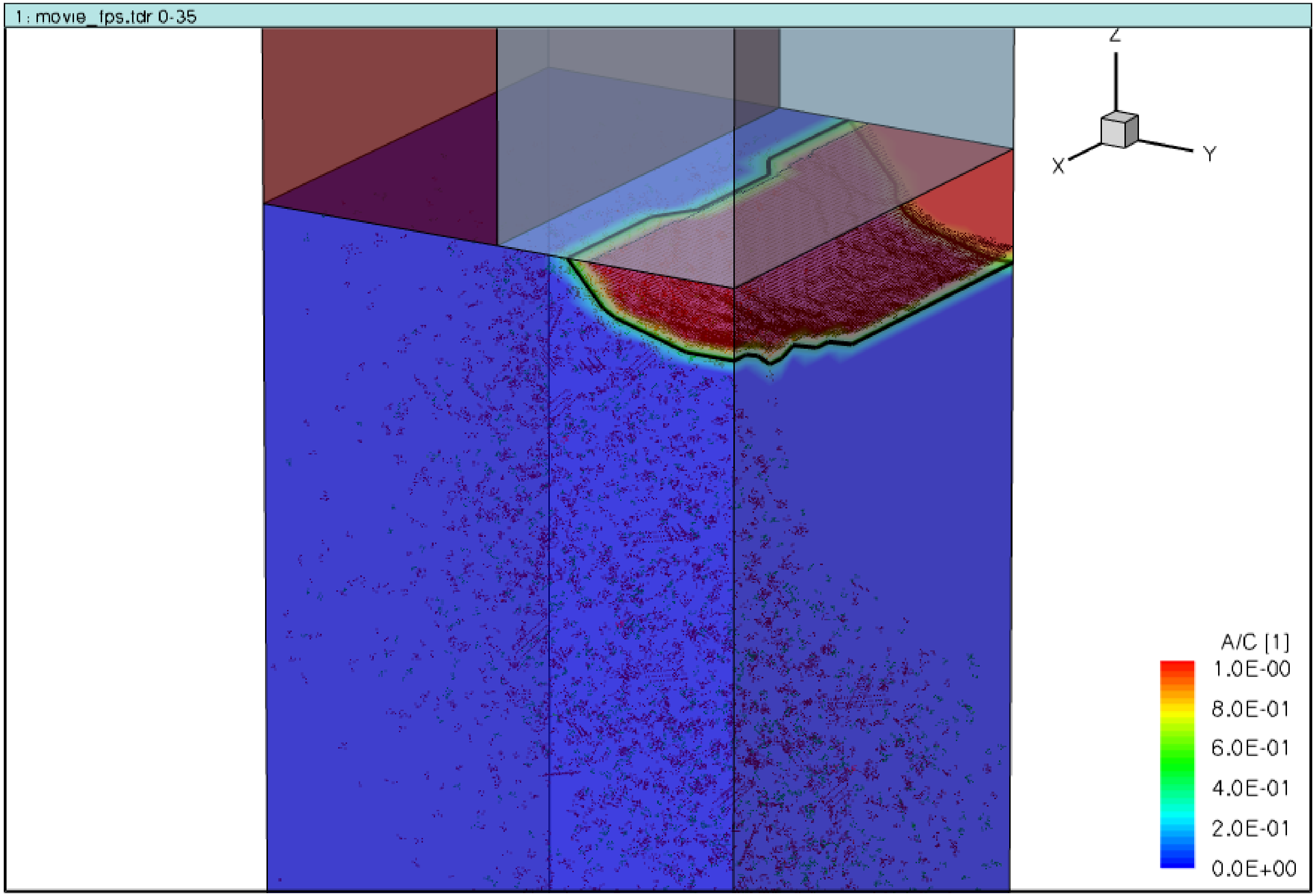
