Multiscale modelling of materials chemomechanics: brittle fracture of oxides and semiconductors

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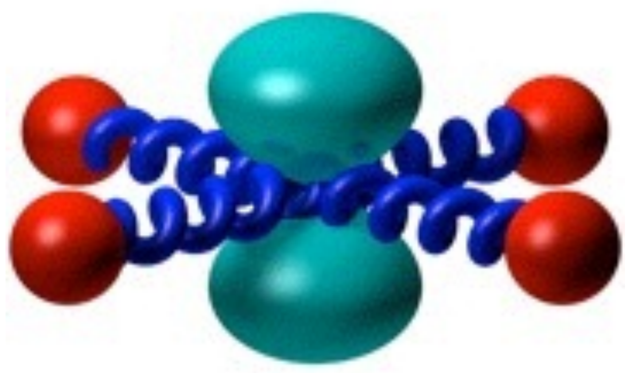
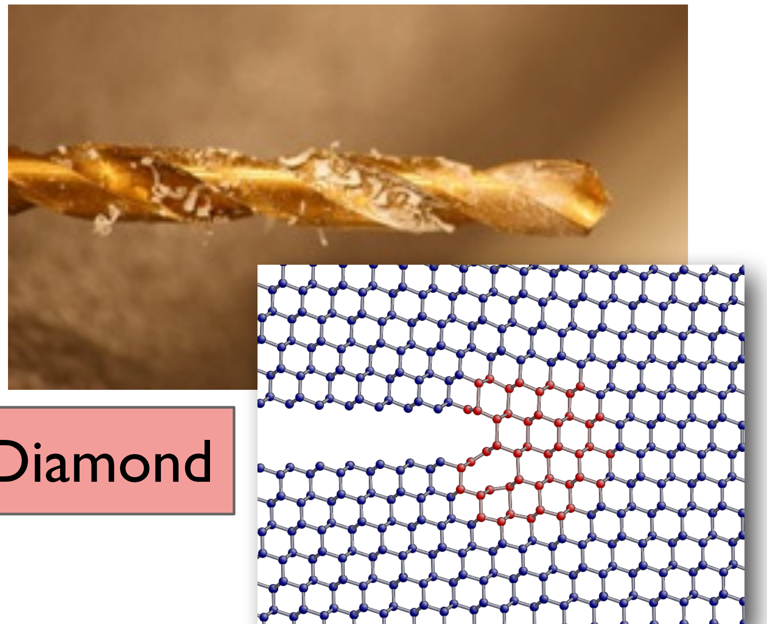
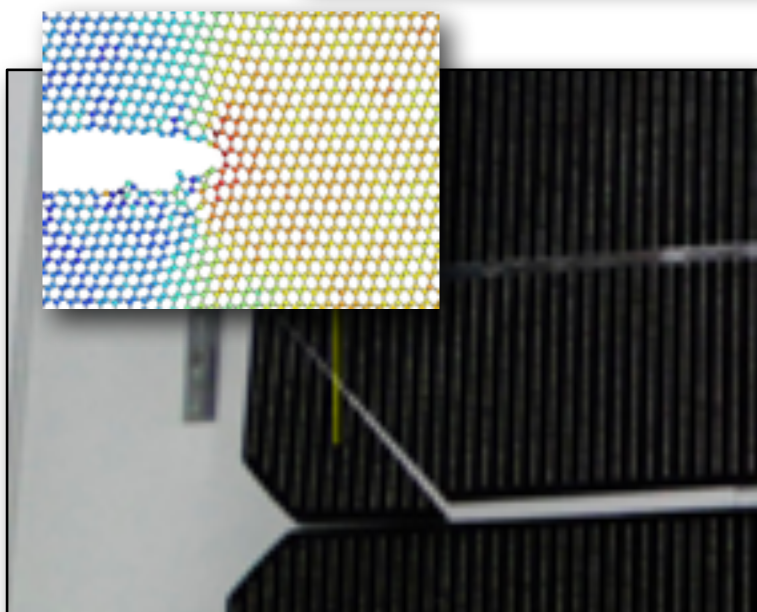


Multiscale Modelling of “Chemomechanical” Materials Failure Processes

Covalent Materials



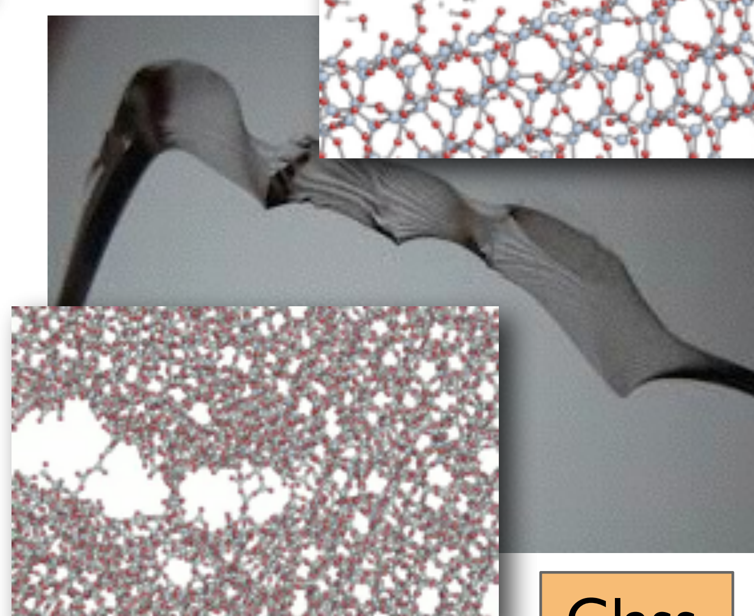
Diamond



Silicon Photovoltaics

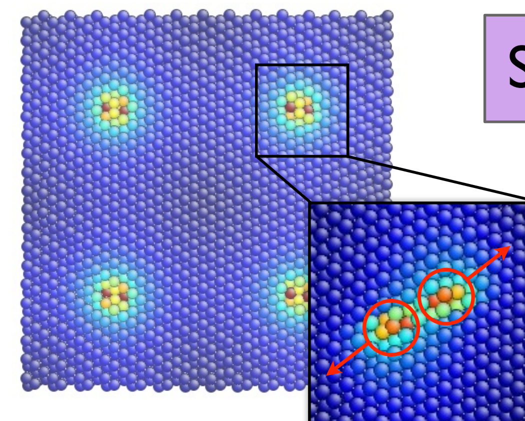
Oxides

Rocks

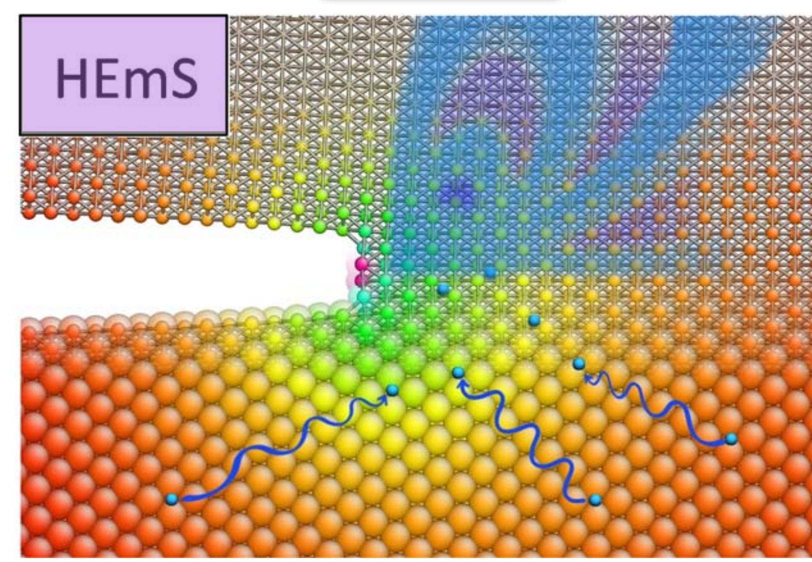


Glass

Metals

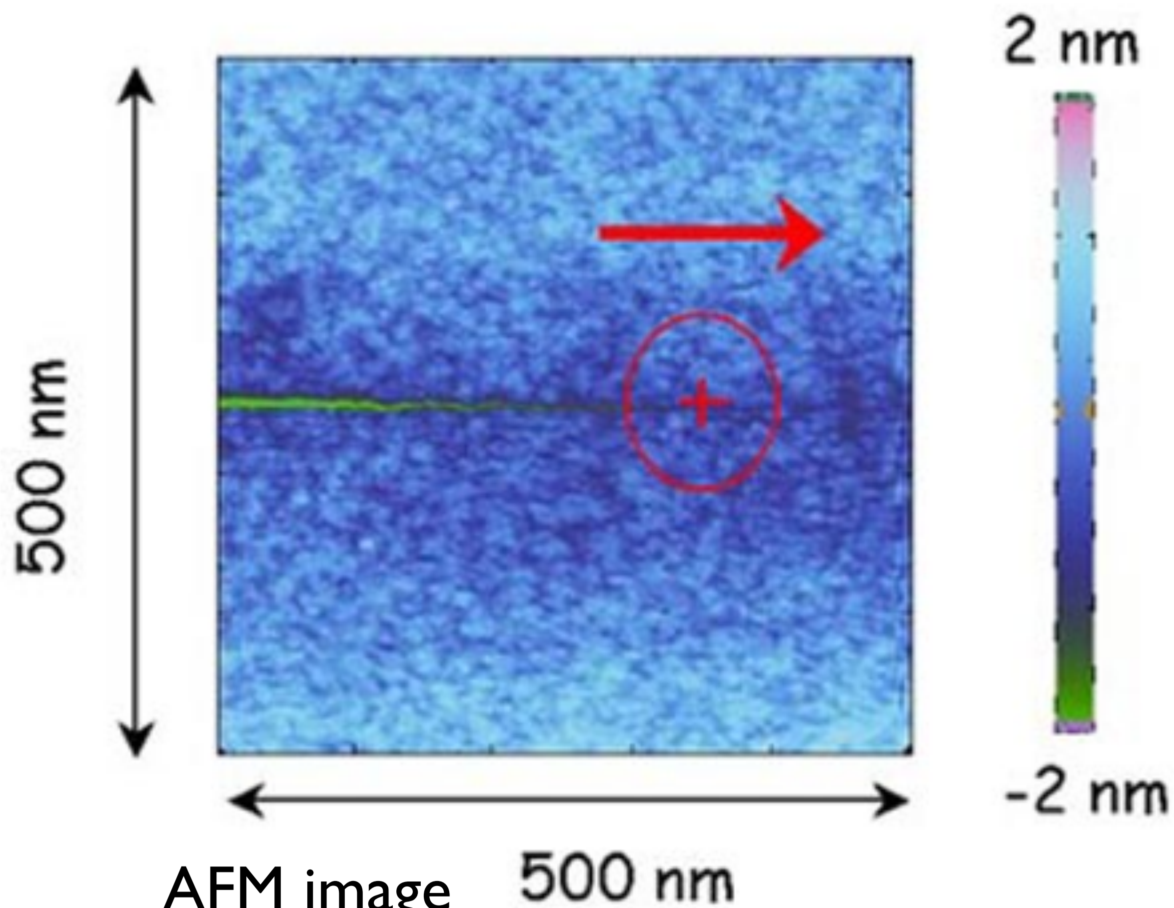


Superalloys



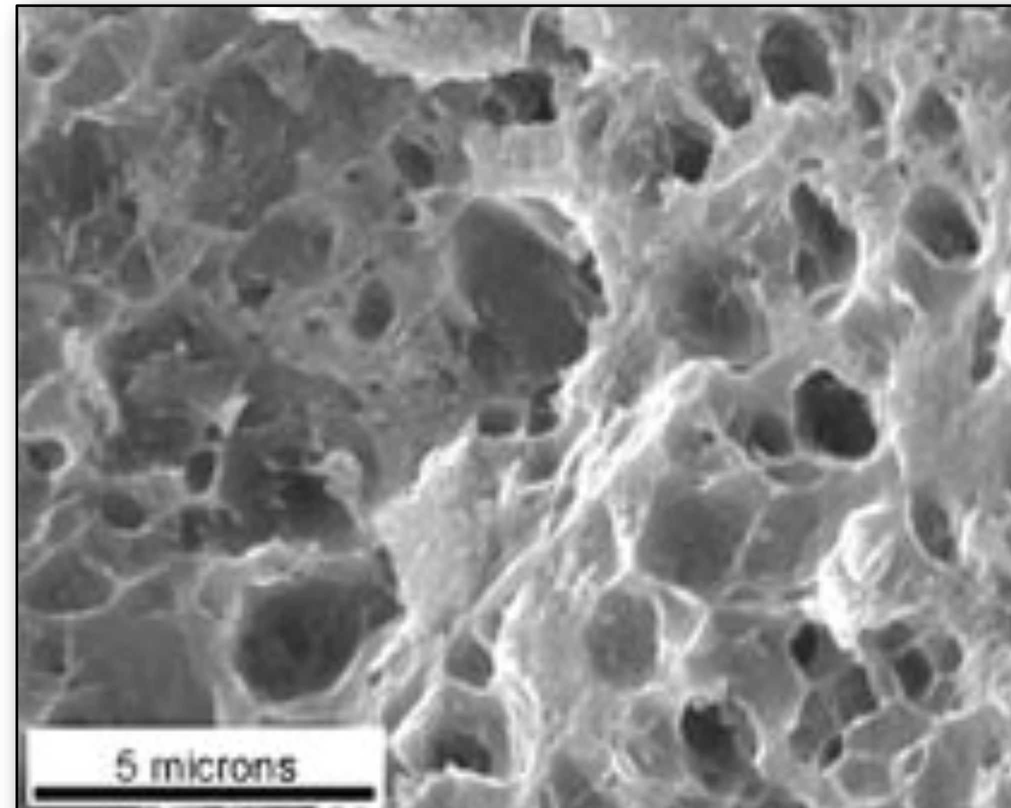
HEmS

Brittle Fracture



AFM image

Ductile Fracture

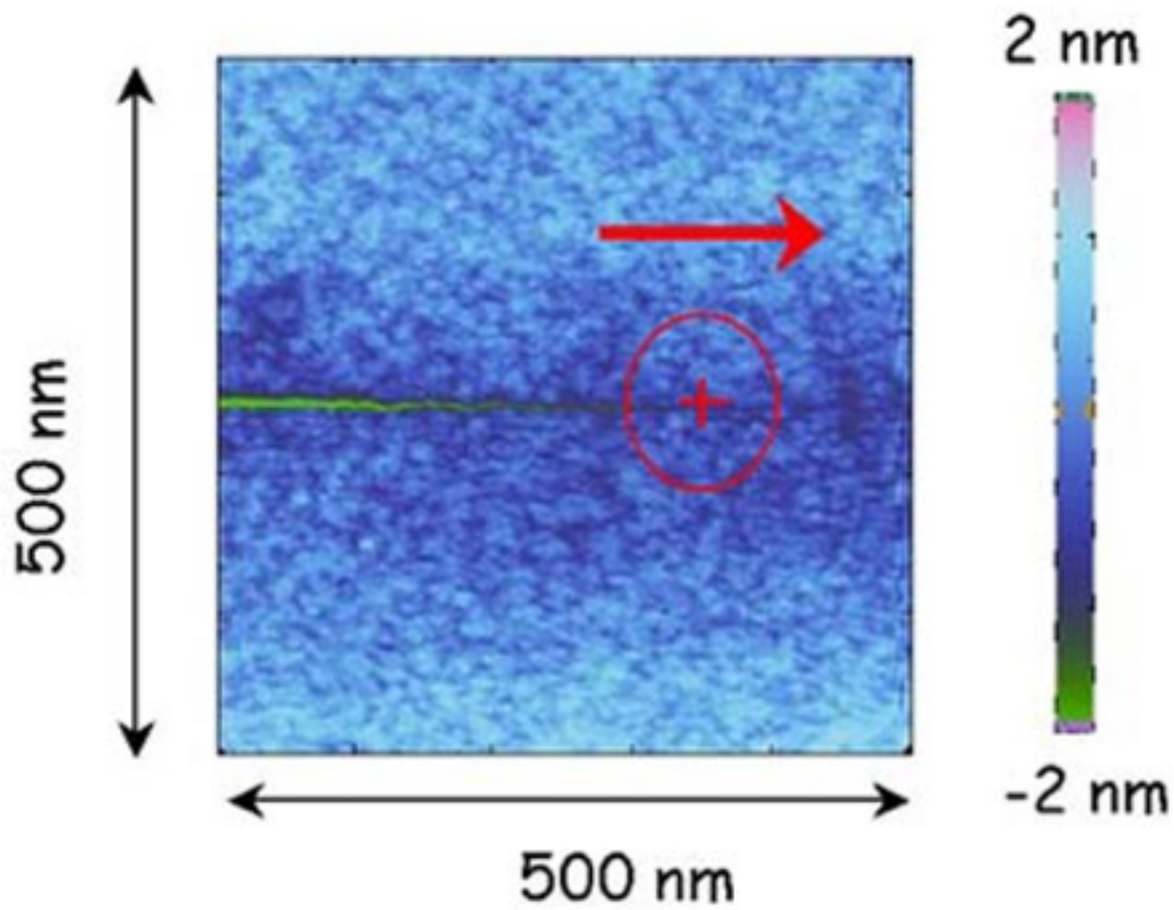


SEM image

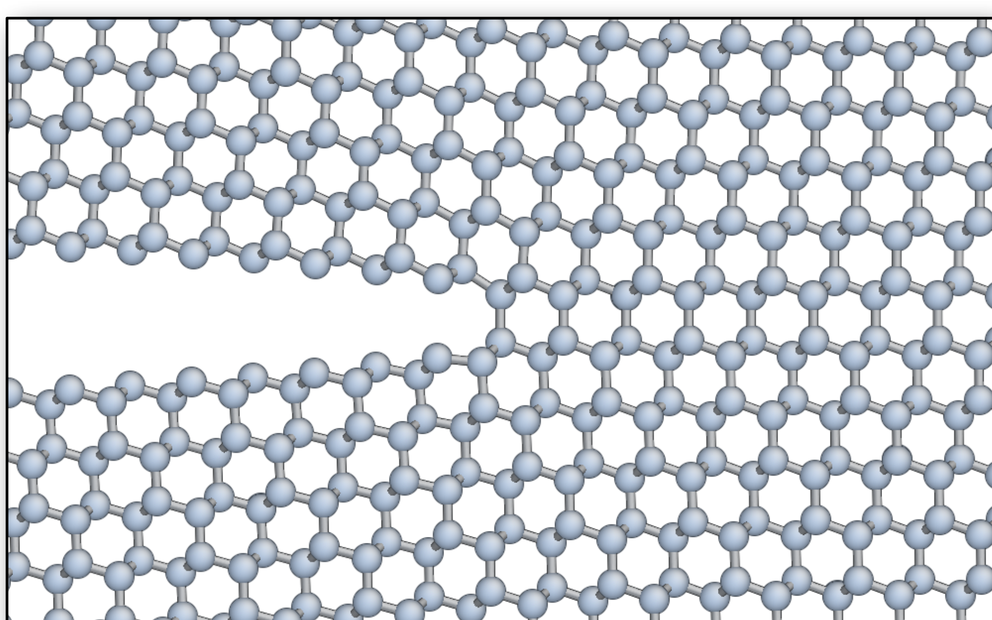
Image credits: C. Marlière, A. Weck, B. Lawn