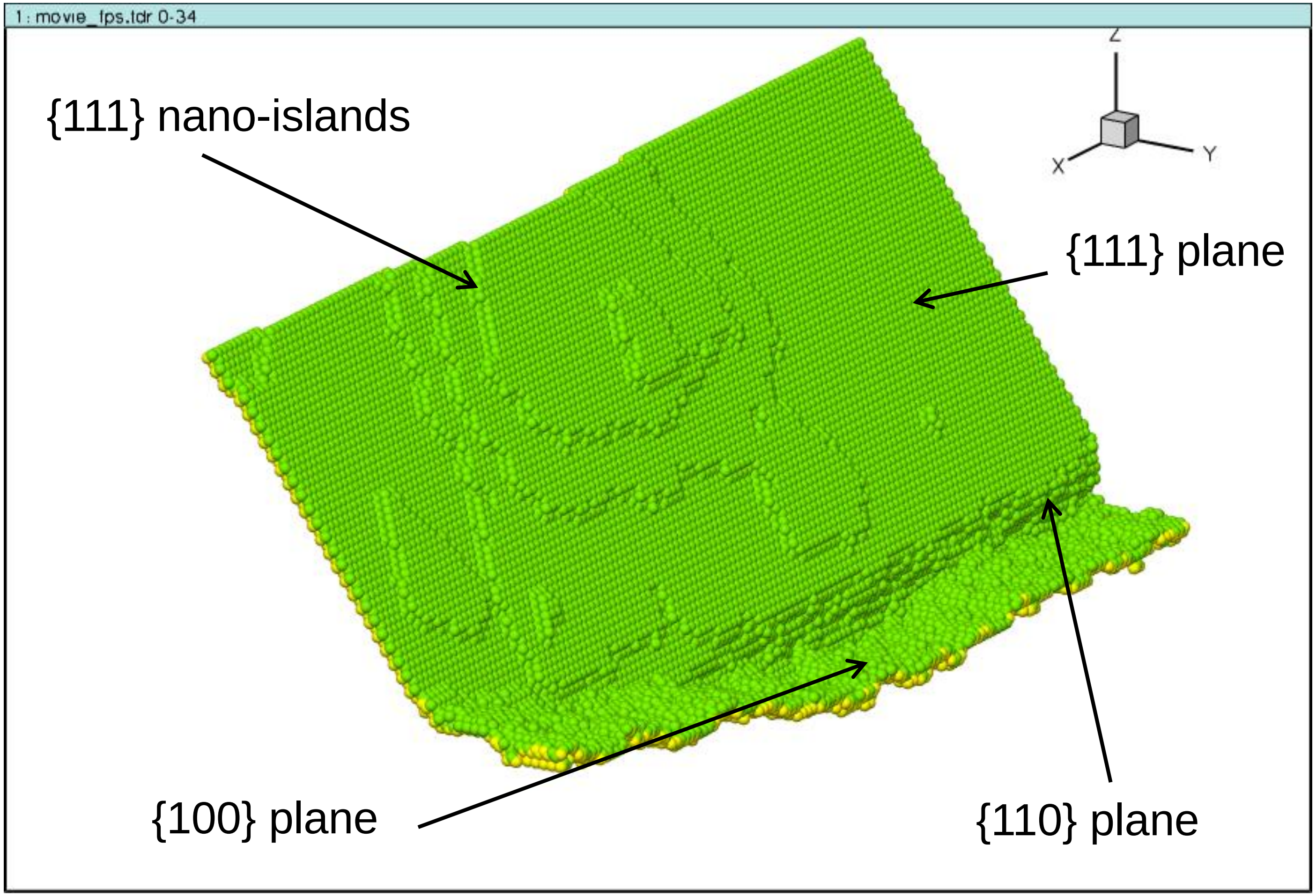
A look at time evolution. -



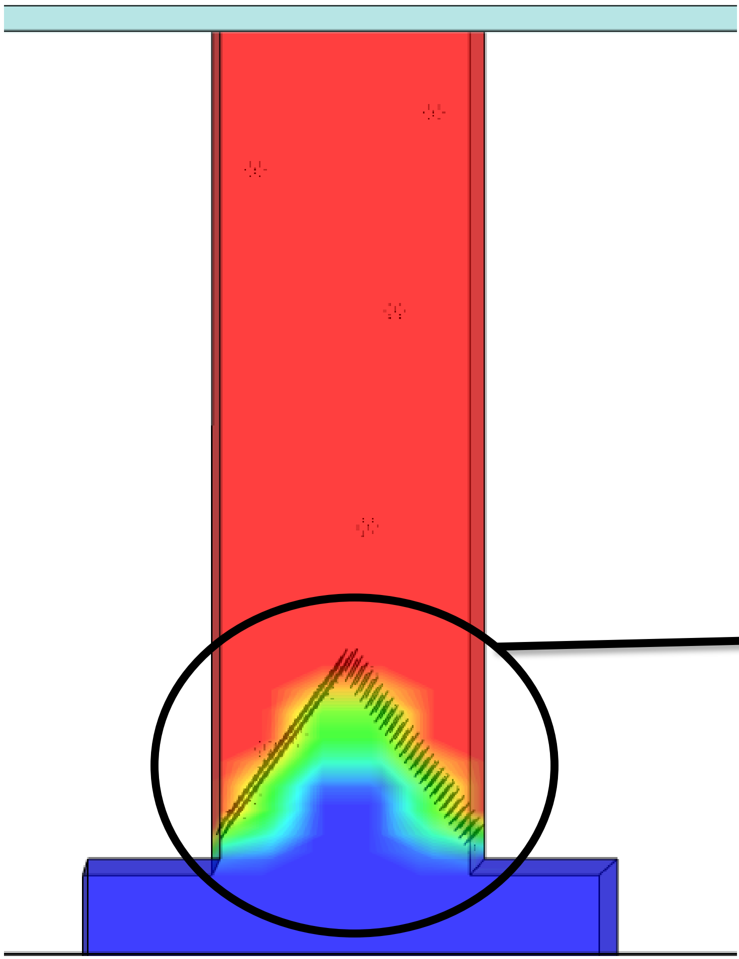
A look at time evolution. |



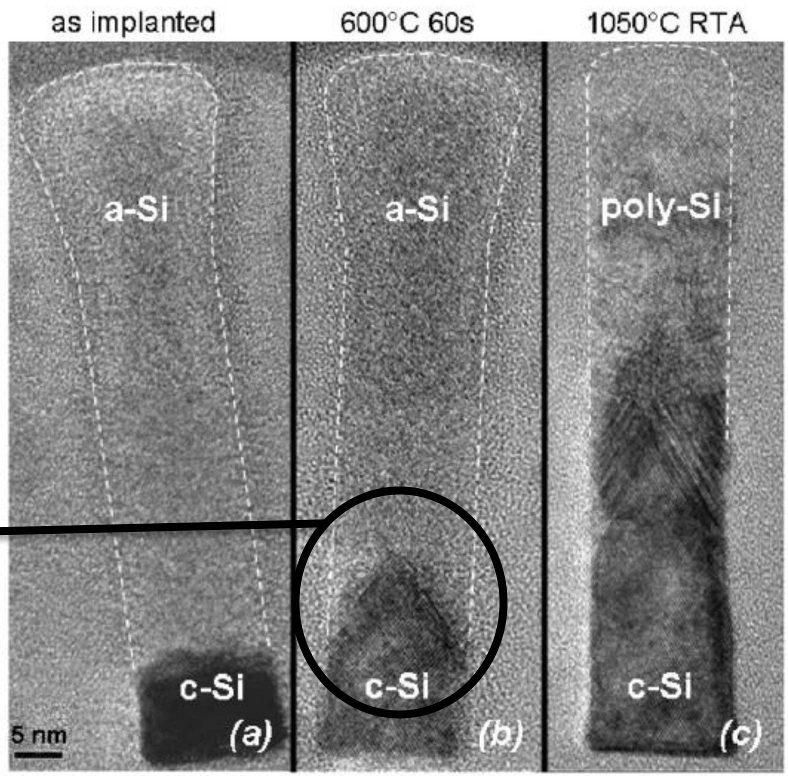
A closer look to the amorphous/crystalline interface



SPER and fins: Faceted growth after fin amorphization.