Fracture at the Microscale

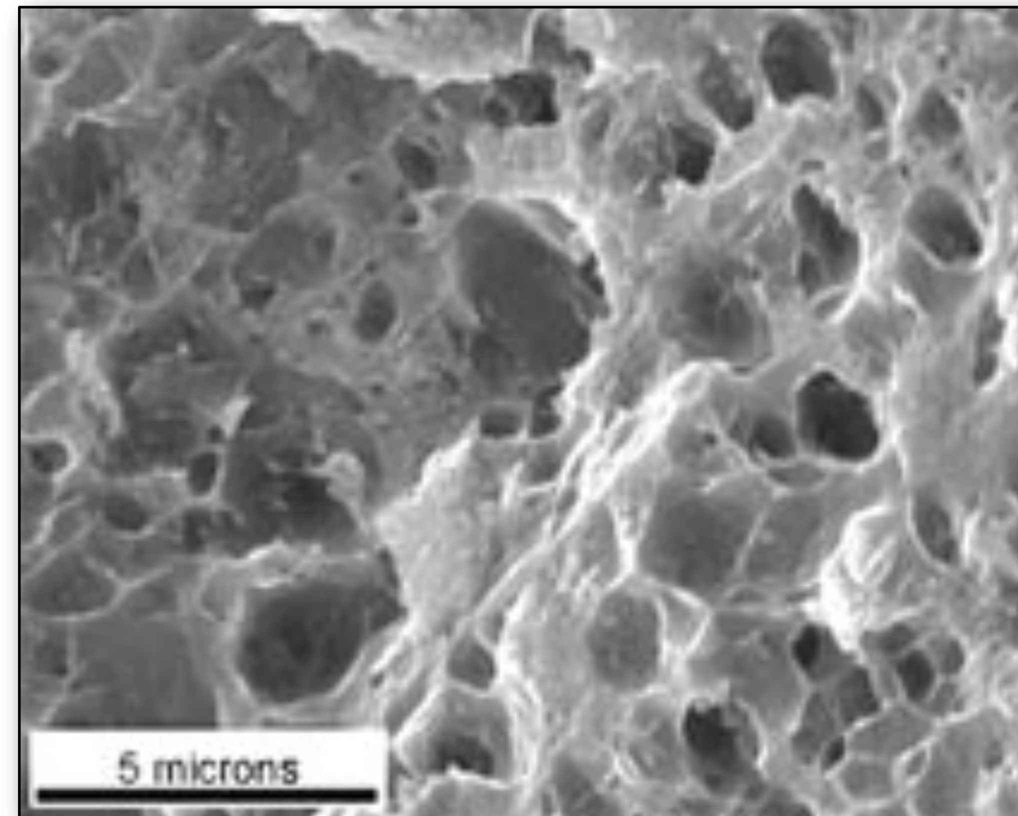
Brittle Fracture



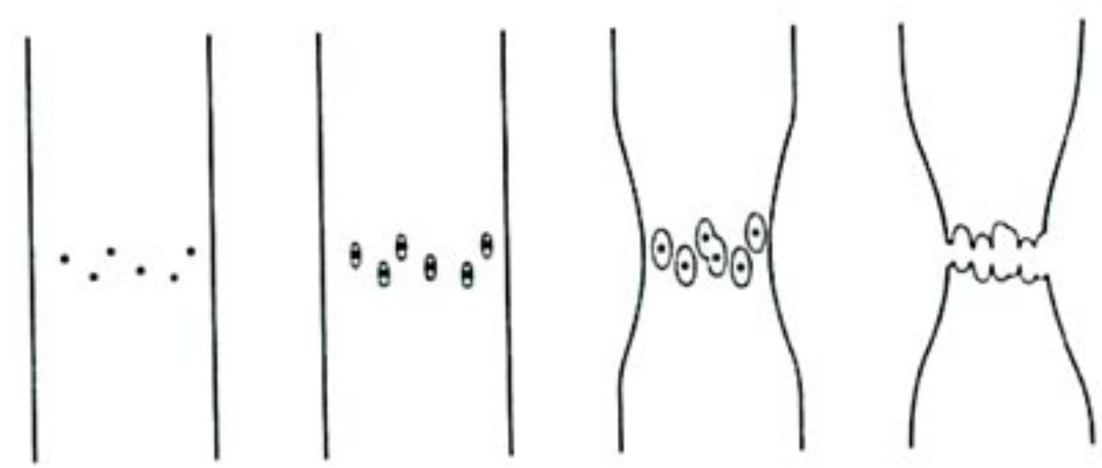
Cleavage in brittle fracture



Ductile Fracture



Void nucleation, growth
and coalescence in ductile fracture



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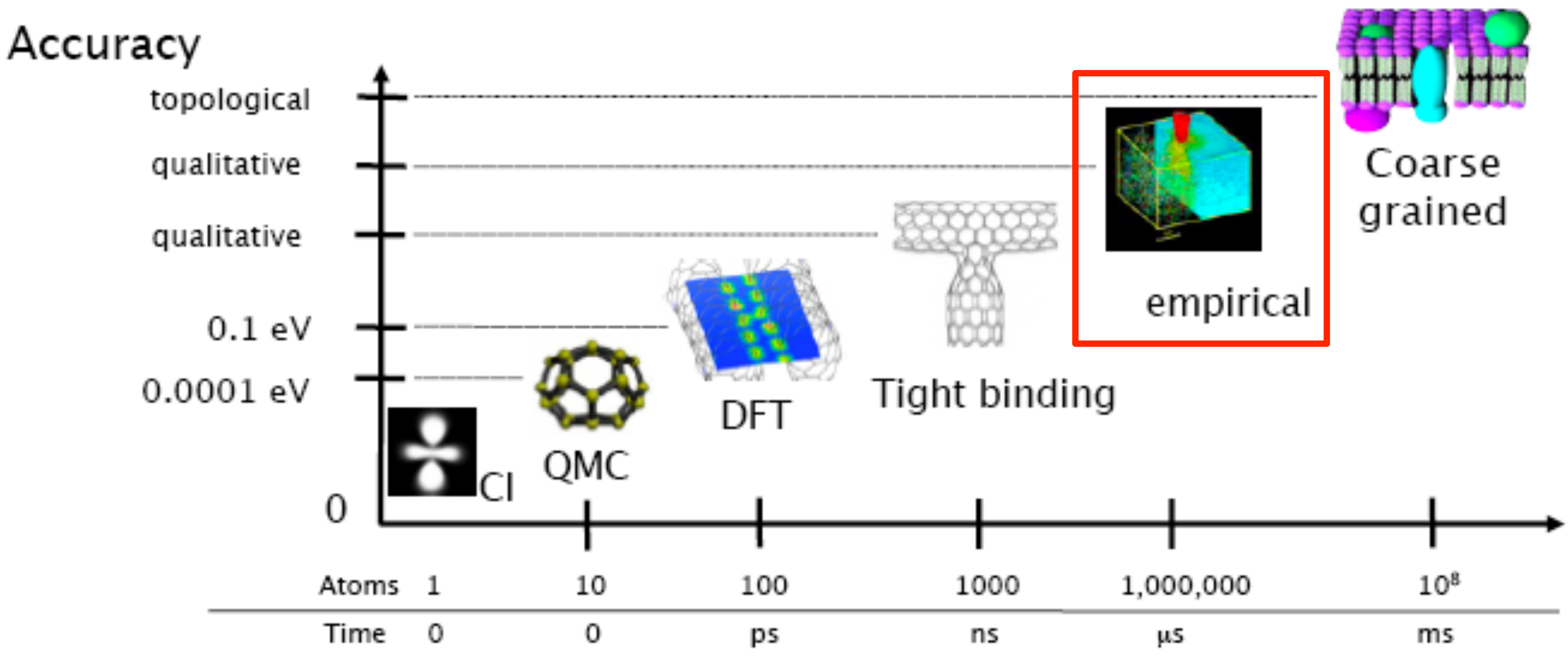
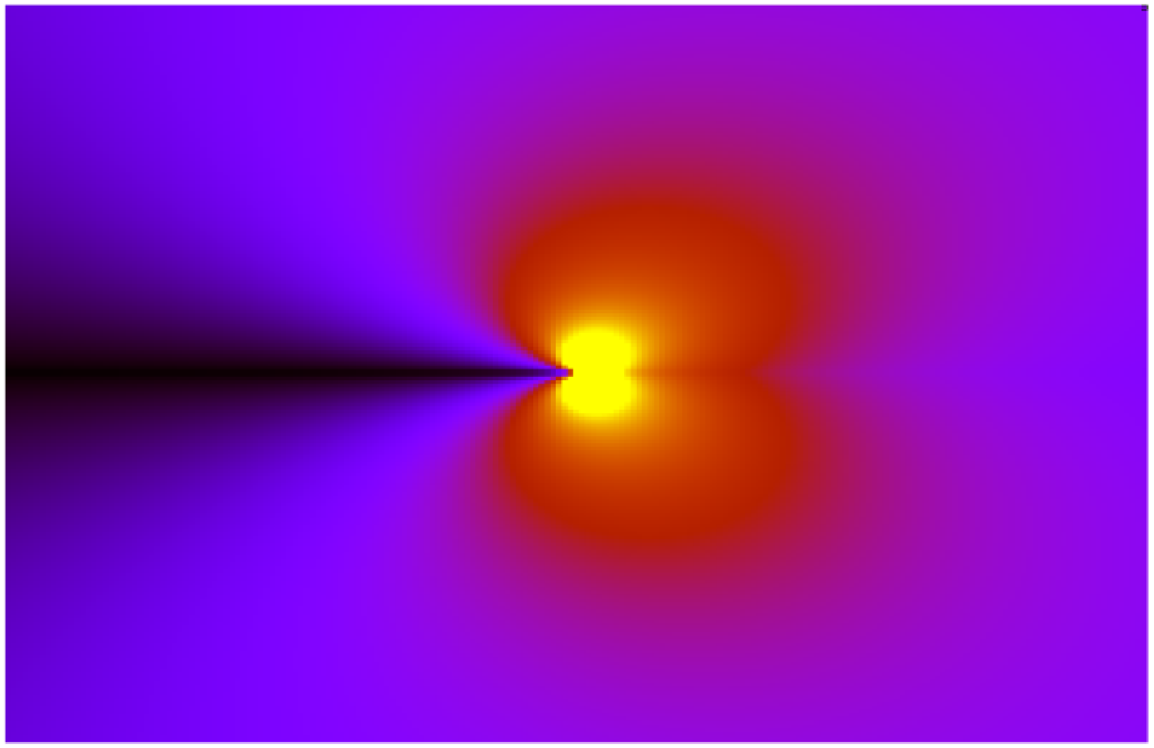
Multiscale Materials Modelling – empirical MD



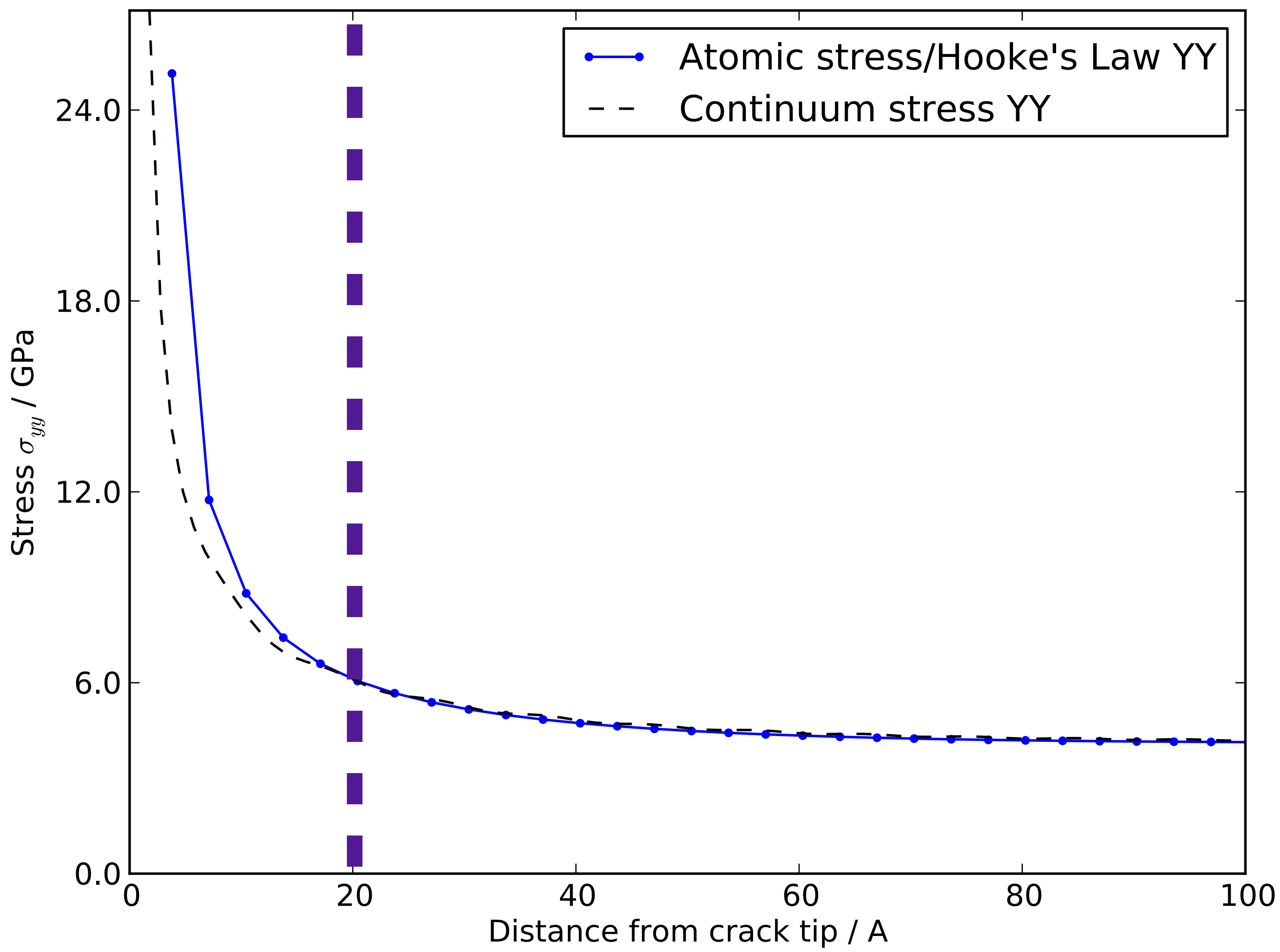
Matching of MD and continuum scale fracture modelling

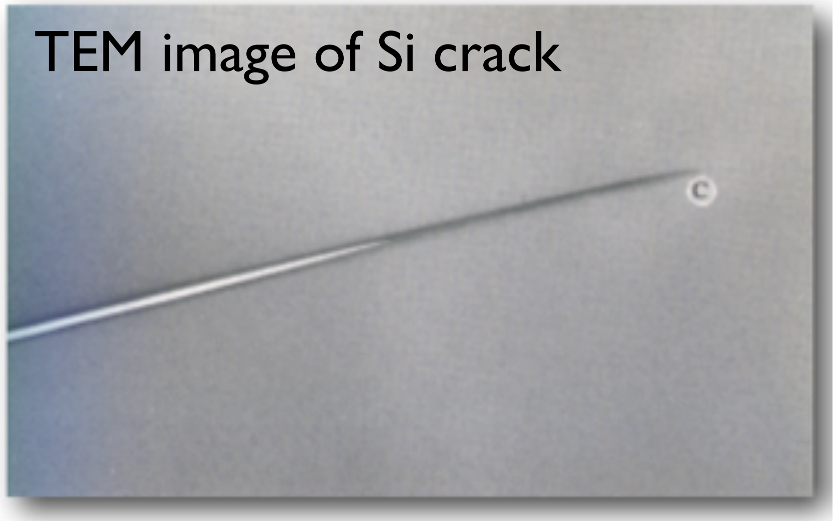


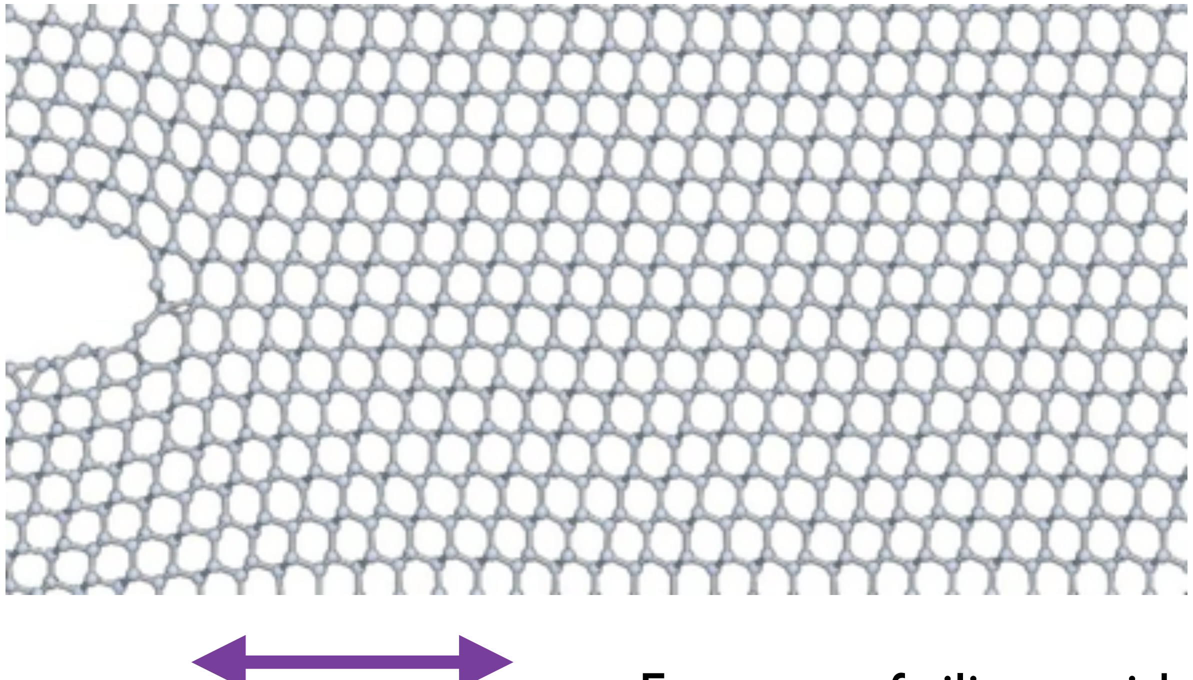
Irwin solution for σ_{yy} near a crack tip

Divergence of stress field near a crack tip

$$\sigma \sim \frac{1}{\sqrt{r}}$$





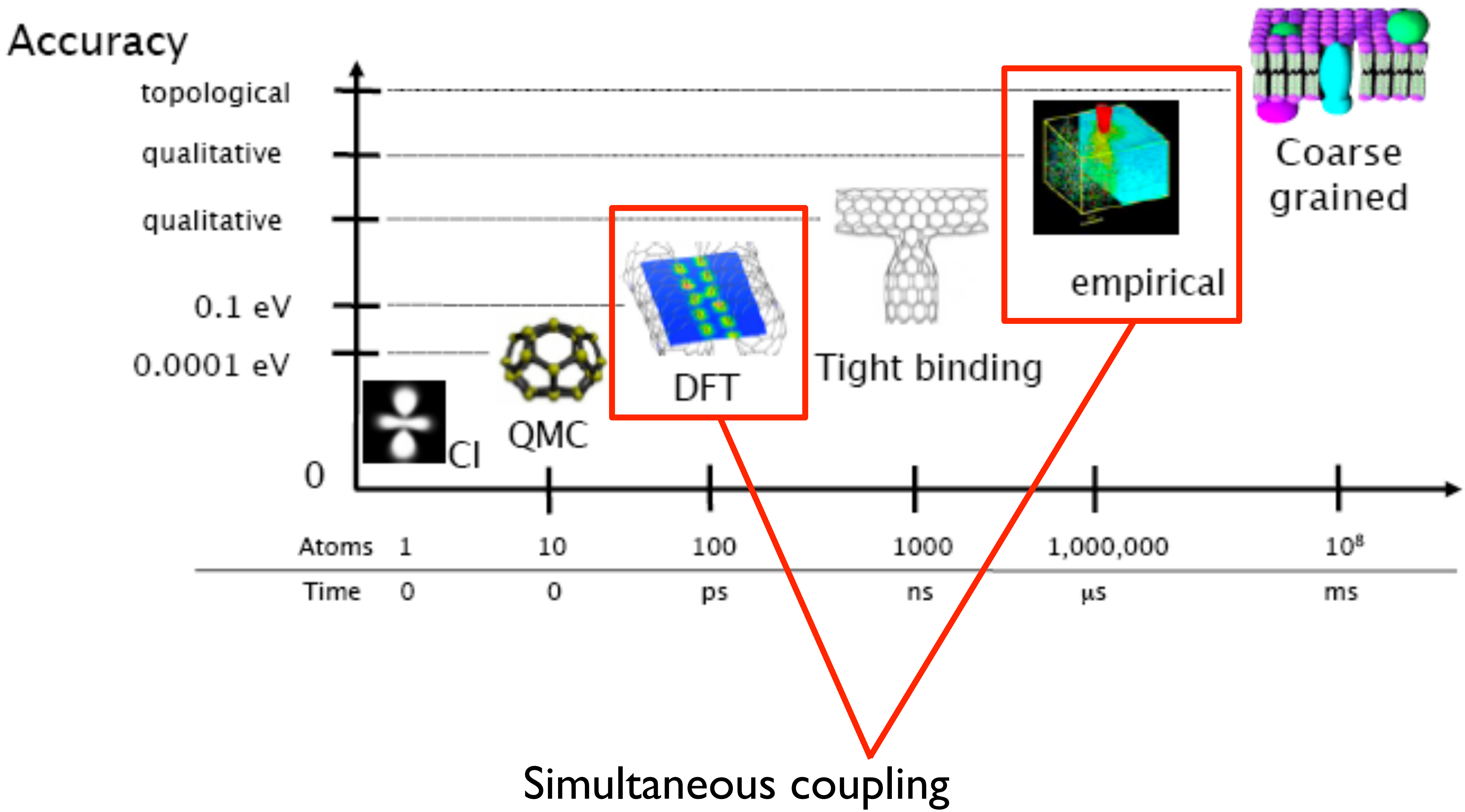


20 A = 2 nm

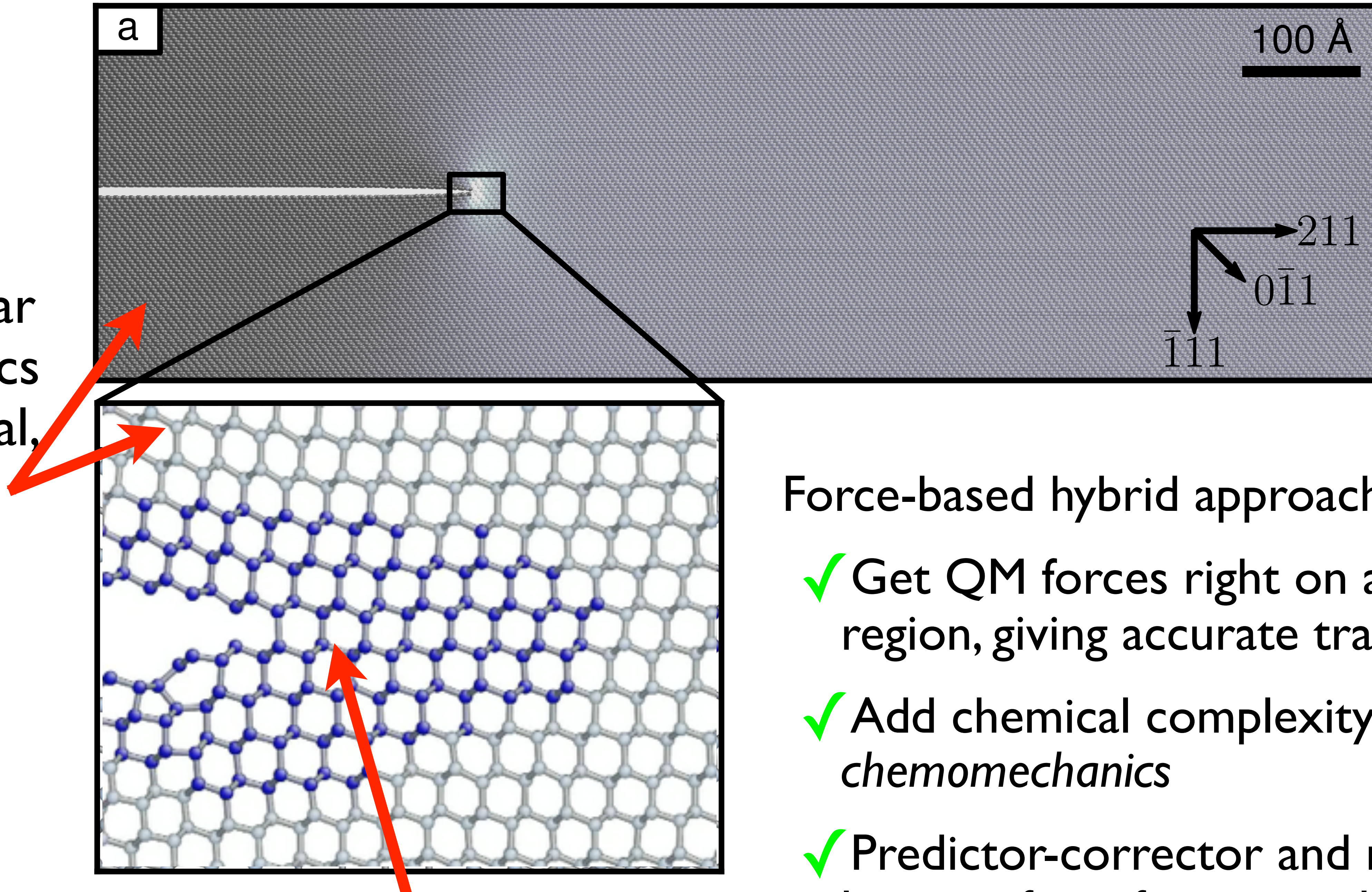
Fracture of silicon with Stillinger-Weber potential

G Singh, JR Kermode, A De Vita and RW Zimmerman, *Submitted*

Multiscale Materials Modelling – QM/MM coupling



Multiscale Materials Modelling – 'Learn on the Fly' scheme



Molecular Mechanics (empirical, fast)

Quantum Mechanics (accurate, slow)

Force-based hybrid approach (cf. QM/MM)

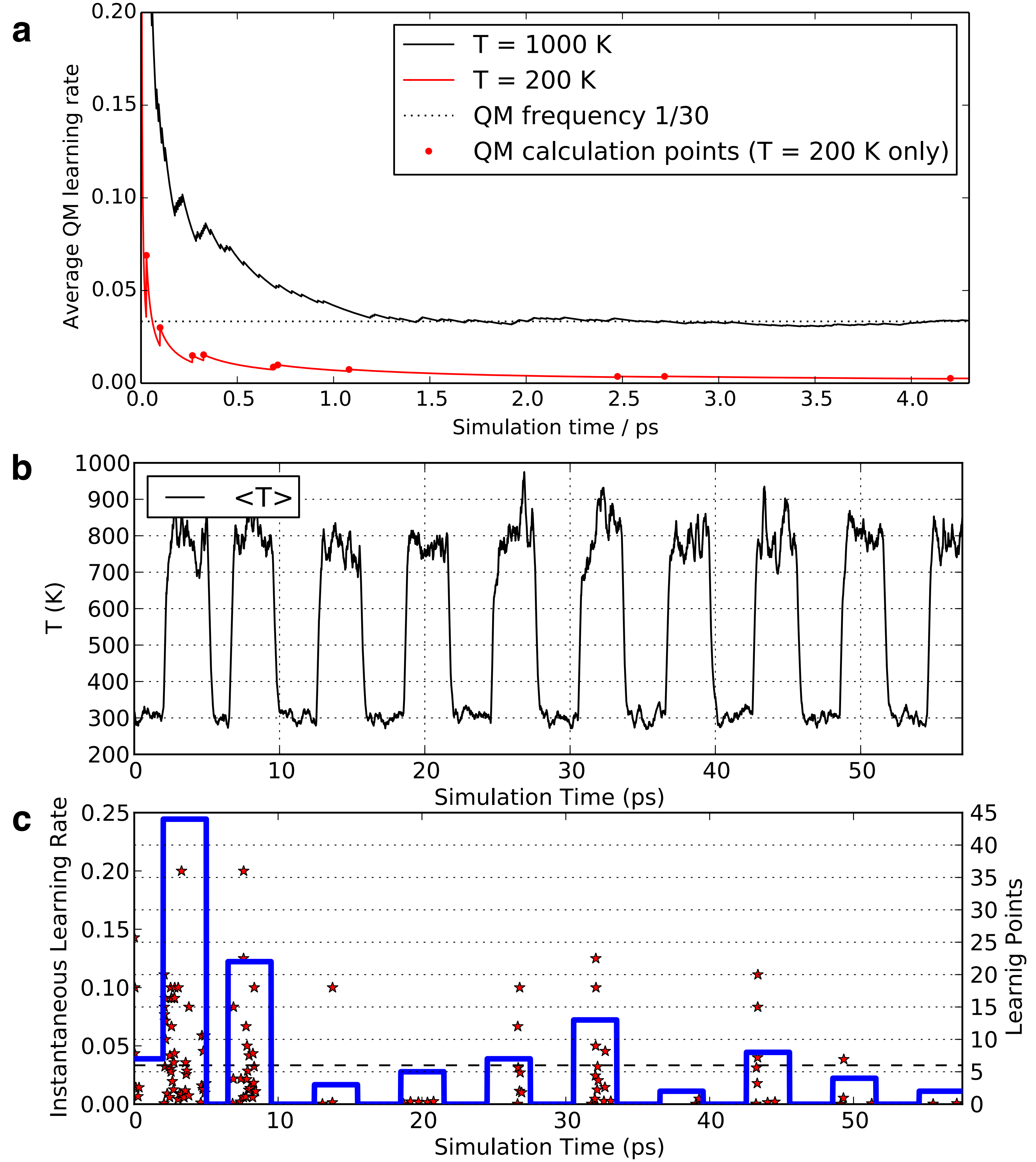
- ✓ Get QM forces right on a moving region, giving accurate trajectories
- ✓ Add chemical complexity near tip: *chemomechanics*
- ✓ Predictor-corrector and machine learning for informational efficiency