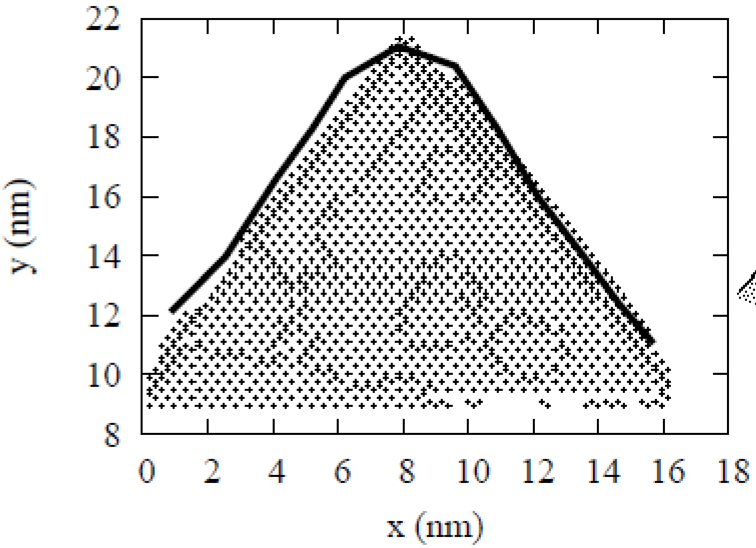


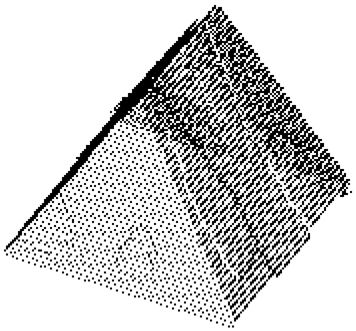
Experimental results from Duffy et al. Appl. Phys. Lett. 90, 241912 (2007)



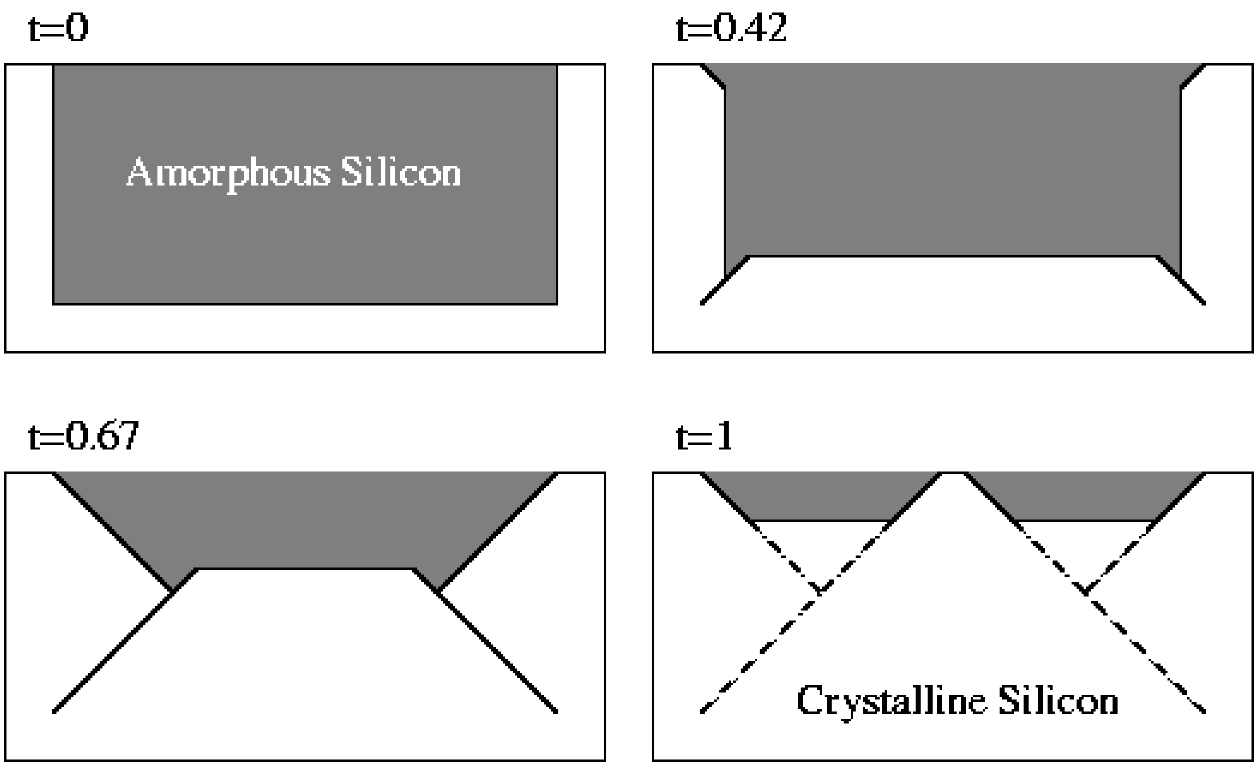
SPER and fins. Experiment vs. simulation comparison.

Experimental results from Duffy et al. Appl. Phys. Lett. 90, 241912 (2007)
Lines: Experiment, symbols, LKMC simulation.



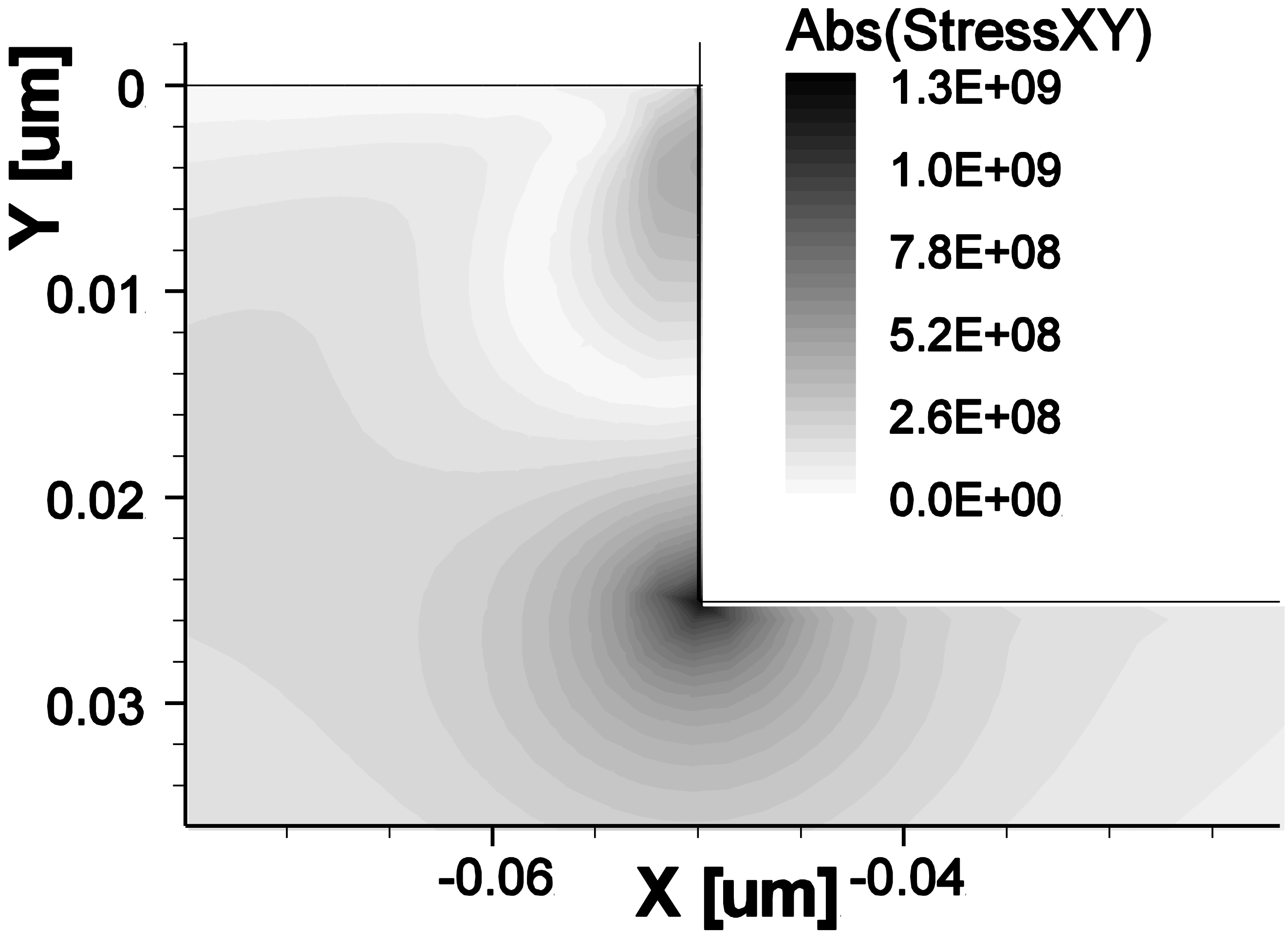


Recrystallization of rectangular shapes:



K.L. Saenger et al. J. Appl. Phys. 101, 084912 (2007)