A. De Vita and R. Car, MRS Proc **491**, 473 (1998)
G Csányi *et al.* Phys. Rev. Lett. **93** 175503 (2004)

N Bernstein *et al.* Rep. Prog. Phys. **72** 026501 (2009)
Z Li, JR Kermode and A De Vita, *Submitted* (2014)

Multiscale Materials Modelling – new machine learning scheme

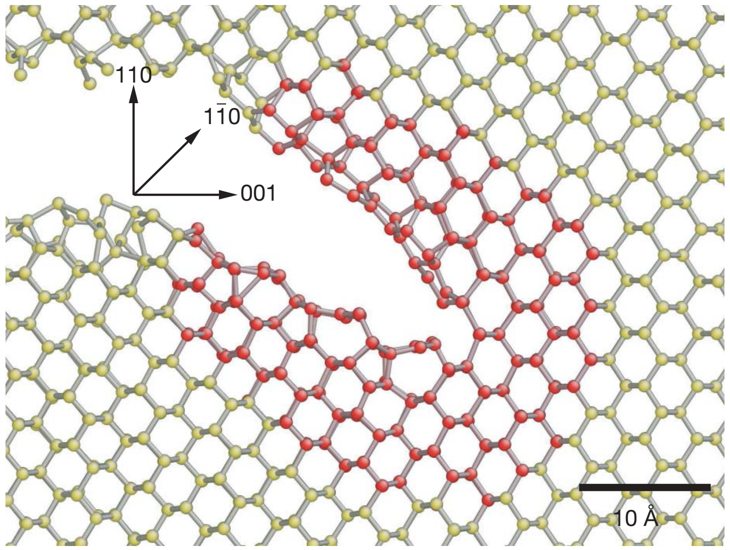
- Forces on atoms are:
  - *Either* predicted by ML using Bayesian inference
  - *Or*, if necessary, computed on-the-fly and added to a growing ML database
- e.g. bulk Si at low and high temperatures:
  - High *T* – only need QM calc every 30 time steps
  - Low *T* – long periods where nothing new happens (> 1 ps)
- Alternating between 300 K and 800 K – fewer QM calculations needed on 2nd and subsequent cycles



Z Li, JR Kermode and A De Vita, *Submitted* (2014)

Overview of Fracture Modelling Applications

Dynamical instabilities in Si



JR Kermode *et. al.*
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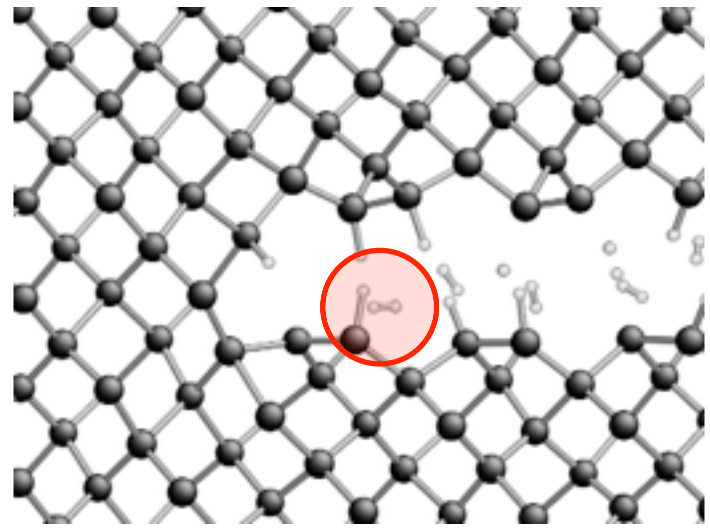
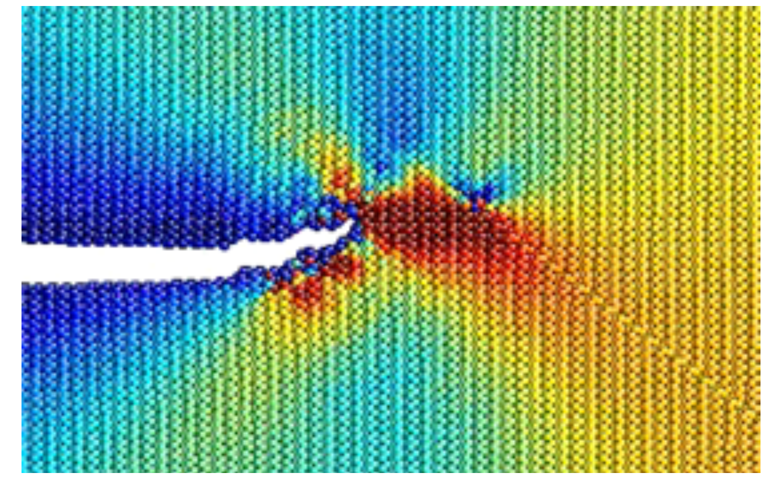


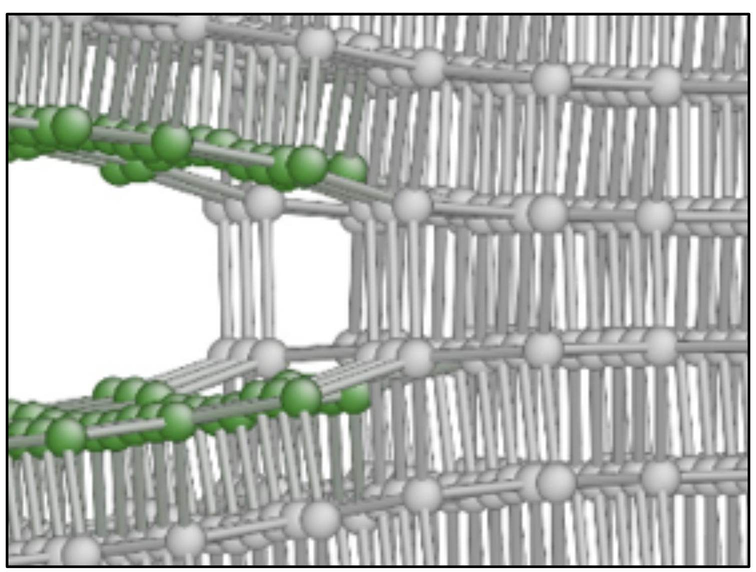
G Moras *et al.* Phys. Rev. Lett.
105, 075502 (2010)

Crack-dislocation interactions



C Gattinoni, JR Kermode and
A De Vita, In *prep* (2014)

Three dimensional effects



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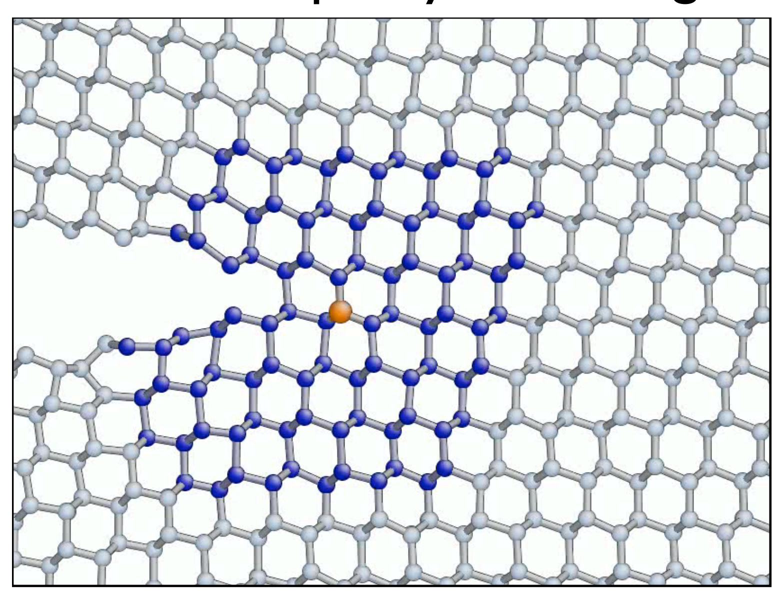
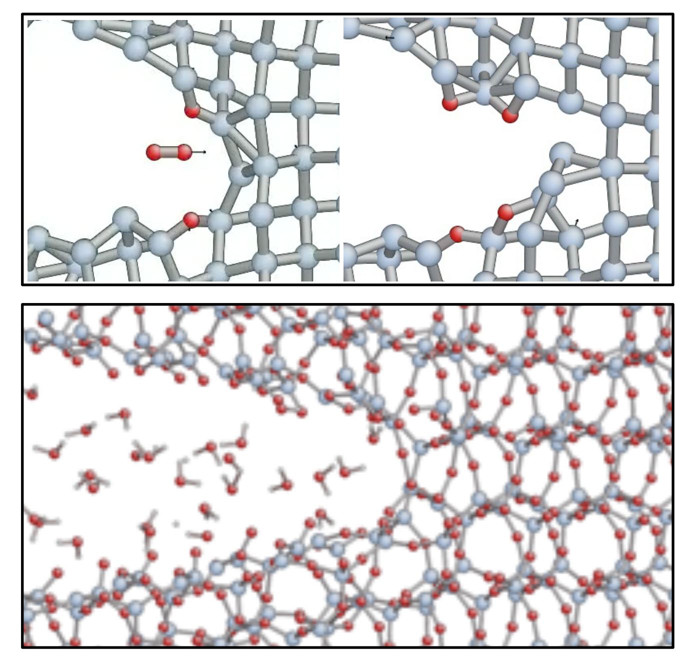
D Sherman and A De Vita, *In prep* (2014)

Crack-impurity scattering



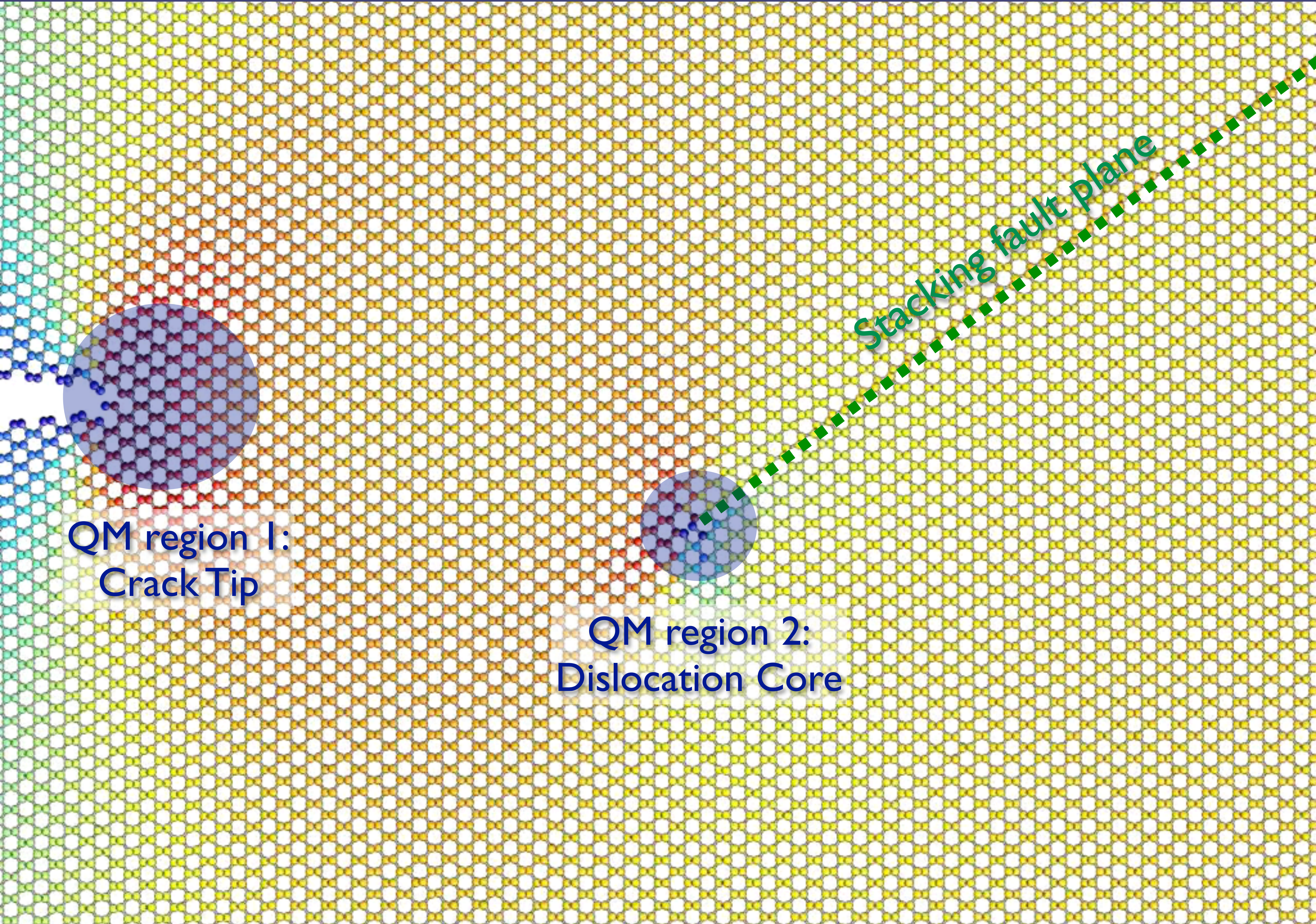
JR Kermode, L Ben-Bashat, F Atrash,
JJ Cilliers, D Sherman and A. De Vita.,
Nat. Commun. **4** 2441 (2013)

Stress corrosion cracking



A Glazier, G Peralta, JR Kermode,
A De Vita and D Sherman, Phys. Rev. Lett,
112 115501 (2014).

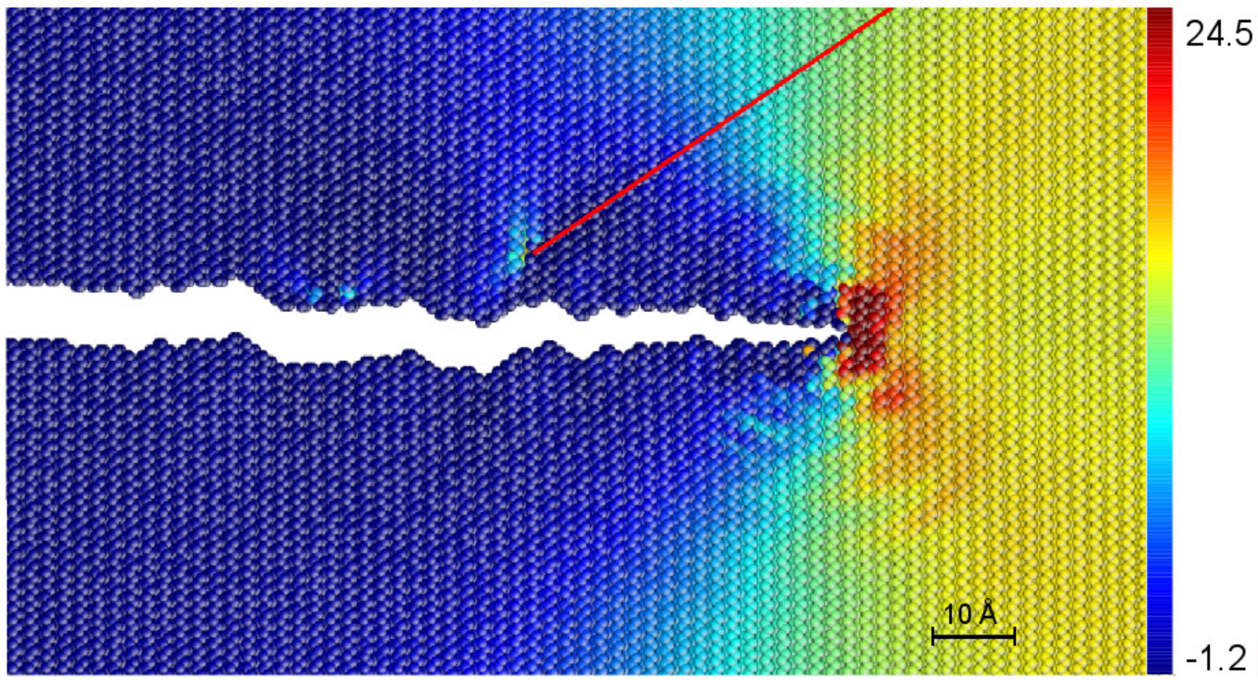
Crack/dislocation interactions – LOTF simulation

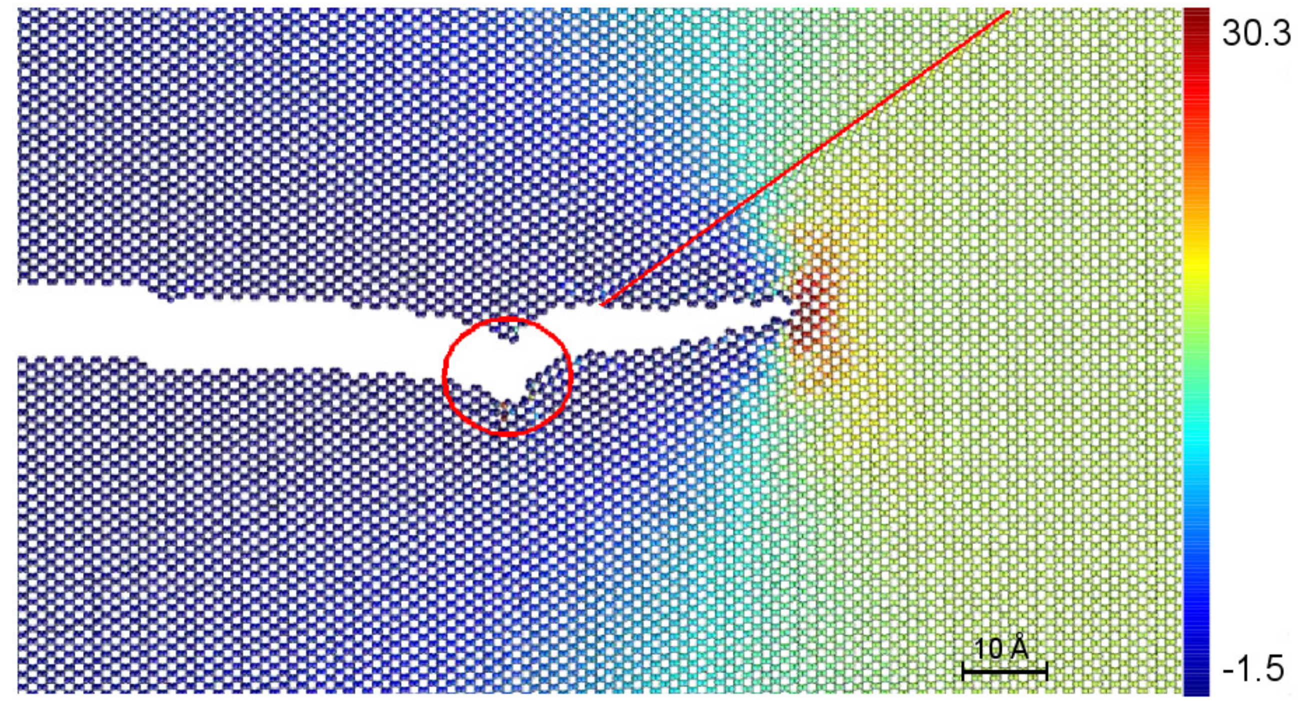


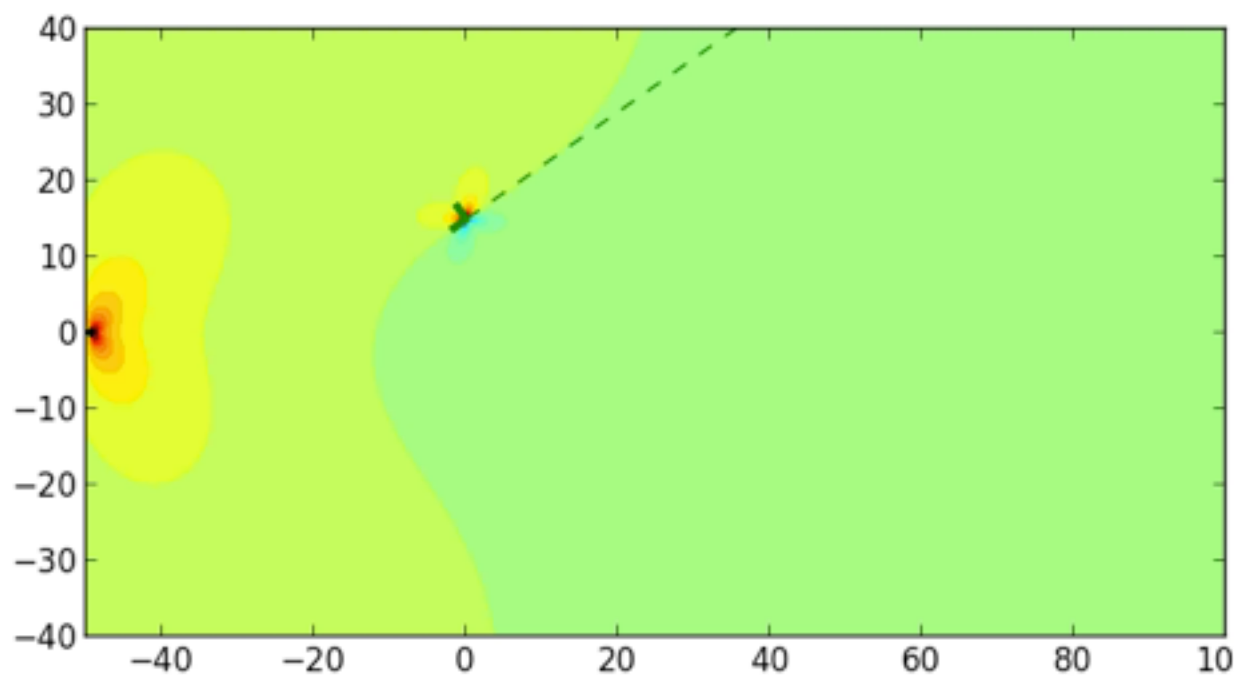
Crack/dislocation interactions – coarse-graining and upscaling