Why corners are different? Stress/Strain as a reason: lattice distortion



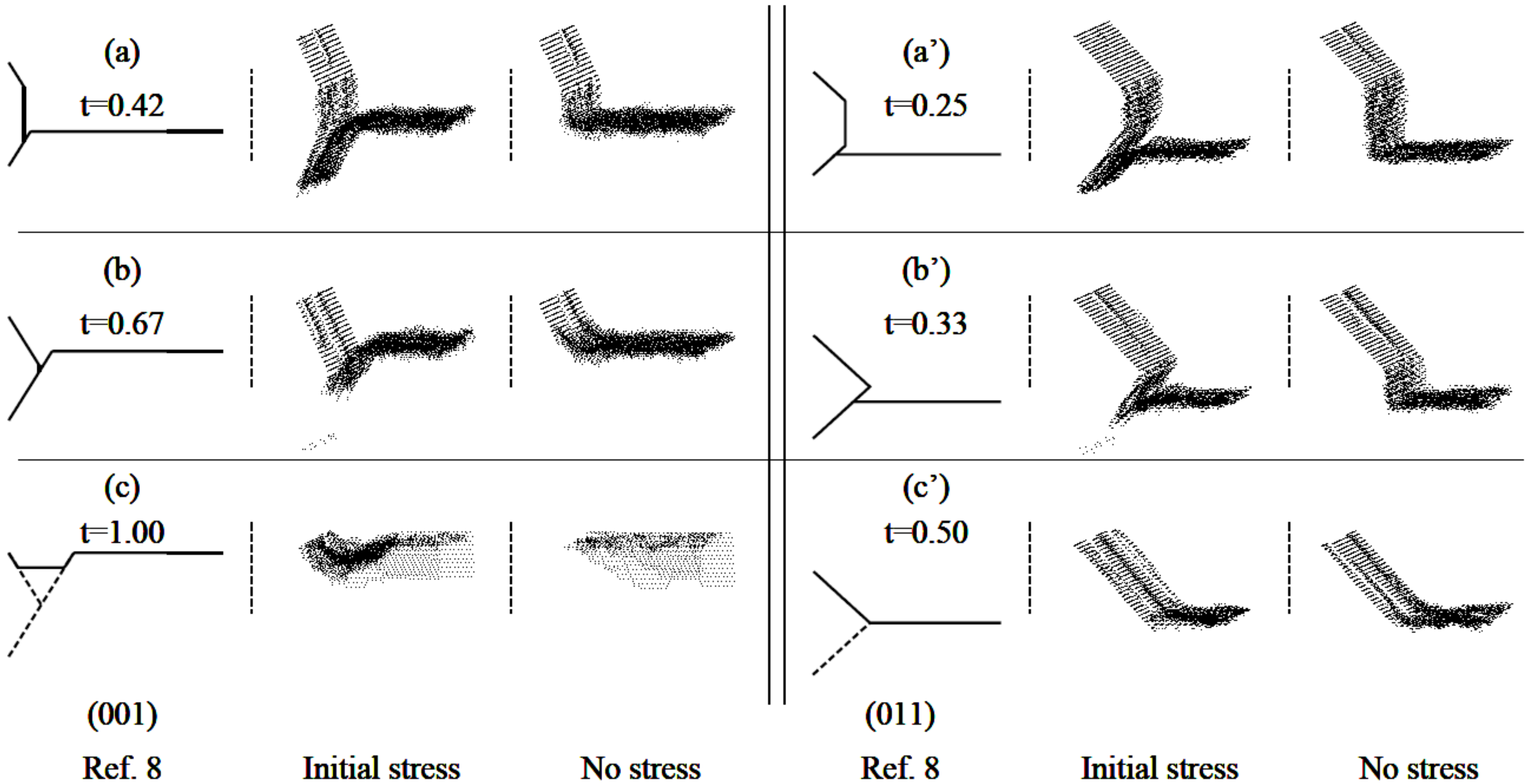
Introducing strain dependency

- The quality of the crystalline lattice template degrades when distorted

$$\upsilon = K(n) \times \exp(-(E + \lambda\left|\varepsilon_{xy}\right|) / K_B T)$$