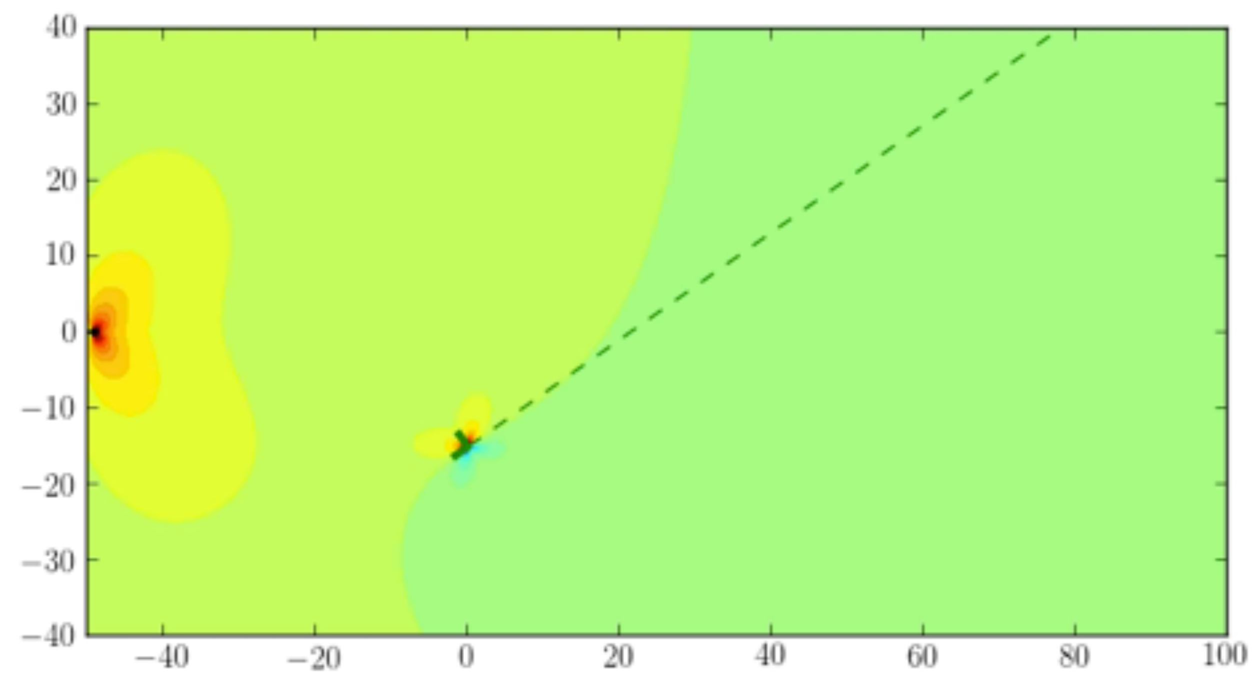
Dislocation core above crack

Dislocation core below crack









C. Gattinoni, J.R. Kermode and A. De Vita, in prep.

Continuum solution: Lin and Thomson (1986)

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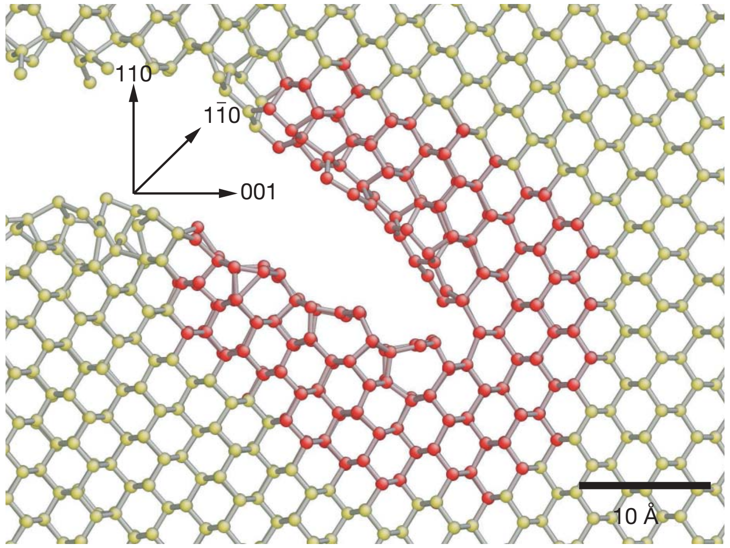

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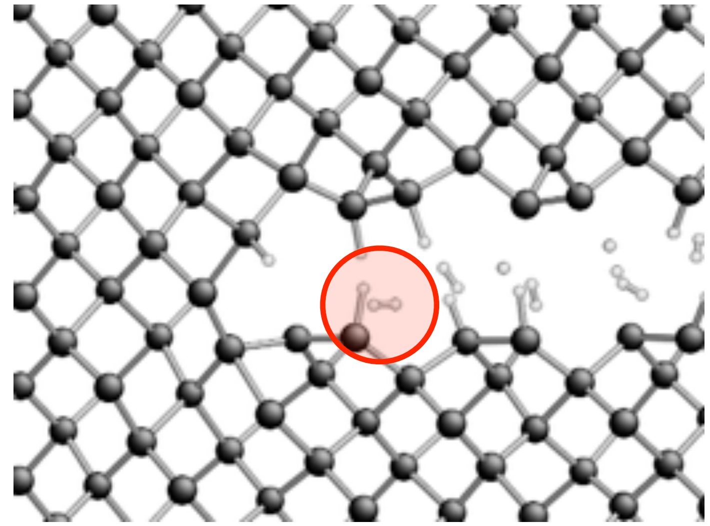

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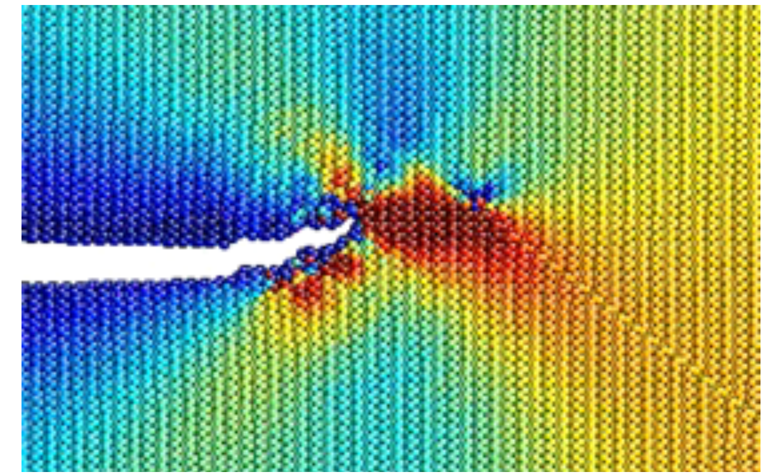

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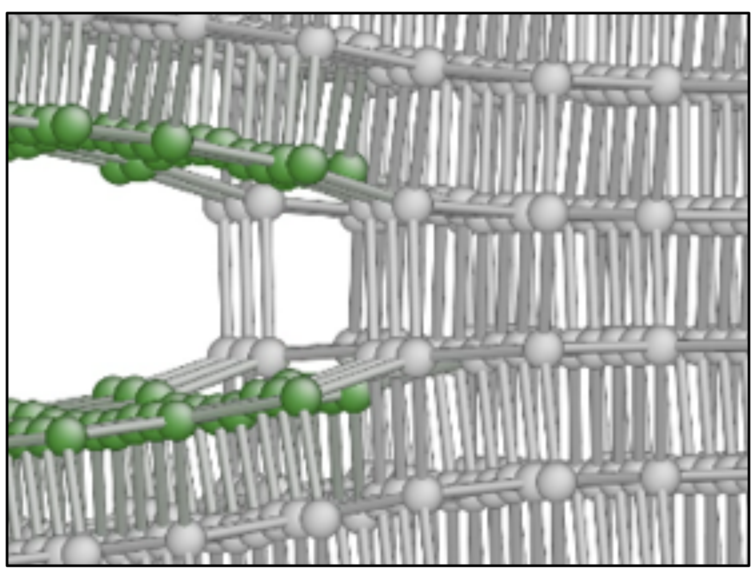

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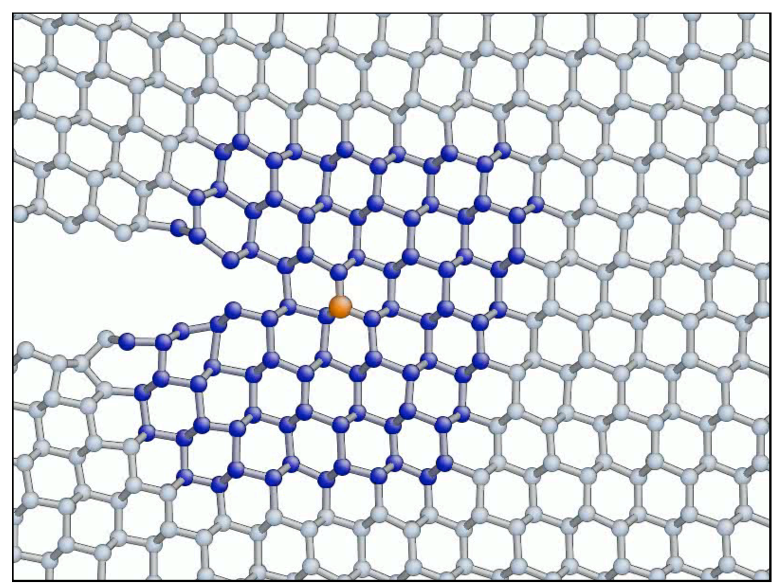
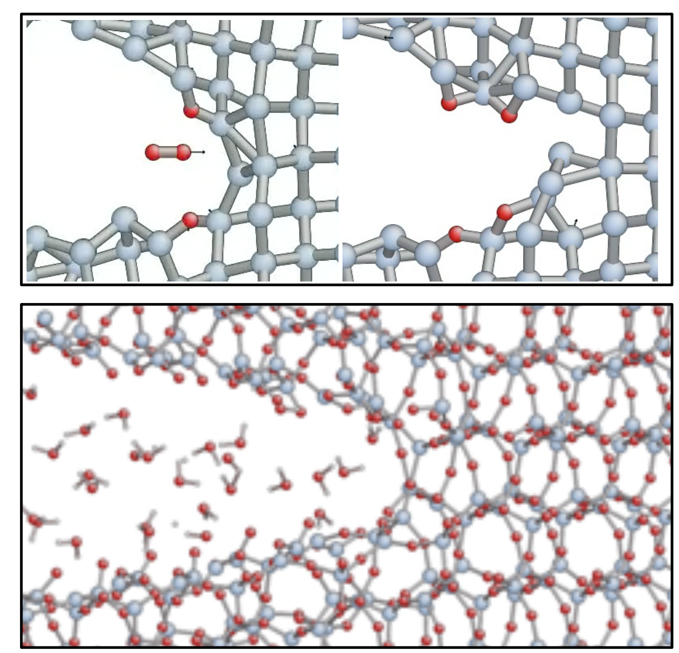


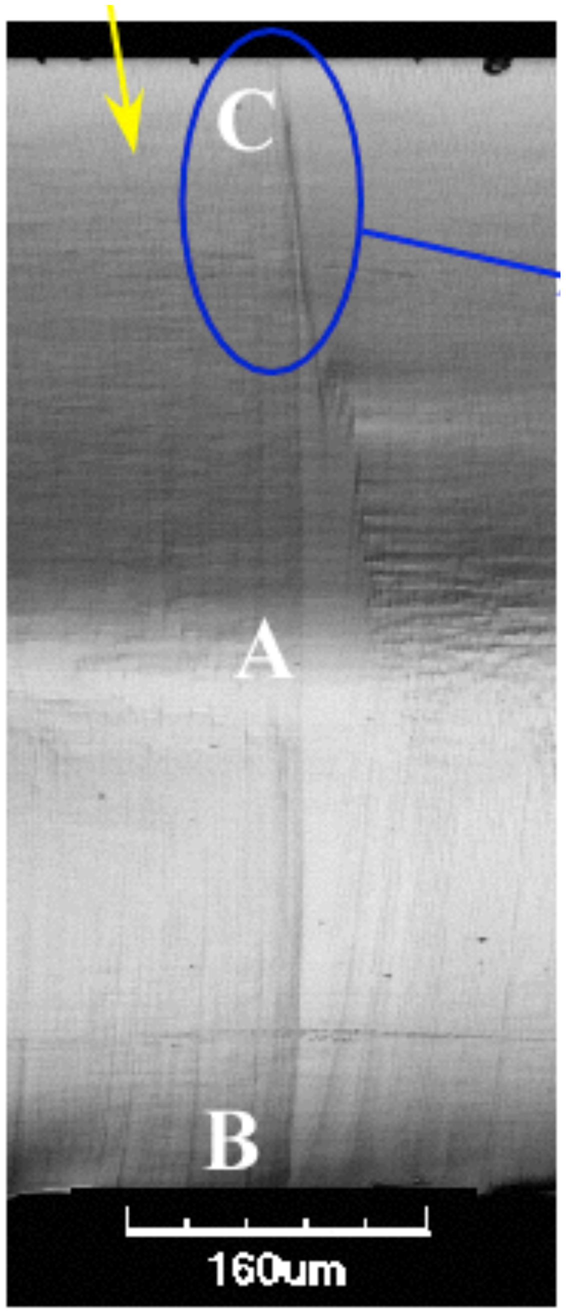
JR Kermode, L Ben-Bashat, F Atrash,
JJ Cilliers, D Sherman and A. De Vita.,
Nat. Commun. **4** 2441 (2013)

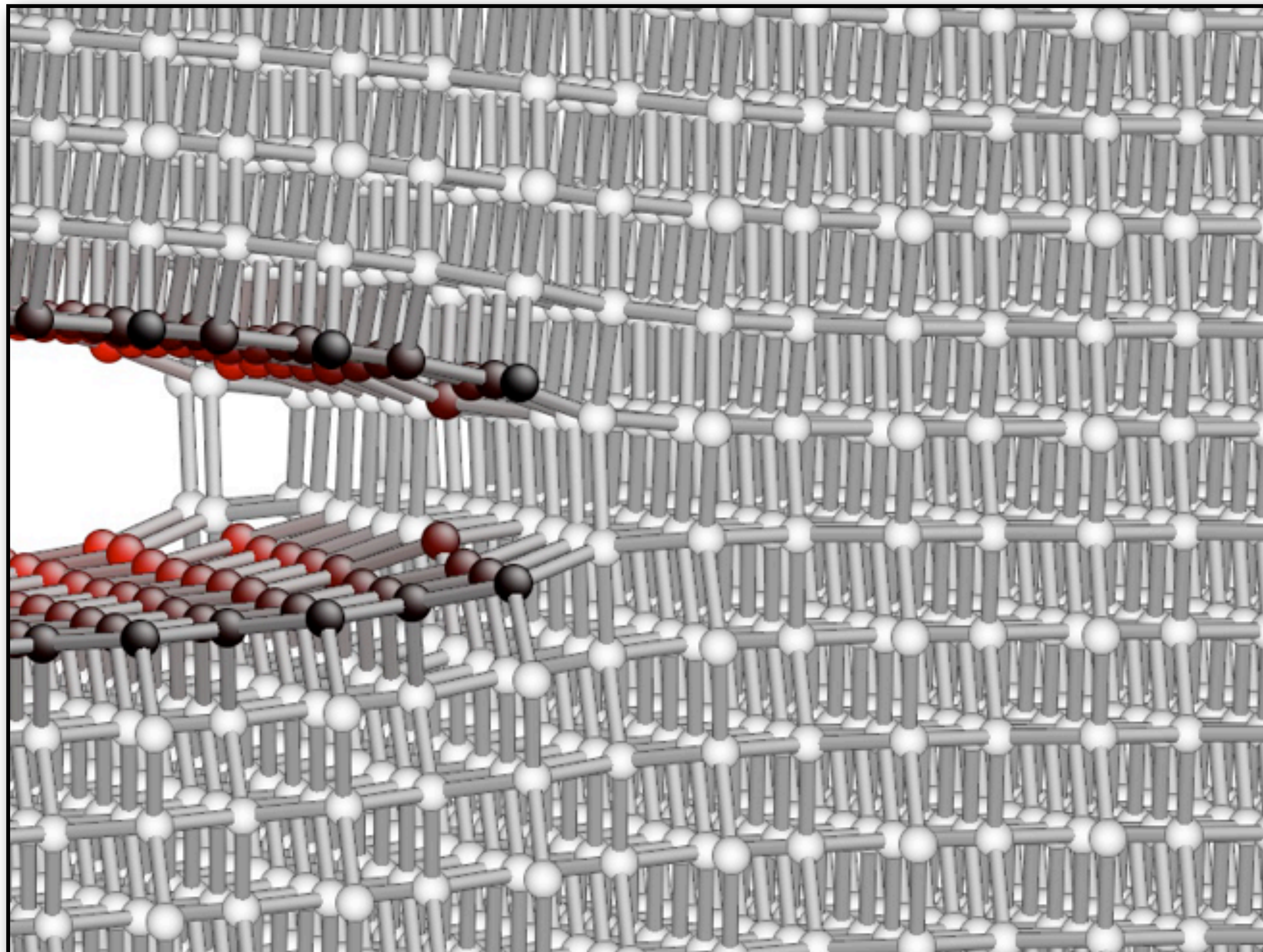
Stress corrosion cracking



A Glazier, G Peralta, JR Kermode,
A De Vita and D Sherman, Phys. Rev. Lett,
112 115501 (2014).

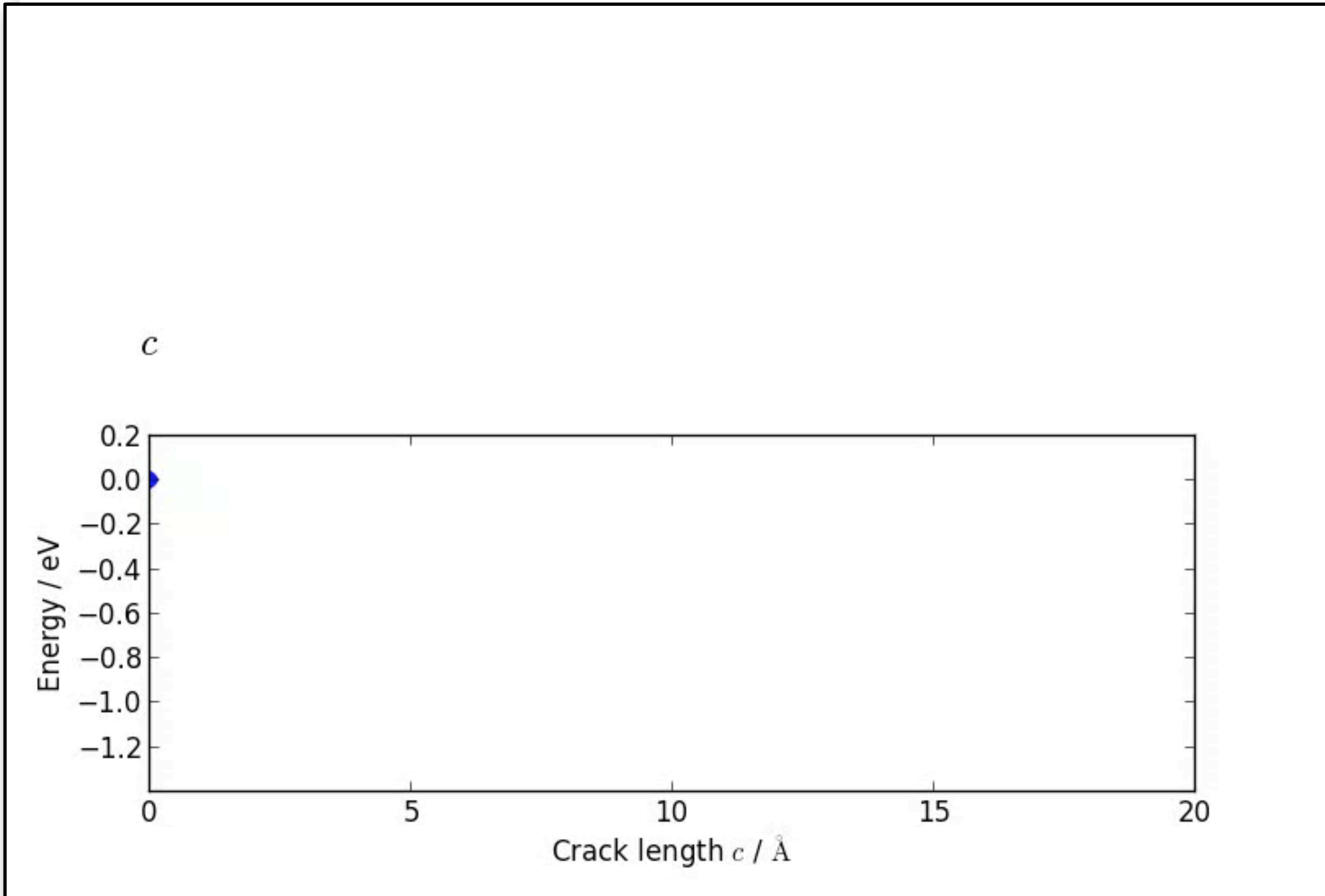
Crack speed measurements in 3D simulations





Experiments: Anna Glazier and Dov Sherman, Technion, Israel

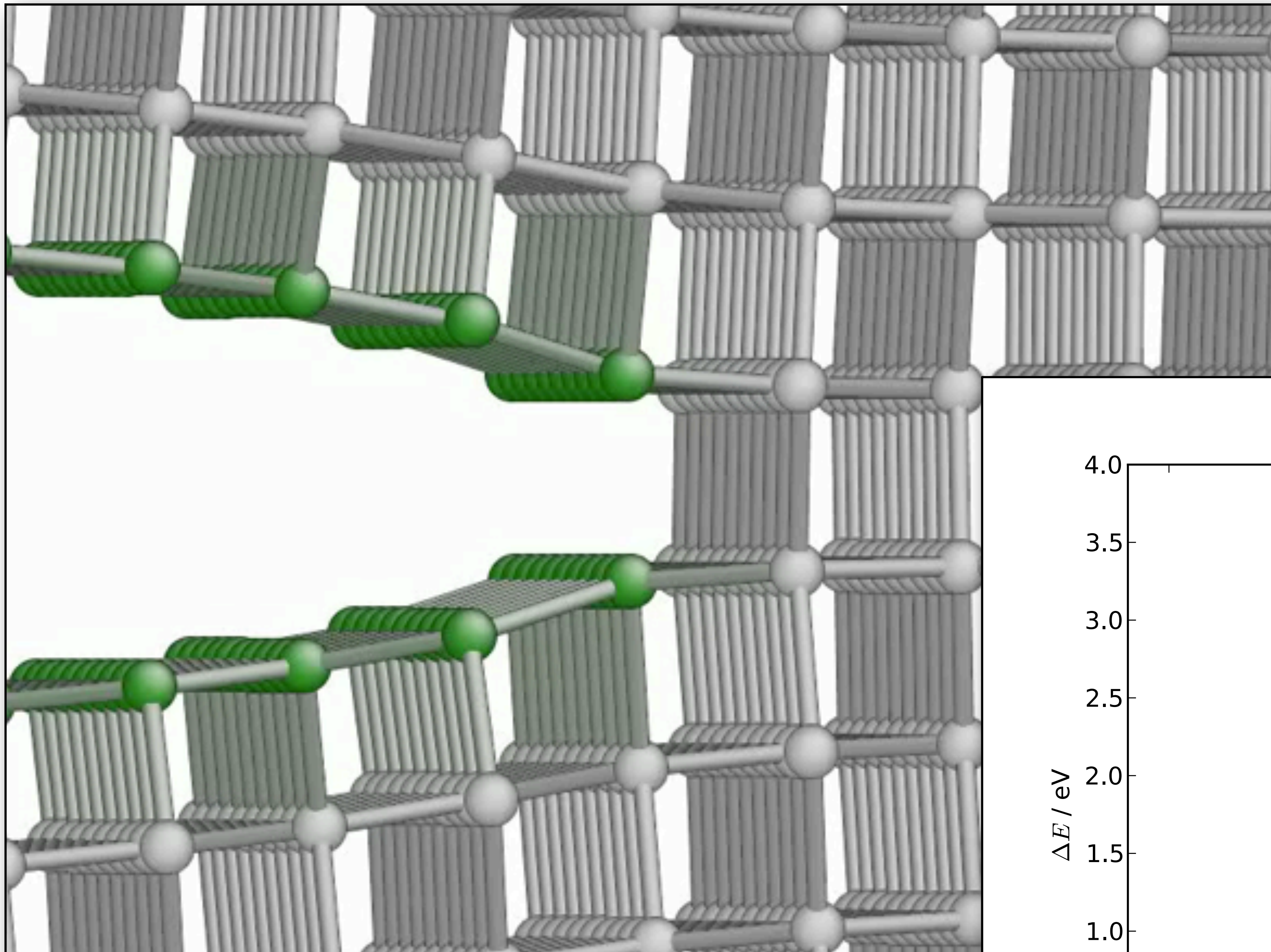
Energetics of Fracture – atomistic picture



$$E_{qs} = (-G + 2\gamma)c - \frac{\gamma_t a_x}{\pi} \sin \frac{2\pi c}{a_x}$$

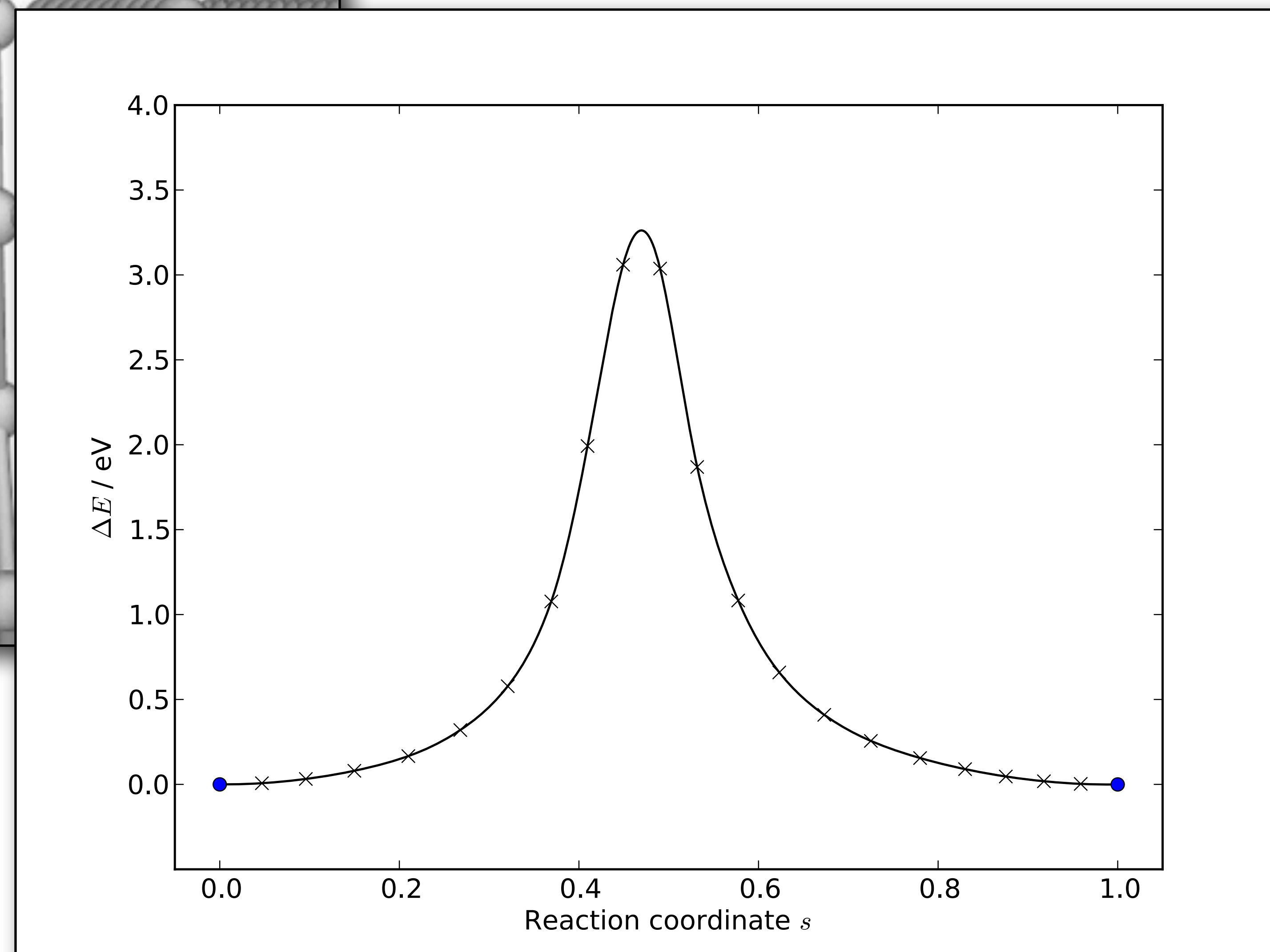
Sinclair, J. E., & Lawn, B. R. Proc. R. Soc. Lond. **329** 83 (1972).

3D fracture – simultaneous bond rupture



10 layers and ~100,000 atoms
Periodic along z

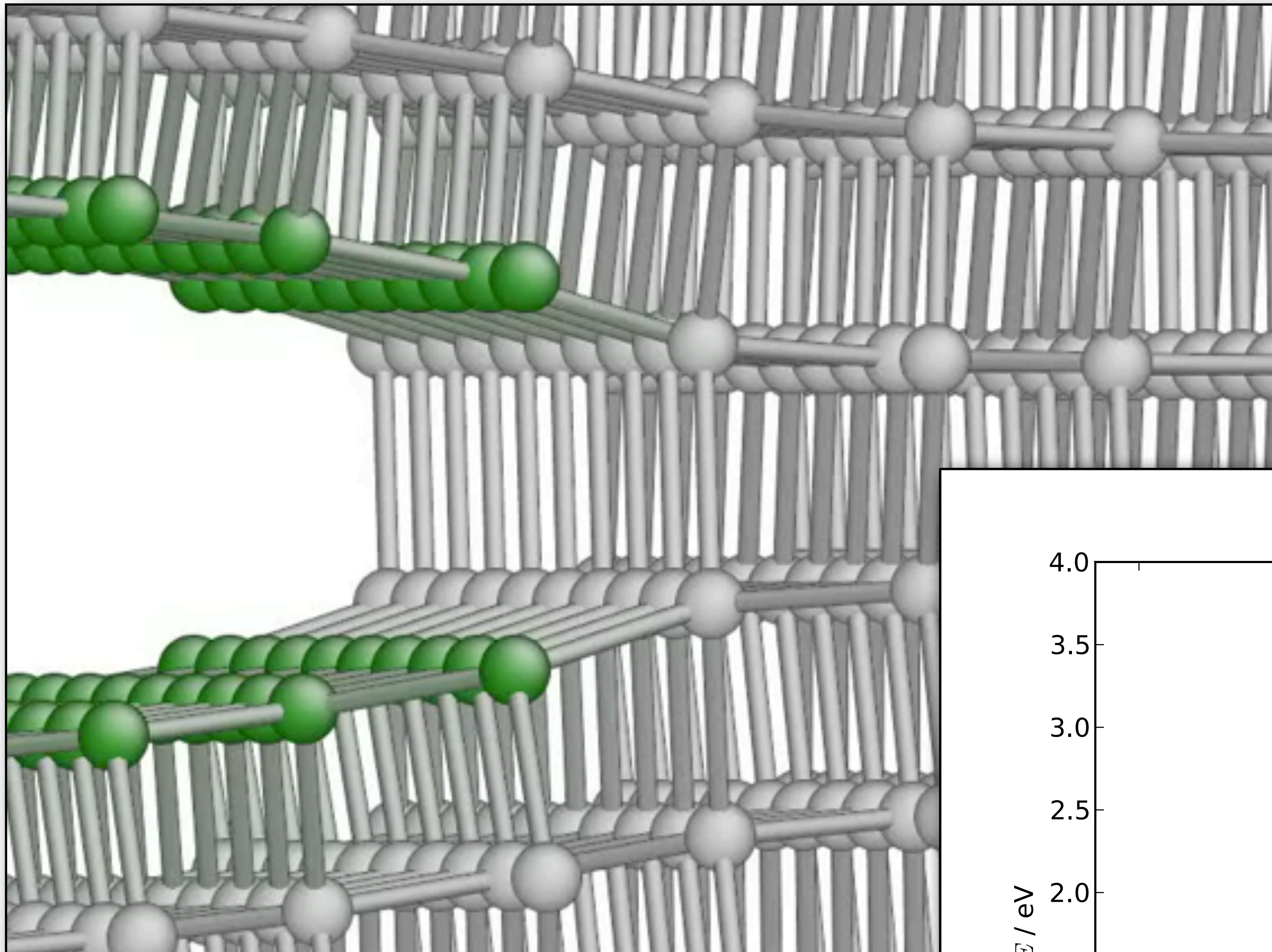
Griffith critical load



Classical NEB calculation

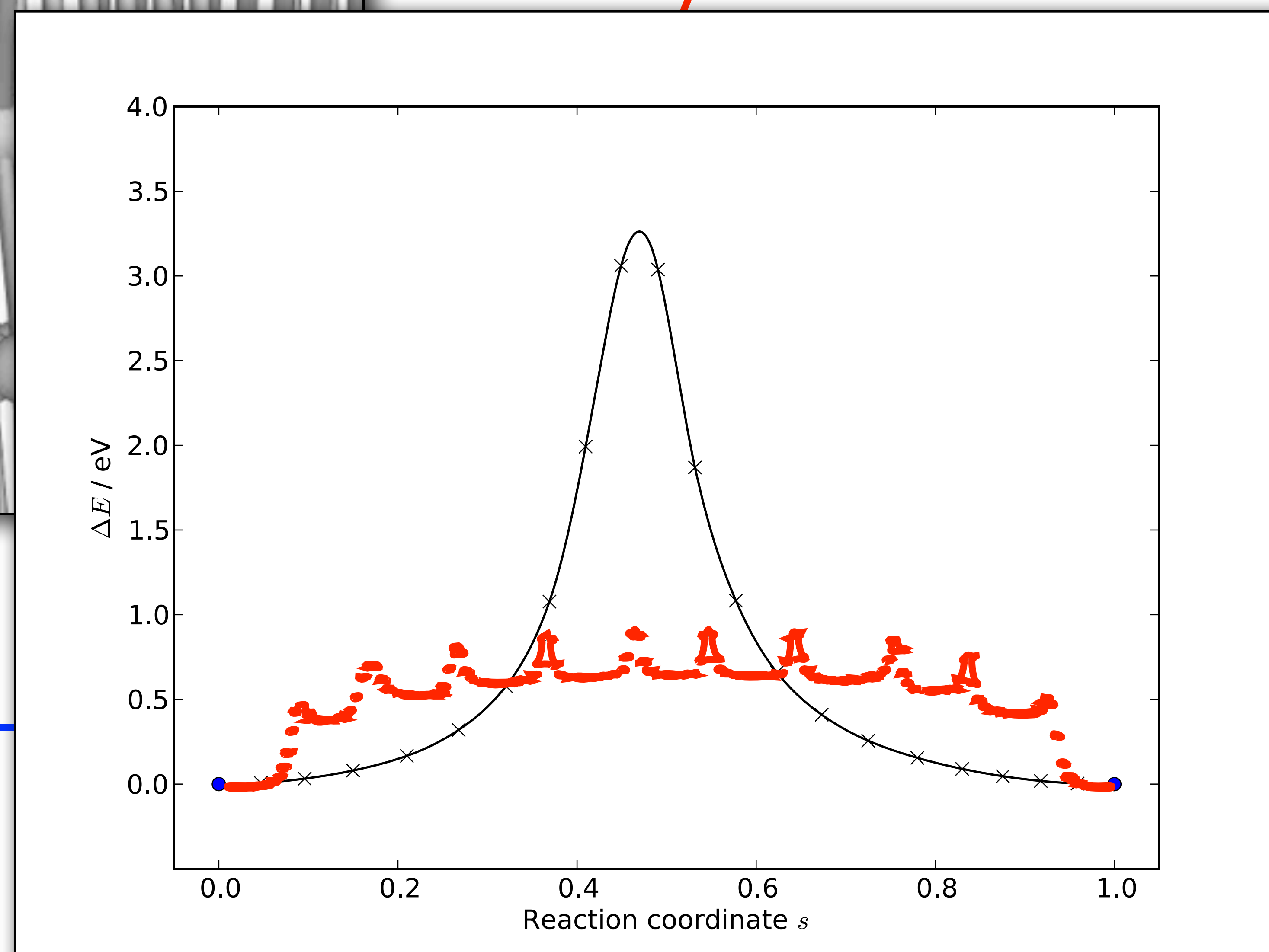
cf. T Zhu, J Li, & S Yip, Phys. Rev. Lett. (2004)

3D fracture – sequential bond rupture



10 layers and ~100,000 atoms
Periodic along z

Kink advance barrier
Griffith critical load



Classical NEB calculation

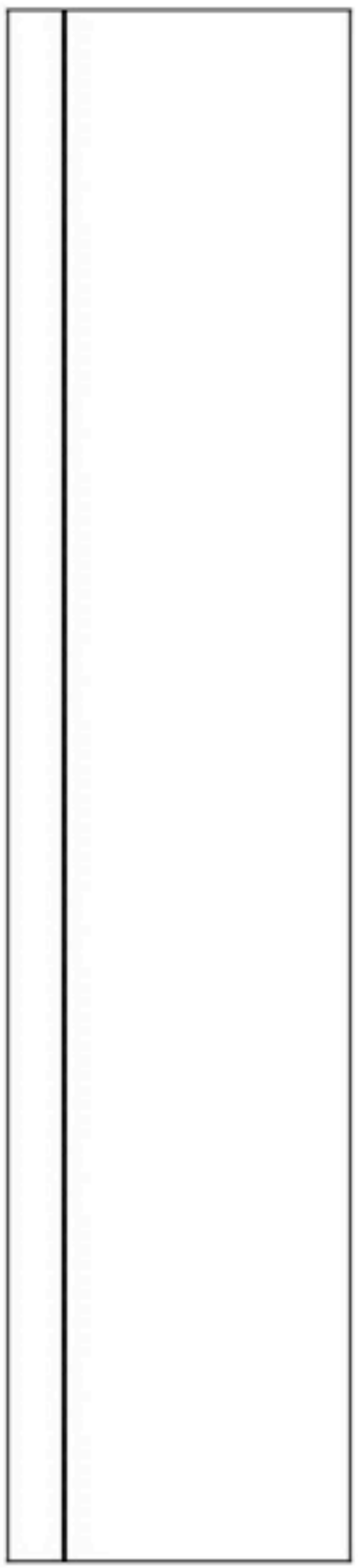
Kink pair
formation barrier

B. Lawn, *J. Mater. Sci.* **10** 469 (1975)

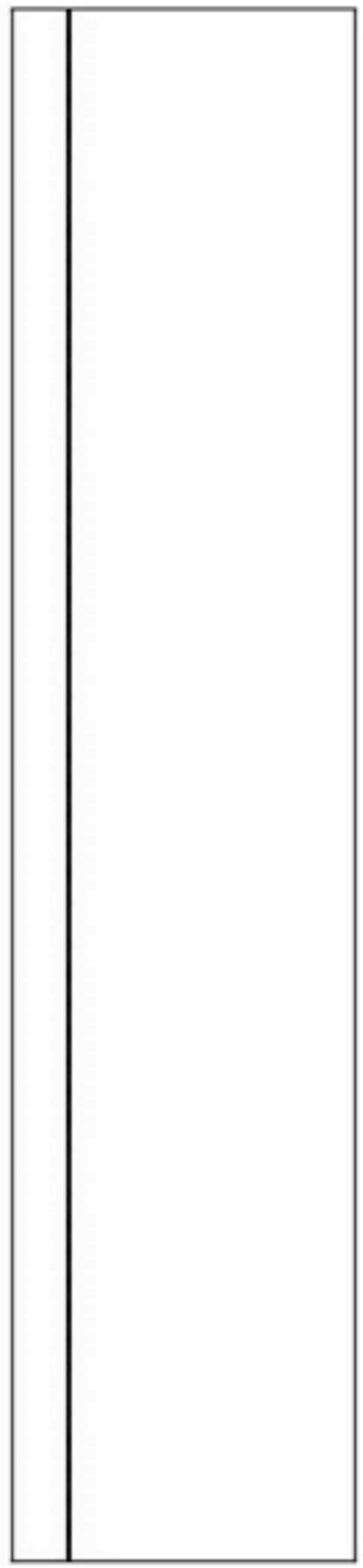
T Zhu, J Li, & S Yip, Phys. Rev. Lett. (2004)

Crack speed measurements in 3D simulations

Mesoscale kinetic Monte Carlo of kink motion

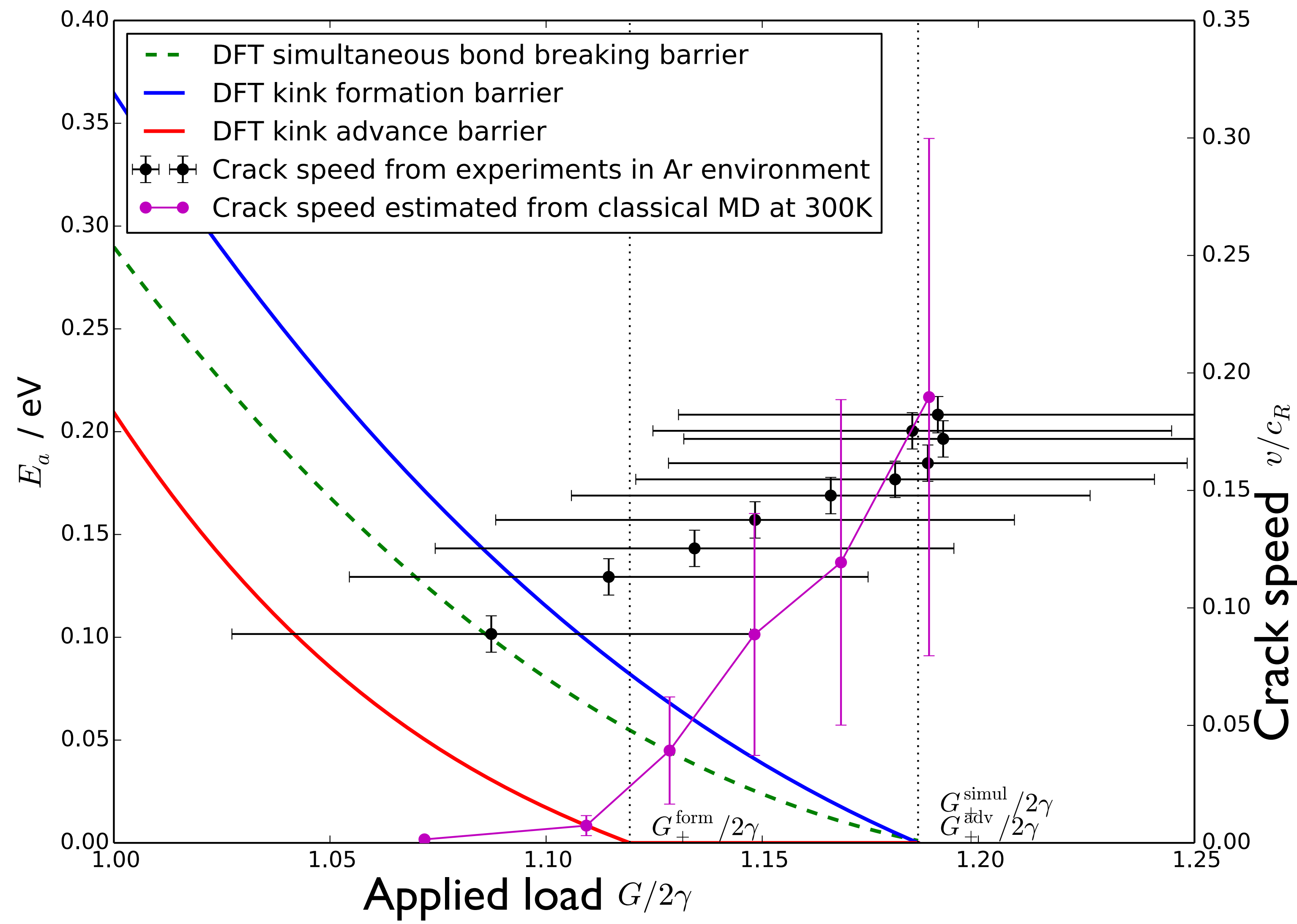


Low load, slow



High load, fast

Crack energy-speed relationship



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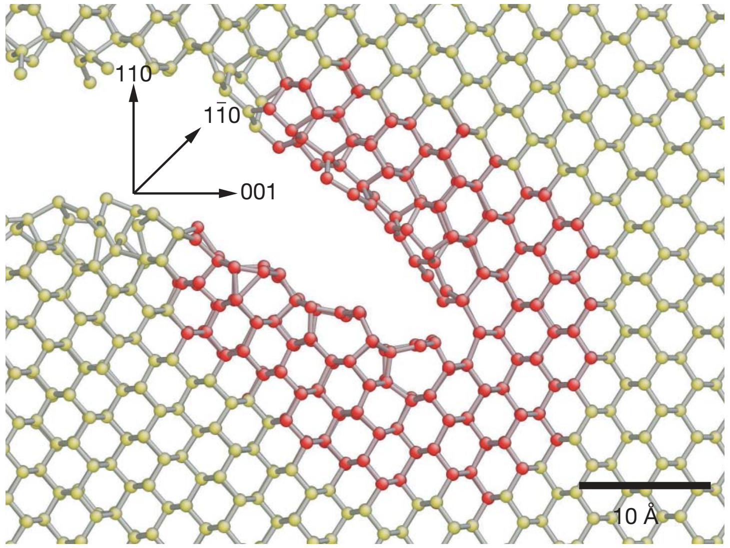

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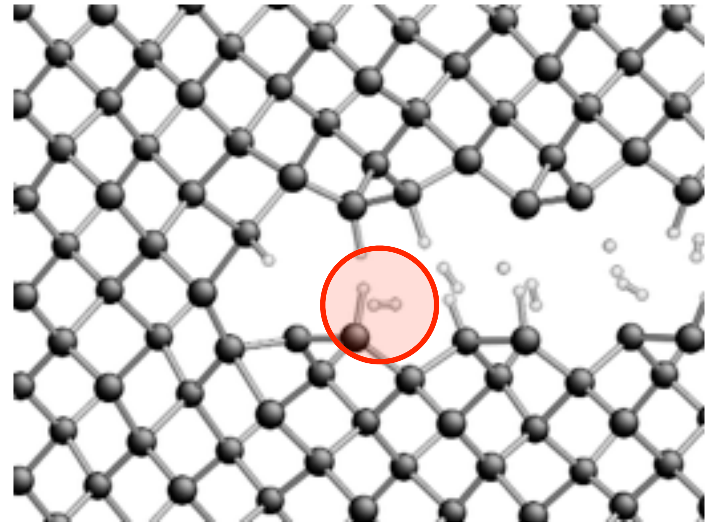

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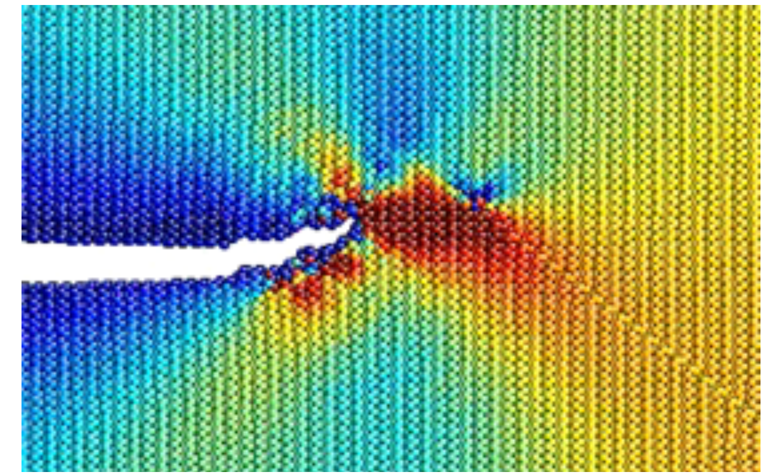

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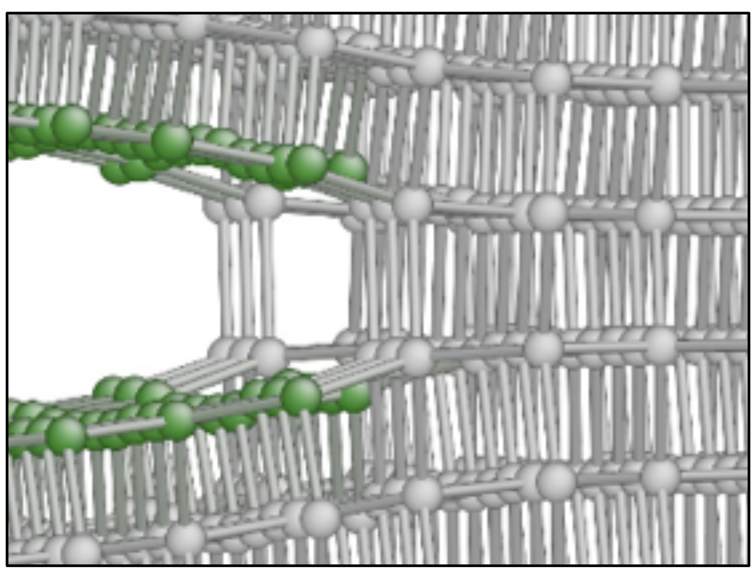