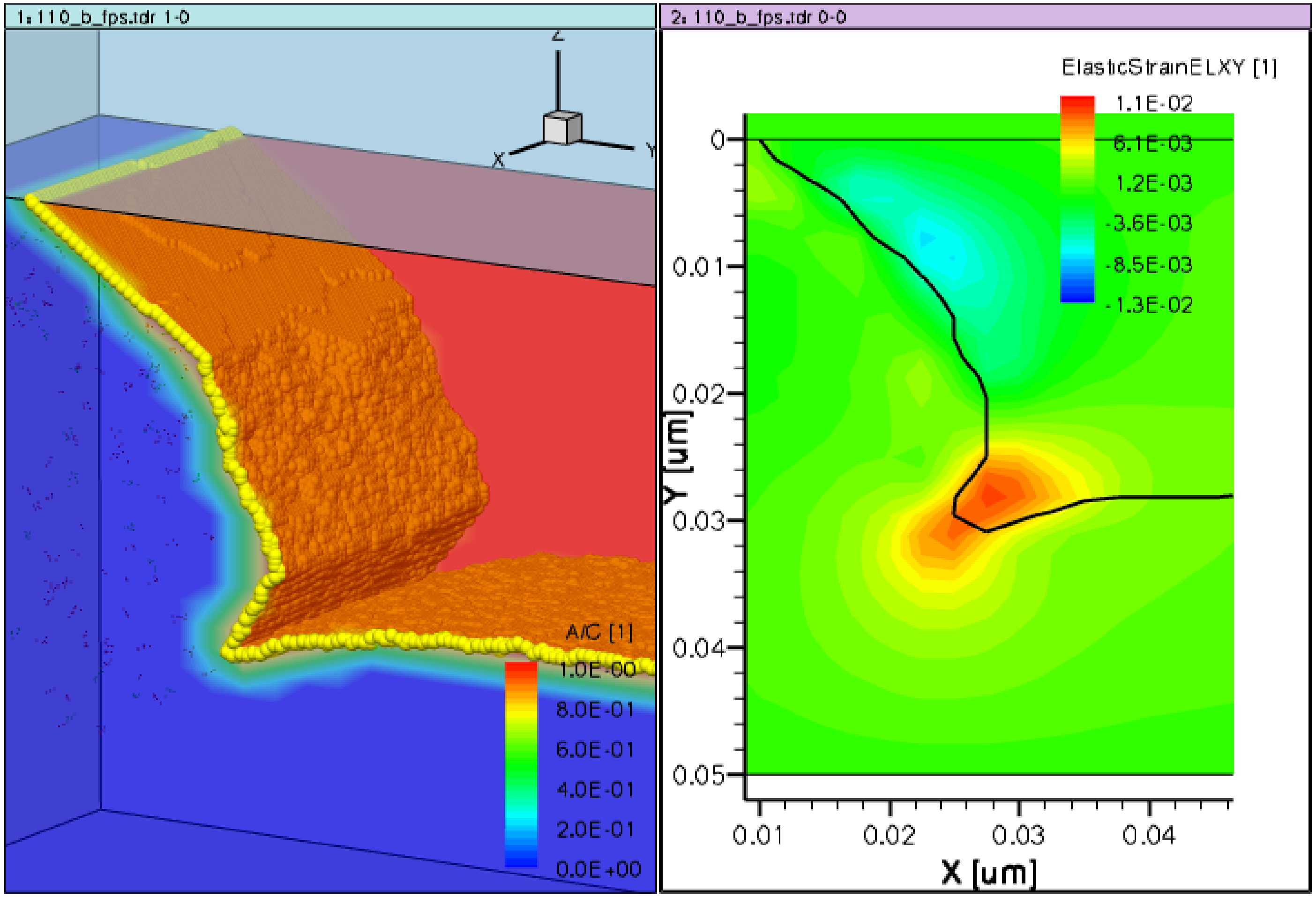
- This is modeled by increasing SPER activation energy by $\lambda|\varepsilon_{xy}|$
- The absolute value is issued because the lattice is distorted regardless of clockwise or counterclockwise shear strain.

Rectangular shape results: λ=5.



I Martin-Bragado and V. Moroz. Appl. Phys. Lett. 95, 123123 (2009)

The strain at the corner generates the trench



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Conclusions

- A LKMC model, based on existing qualitative atomistic ideas, quantitatively explains and reproduces different planar SPER velocities
- The model also satisfactory reproduces facet formation in very thin amorphized fins.
- Finally, it explains anomalous regrowth patters and facet formation in rectangular amorphized (001) and (011) Si substrates.
- Model included in sprocess KMC, 2010.03 release.

Questions?