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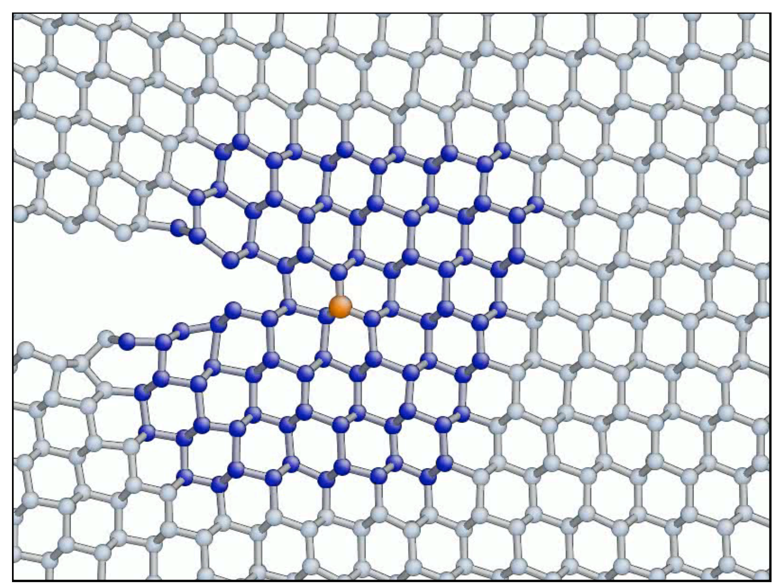

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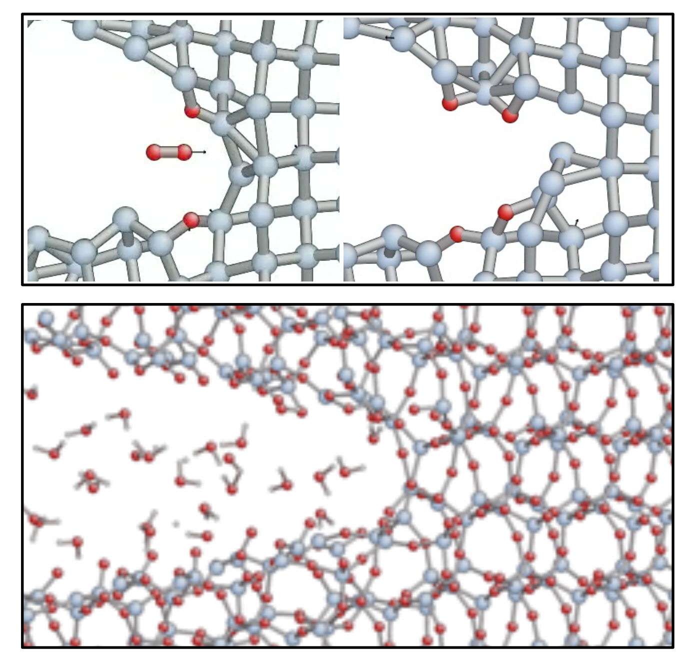
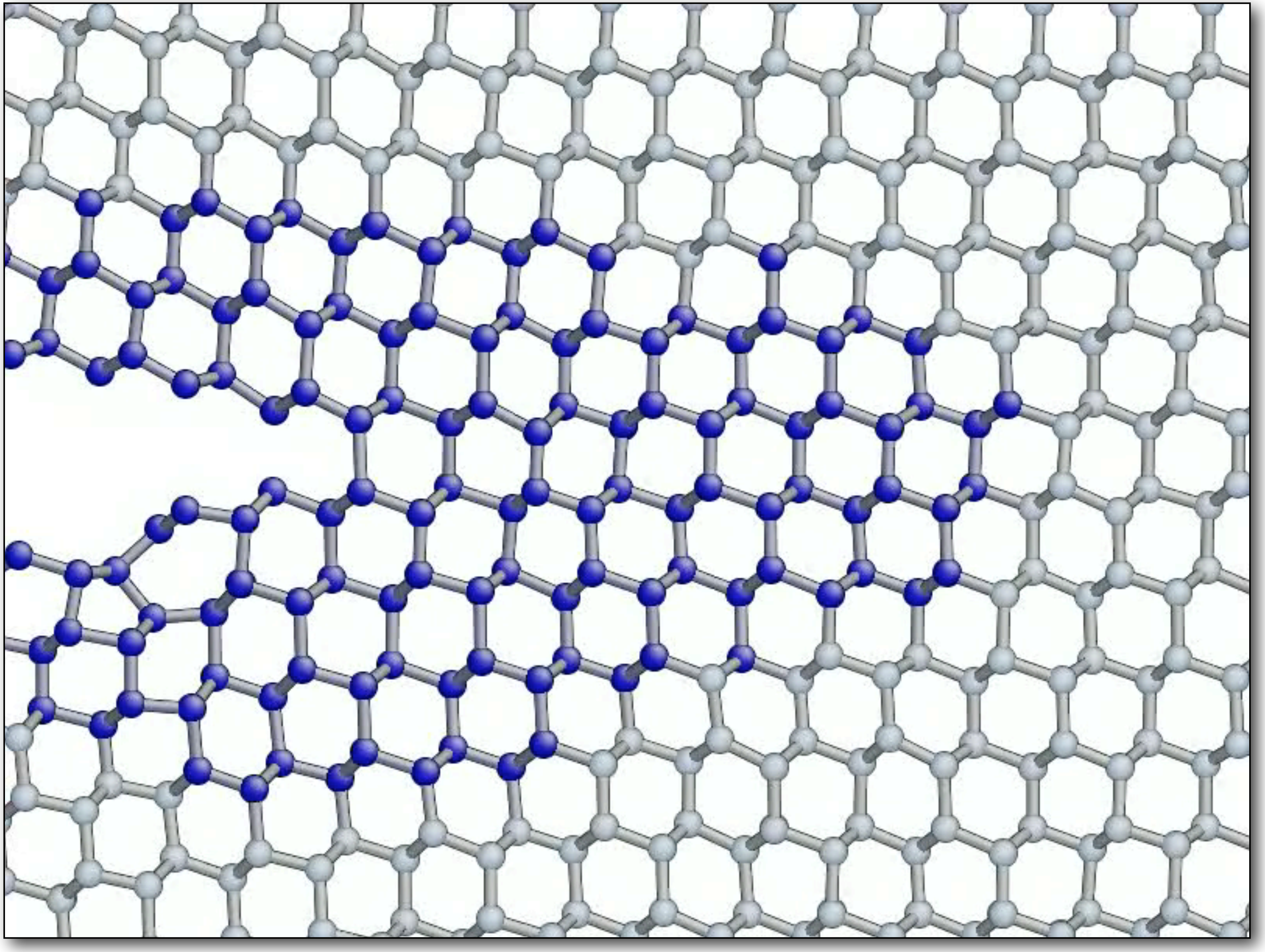
Stress corrosion cracking



A Glazier, G Peralta, JR Kermode,
A De Vita and D Sherman, Phys. Rev. Lett,
112 **115501 (2014).**

Crack propagation vs. chemical impurities – simulation



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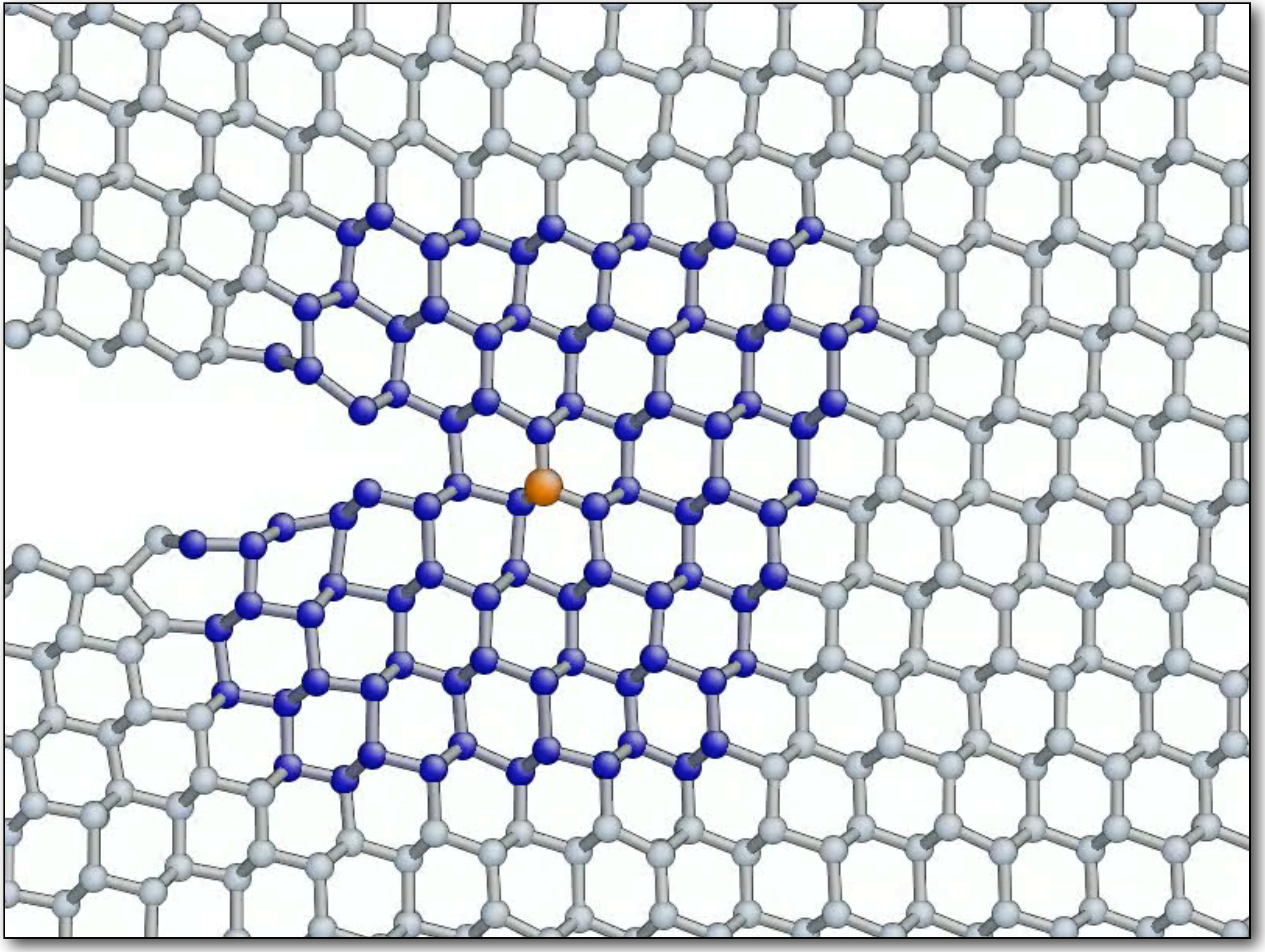

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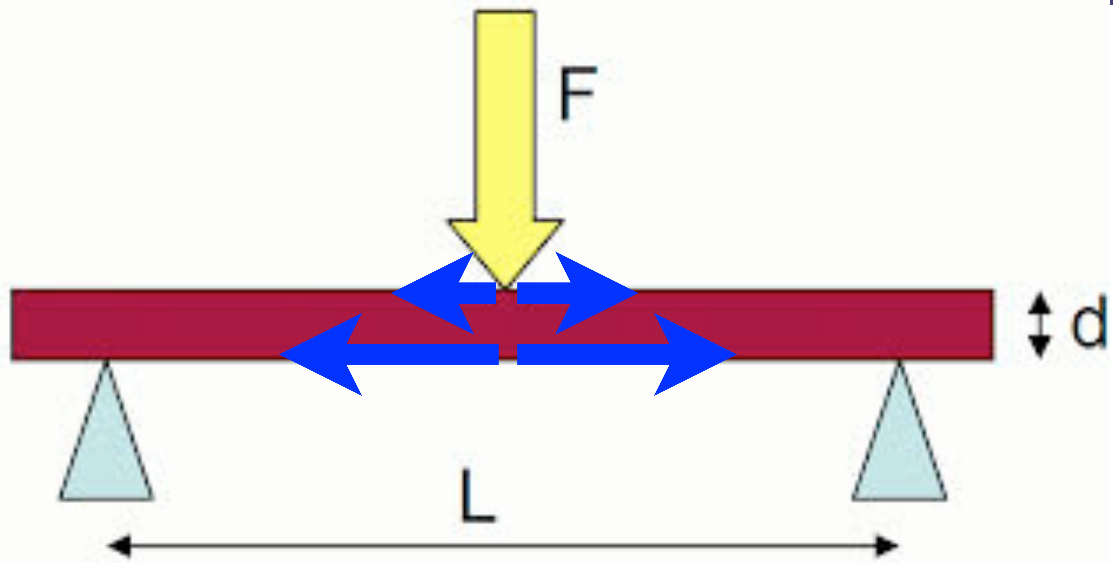
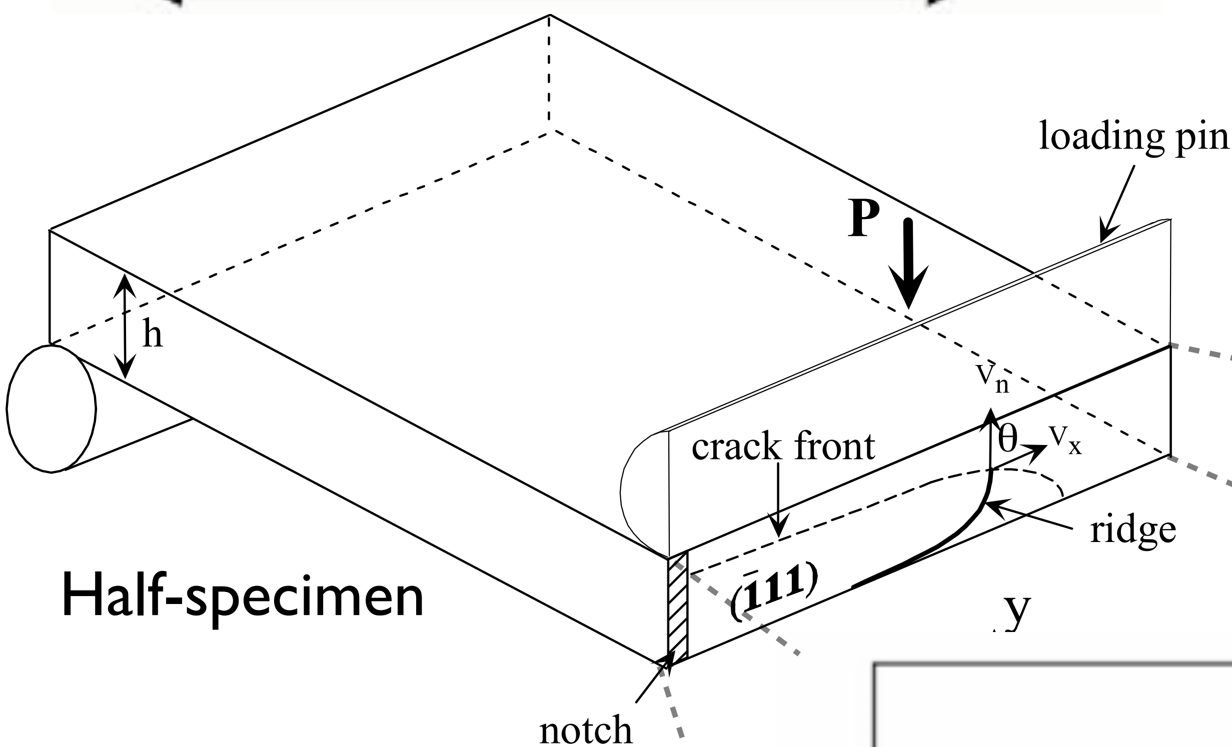
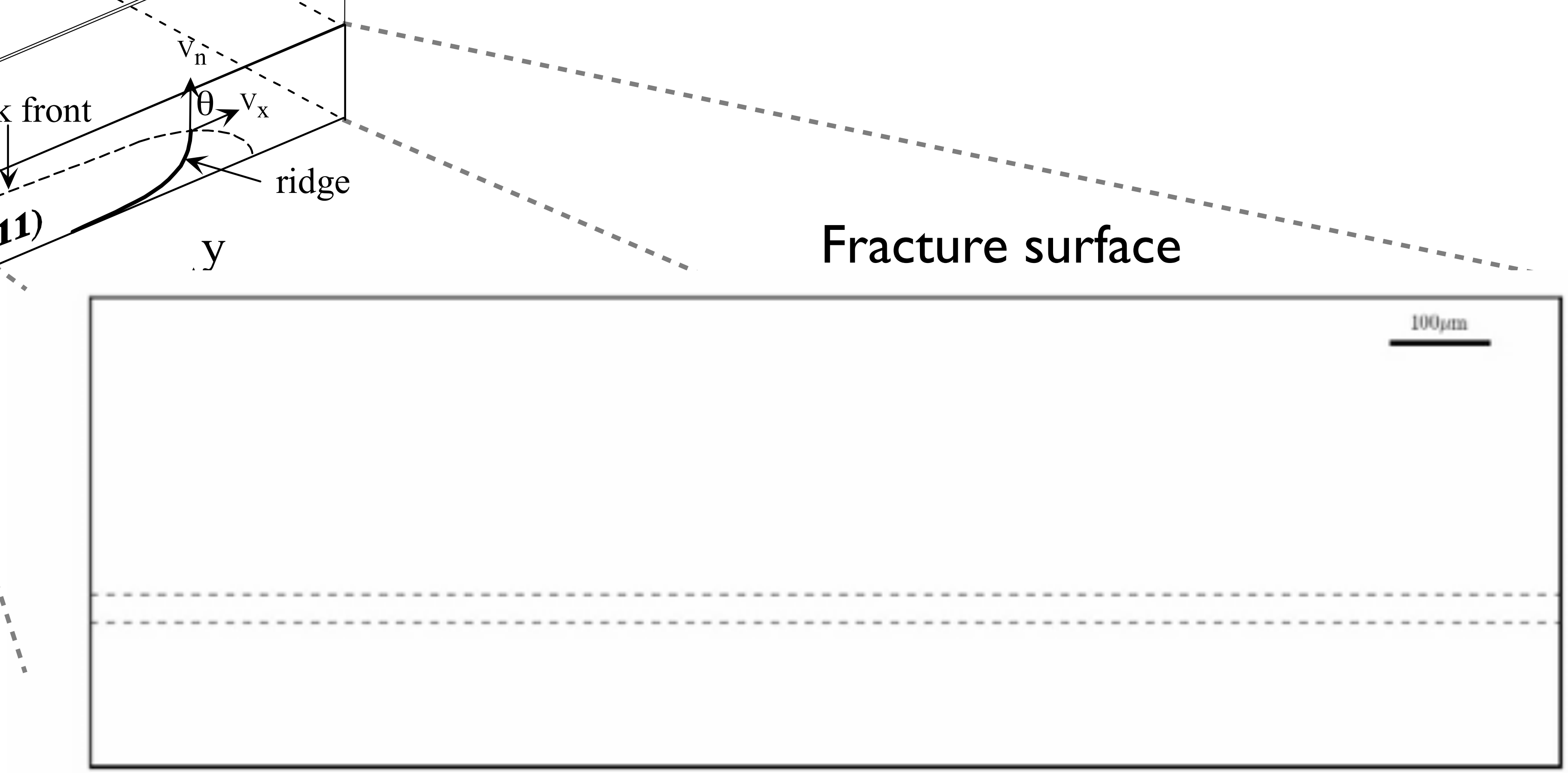
Interaction between crack tips and point defects – experiments



- Three point bending (3PB), crack subjected to maximum tension at bottom of sample
- Crack front is sliding ellipse
- Speed decreasing moving up specimen
- Ridges form out of (111) plane, same as 'down' in simulations





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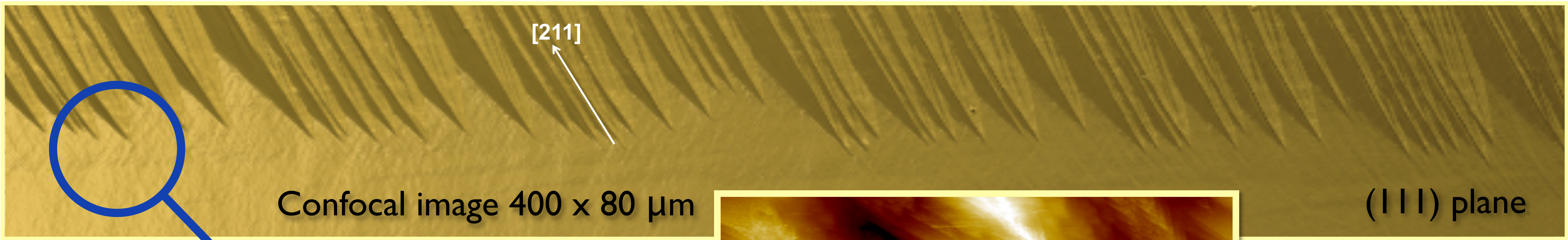
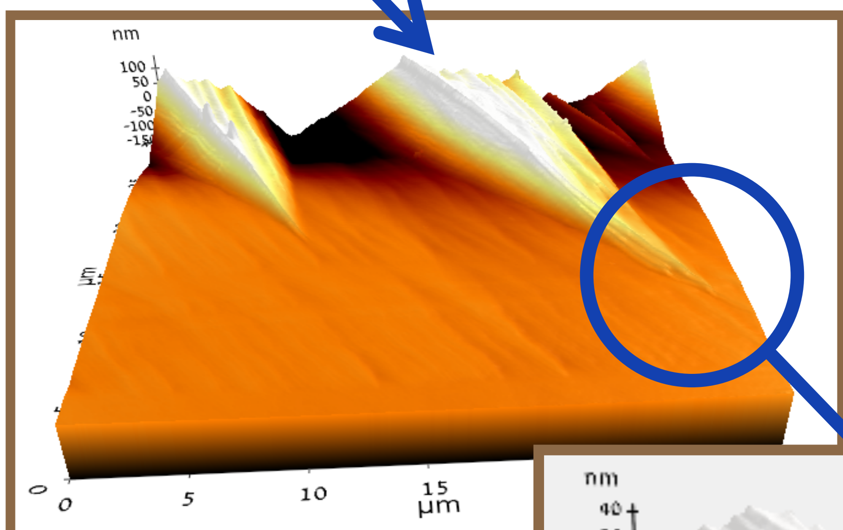
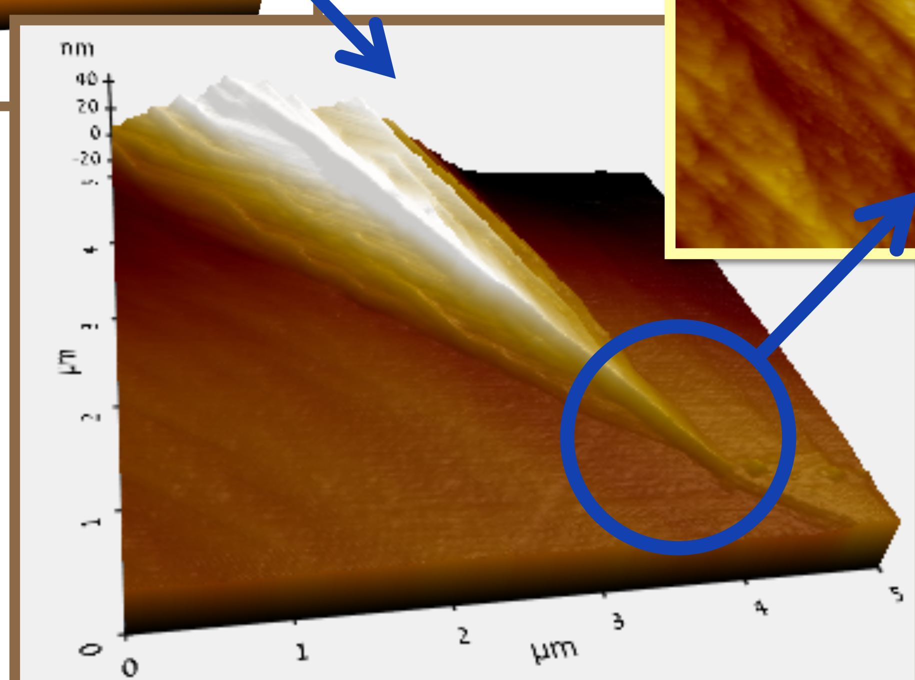


Confocal image 400 x 80 µm

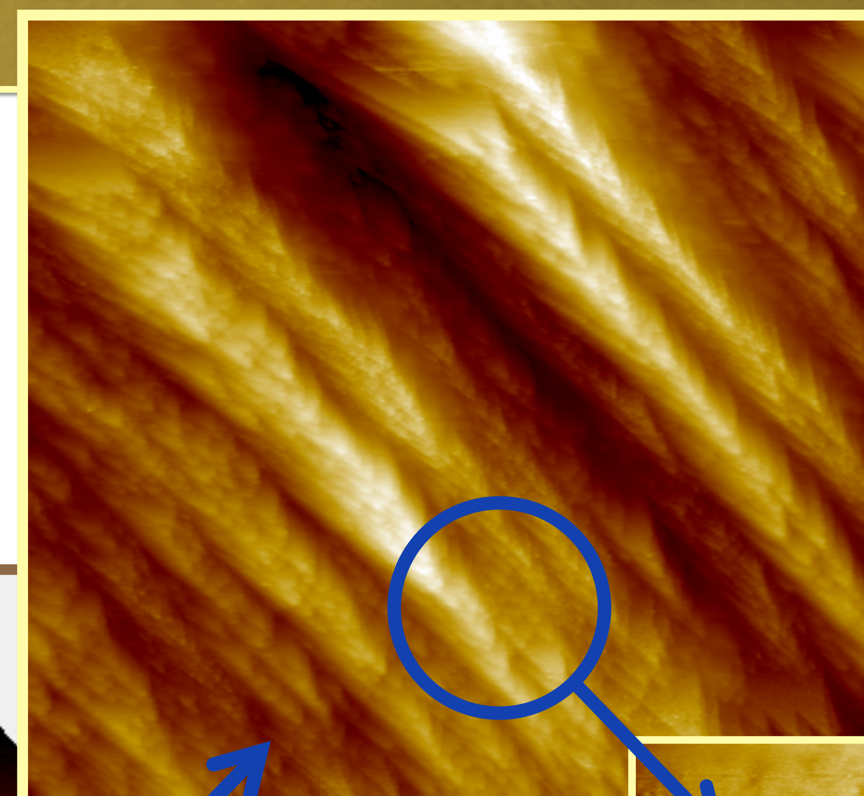
(111) plane



AFM image
30 x 30 µm

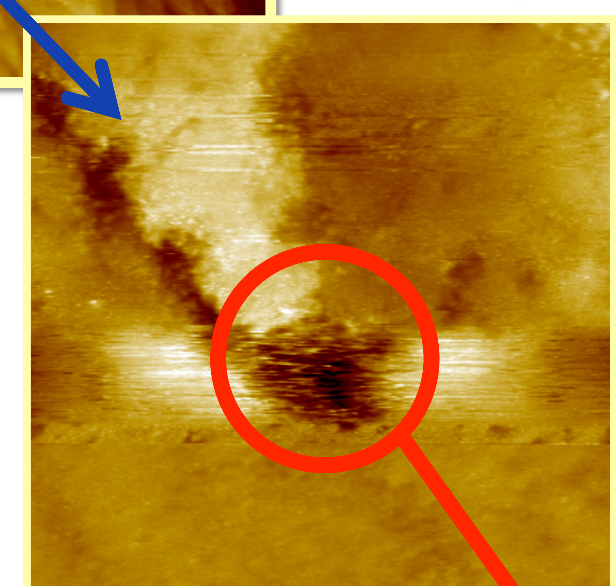


STM image
1.8 µm x 1.8 µm x 6 nm



STM image
3.1 µm x 3.5 µm x 5 nm

STM image 100 x 100 nm



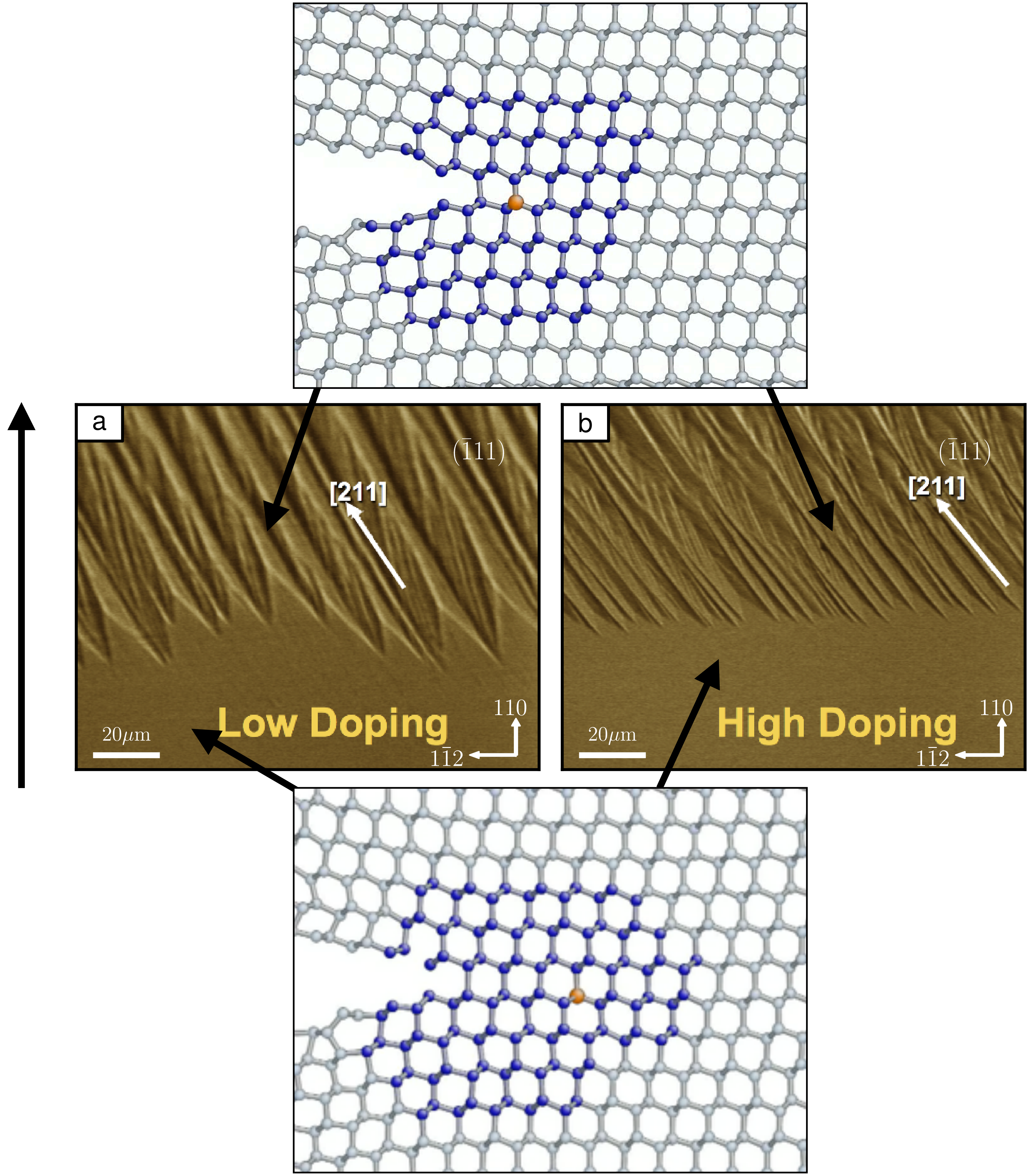
Atomic scale surface feature seen at perturbation edge

JR Kermode, L Ben-Bashat, F Atrash, JJ Cilliers, D Sherman and A. De Vita., Nat. Commun. 4 2441 (2013)

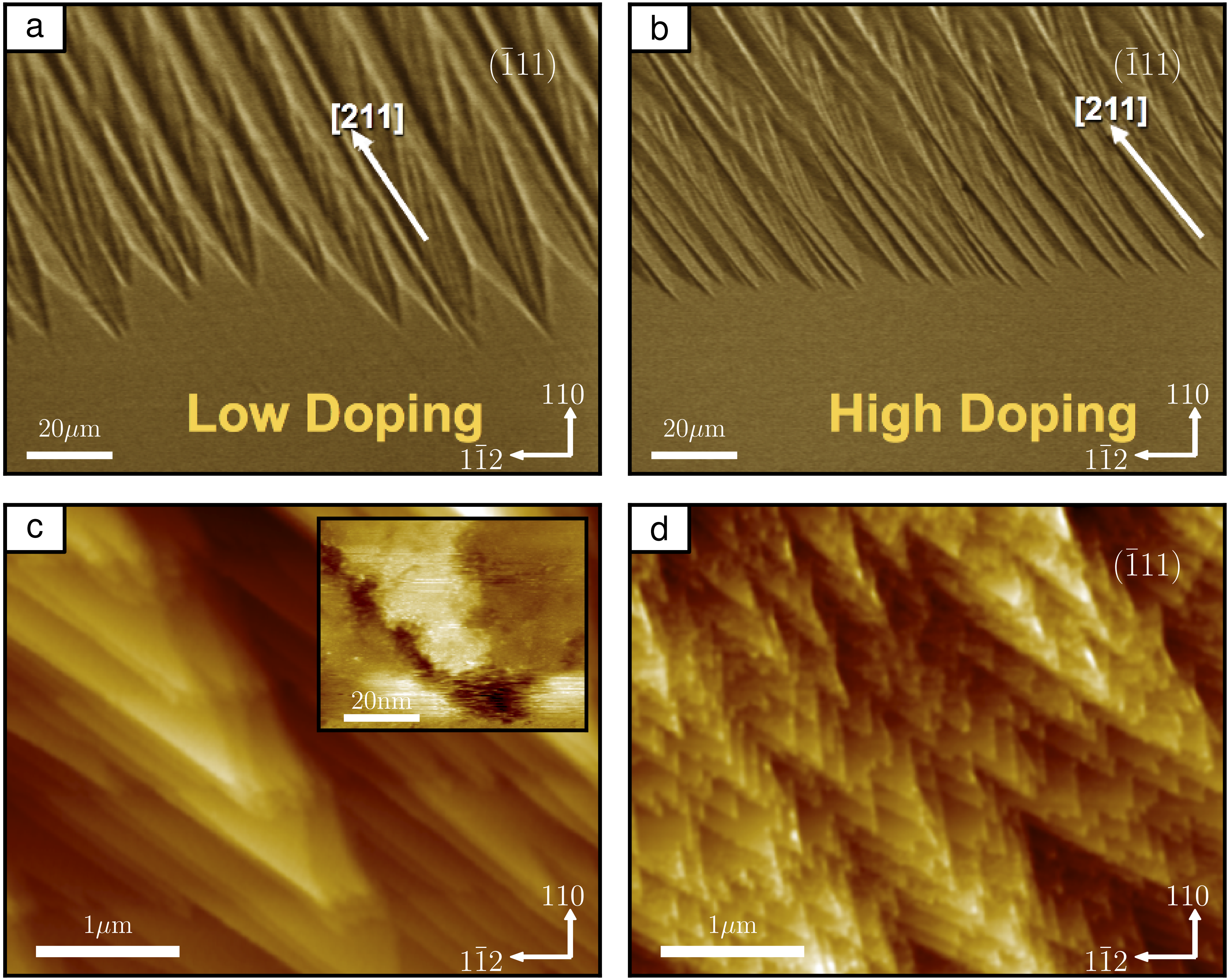
Crack propagation vs. chemical impurities – experiment and theory

Decreasing crack speed,

Increasing chance of interaction with B dopants



Interaction between crack tips and point defects – experiments

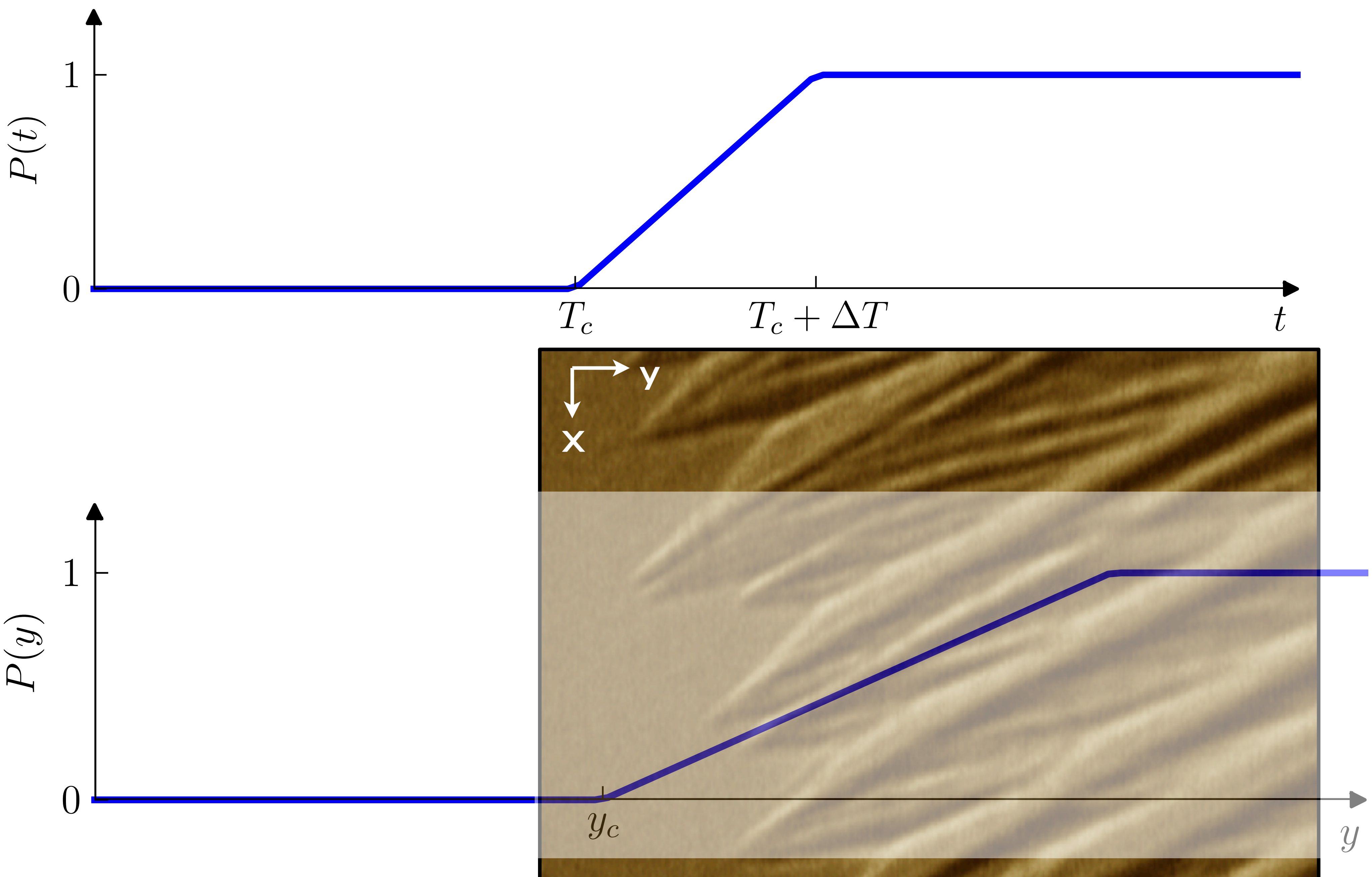


Interaction between crack tips and point defects – model

Going back to our DFT simulations, two time scales are important:

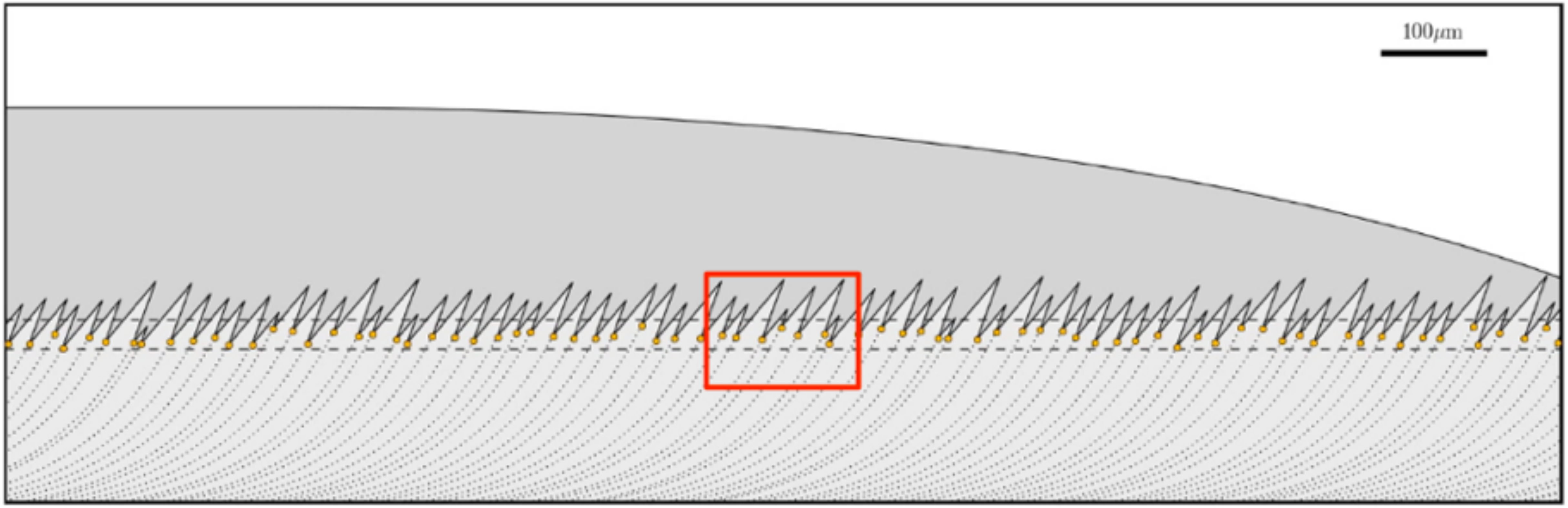
- Minimum time for deflection process to occur T_c
- Time for crack to advance by one bond a/v_c

T_c is 'blurred' by period ΔT of phonon mode that triggers deflection

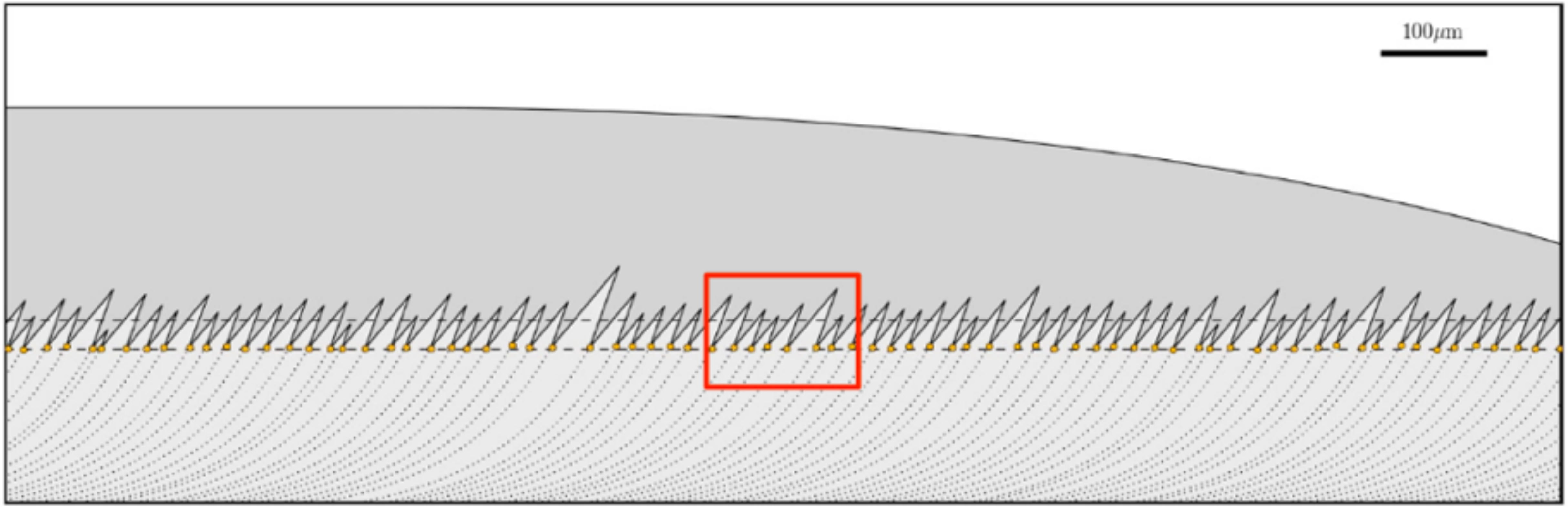


Interaction between crack tips and point defects – model

Low doping

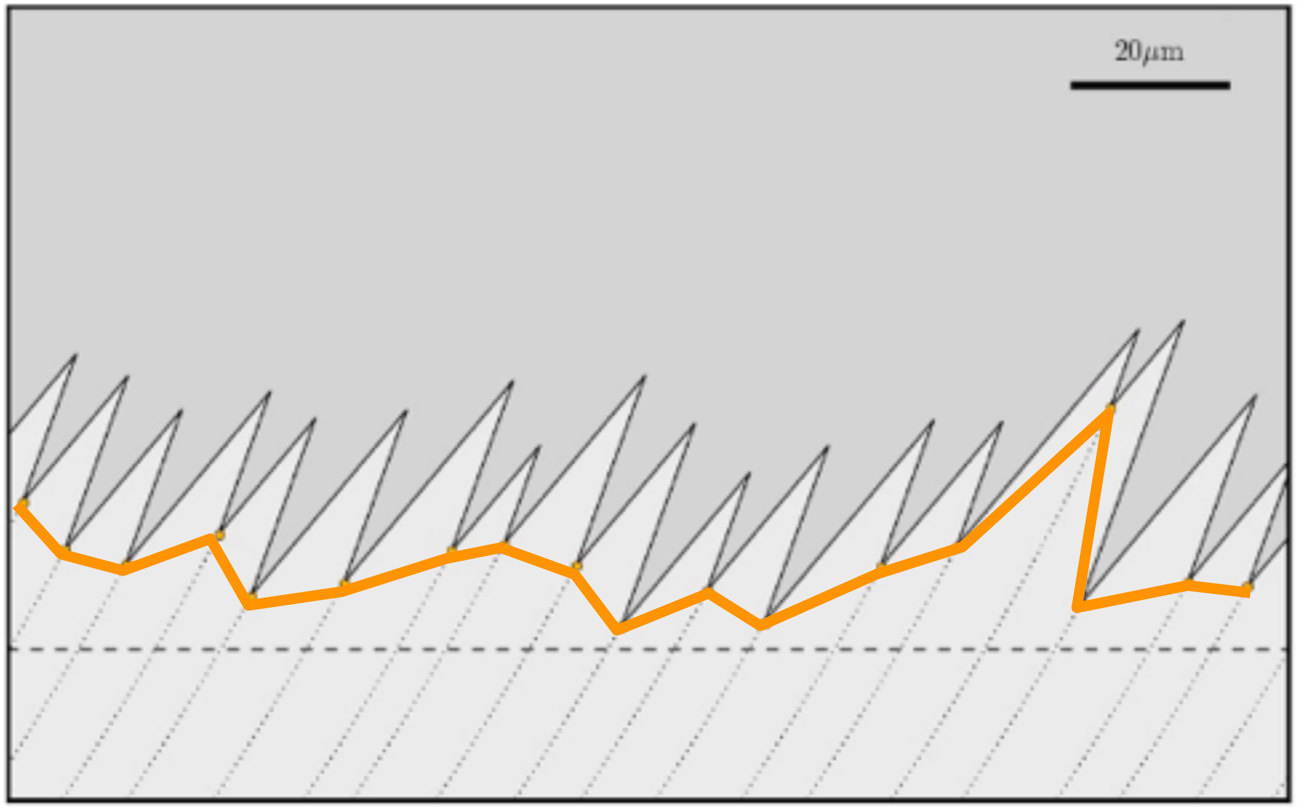


High doping



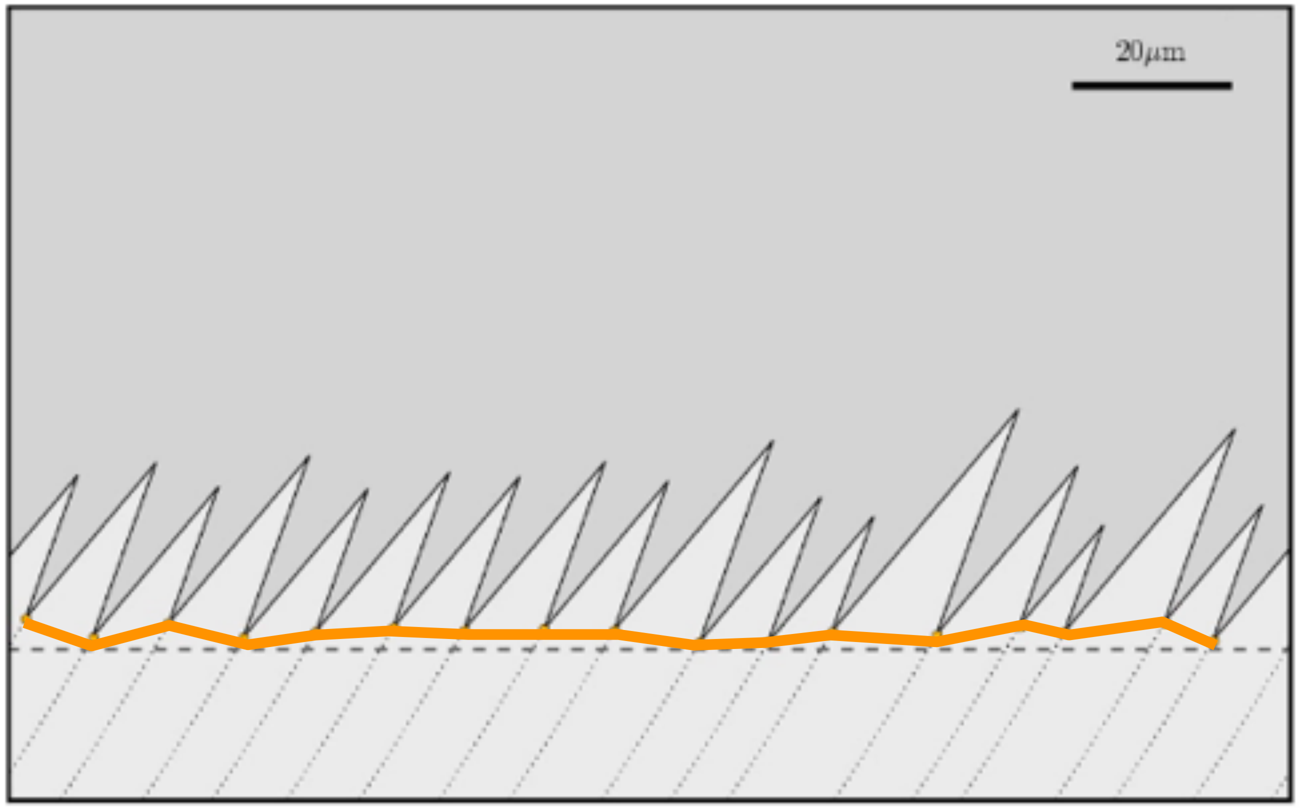
Crack propagation vs. chemical impurities – mesoscale model

Low doping



Roughness ~ 10 micron

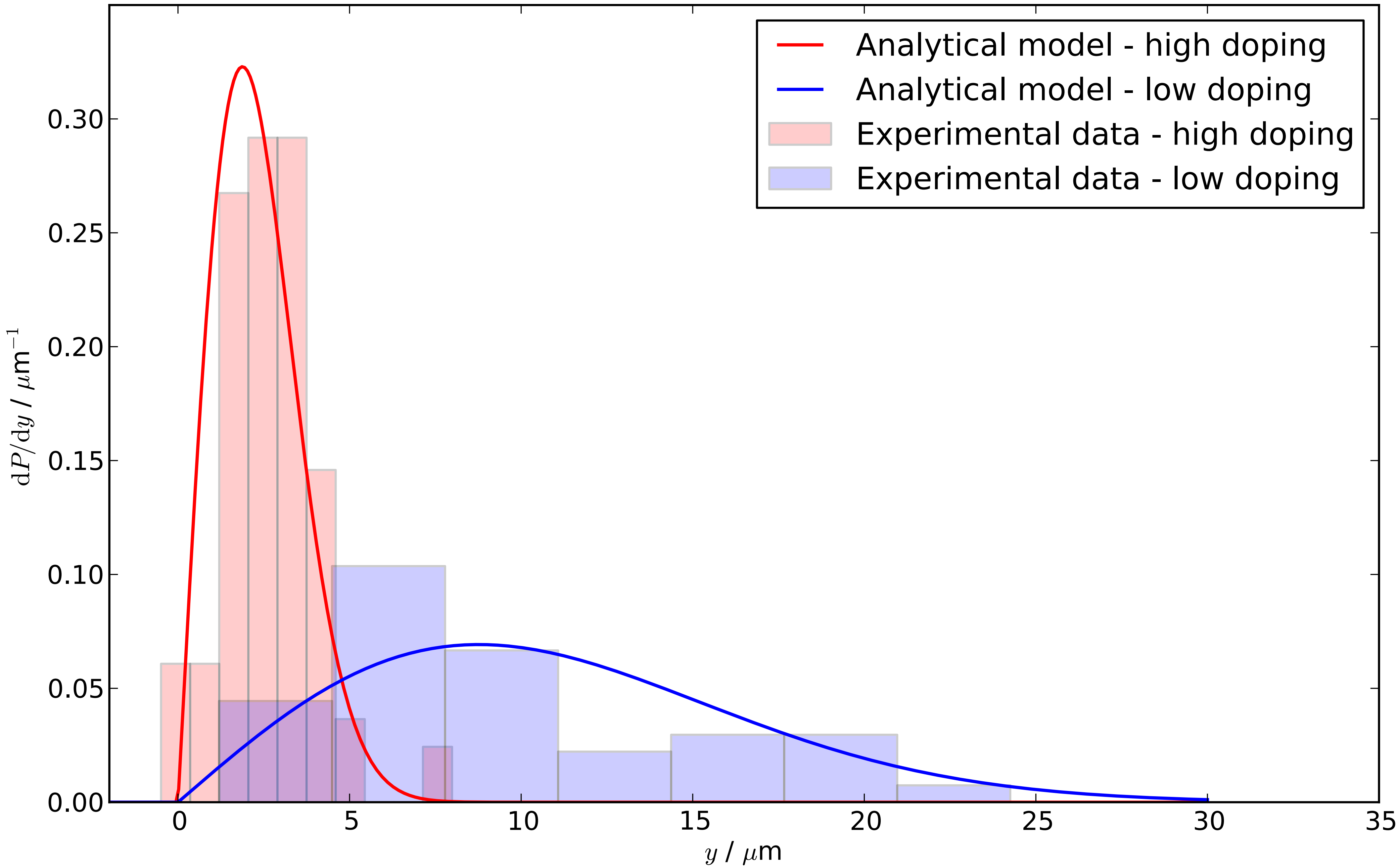
High doping



Roughness ~ 2 micron

JR Kermode, L Ben-Bashat, F Atrash, JJ Cilliers, D Sherman and A. De Vita., Nat. Commun. 4 2441 (2013)

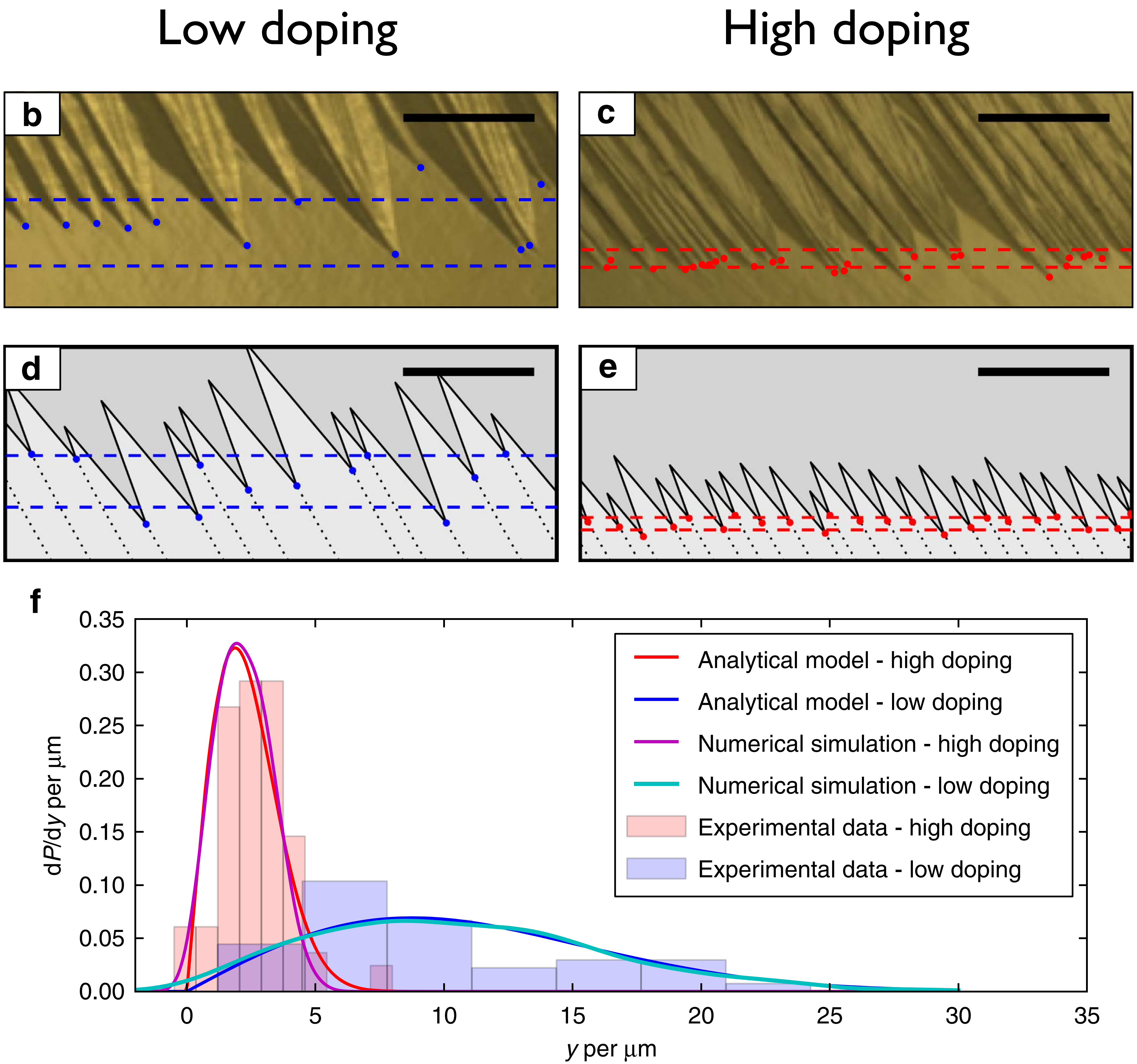
Interaction between crack tips and point defects – model *vs.* expt.



$$\frac{\mathrm{d}R}{\mathrm{d}y} = \frac{y}{\sigma^2} \exp\left(-\frac{y^2}{2\sigma^2}\right) \qquad \sigma = \sqrt{\frac{\Delta T v_c^3}{\alpha n' a g}}$$

JR Kermode, L Ben-Bashat, F Atrash, JJ Cilliers, D Sherman and A. De Vita., Nat. Commun. 4 2441 (2013)

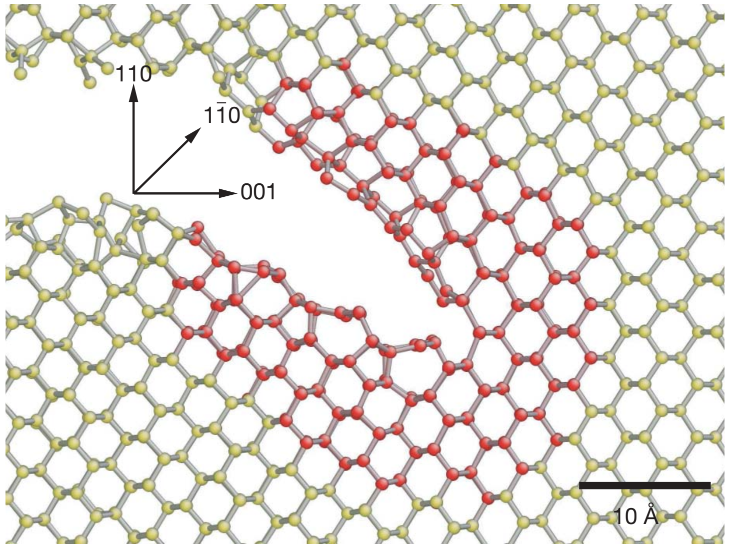
Crack propagation vs. chemical impurities – experiment and theory



JR Kermode, L Ben-Bashat, F Atrash, JJ Cilliers, D Sherman and A. De Vita., Nat. Commun. 4 2441 (2013)

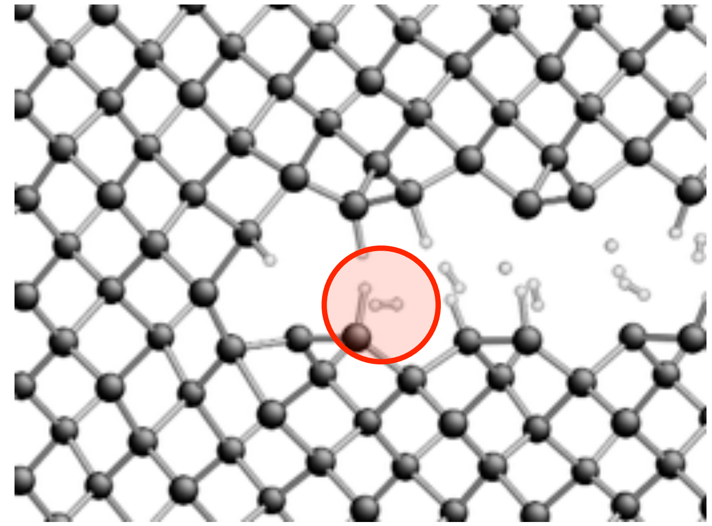
Overview of Fracture Modelling Applications

Dynamical instabilities in Si



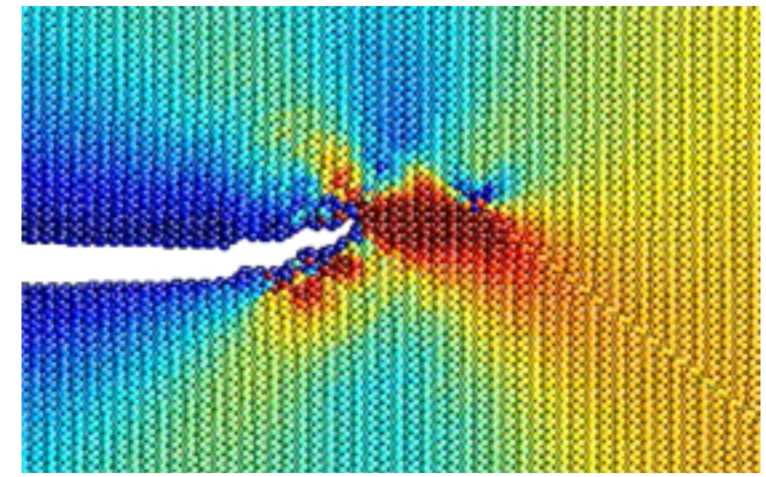
JR Kermode *et. al.*
Nature **455** 1224 (2008)

H induced 'SmartCut'



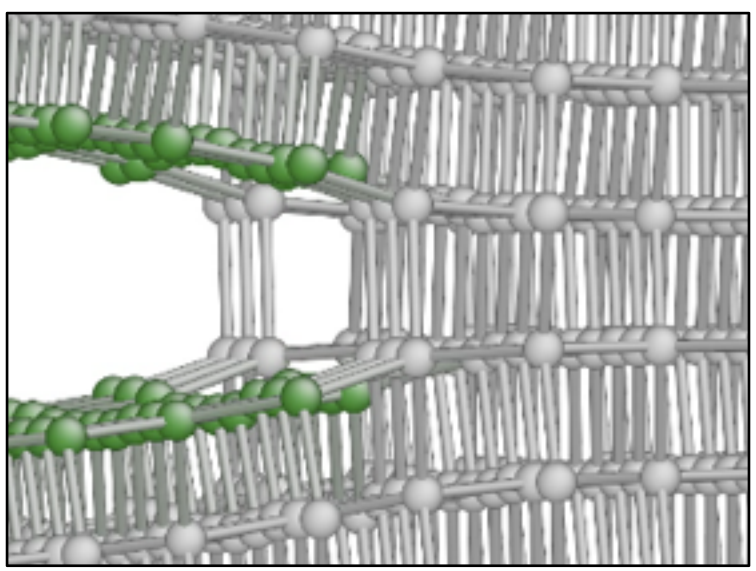
G Moras *et al.* Phys. Rev. Lett.
105, 075502 (2010)

Crack-dislocation interactions



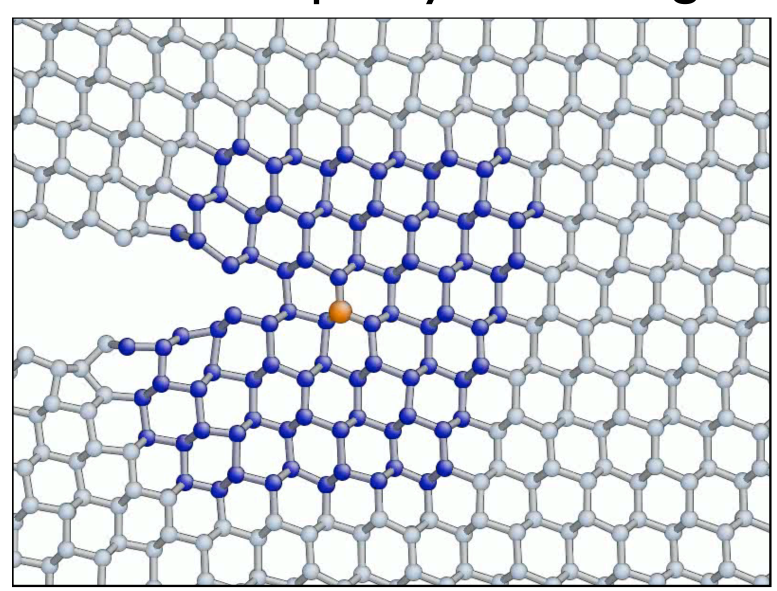
C Gattinoni, JR Kermode and
A De Vita, *In prep* (2014)

Three dimensional effects



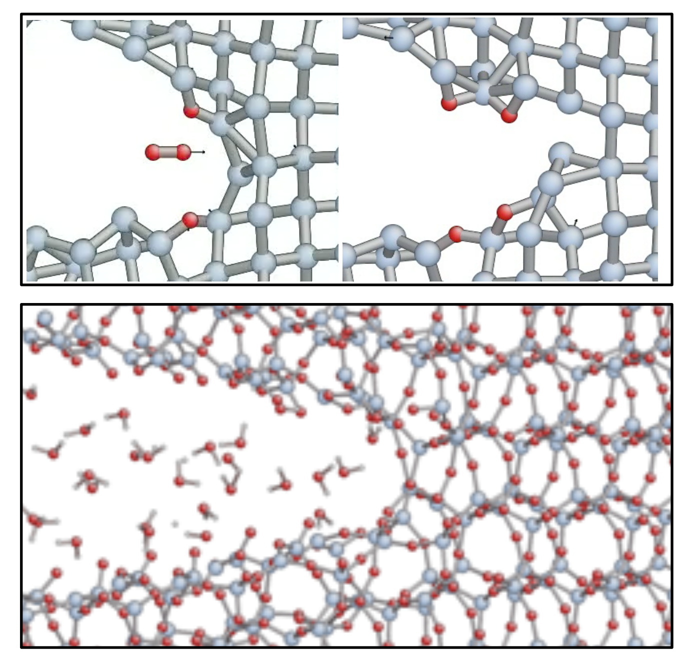
JR Kermode, A. Glazier, G Csányi,
D Sherman and A De Vita, *In prep* (2014)

Crack-impurity scattering



JR Kermode, L Ben-Bashat, F Atrash,
JJ Cilliers, D Sherman and A. De Vita.,
Nat. Commun. **4** 2441 (2013)

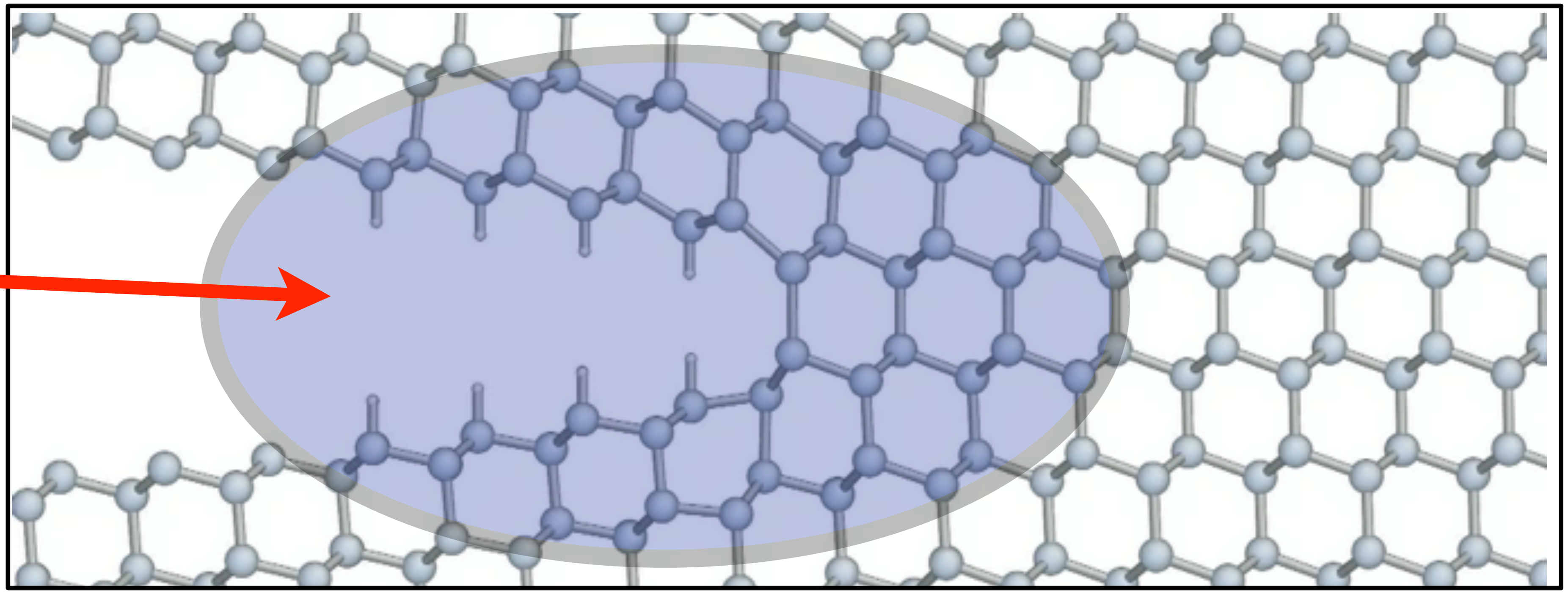
Stress corrosion cracking

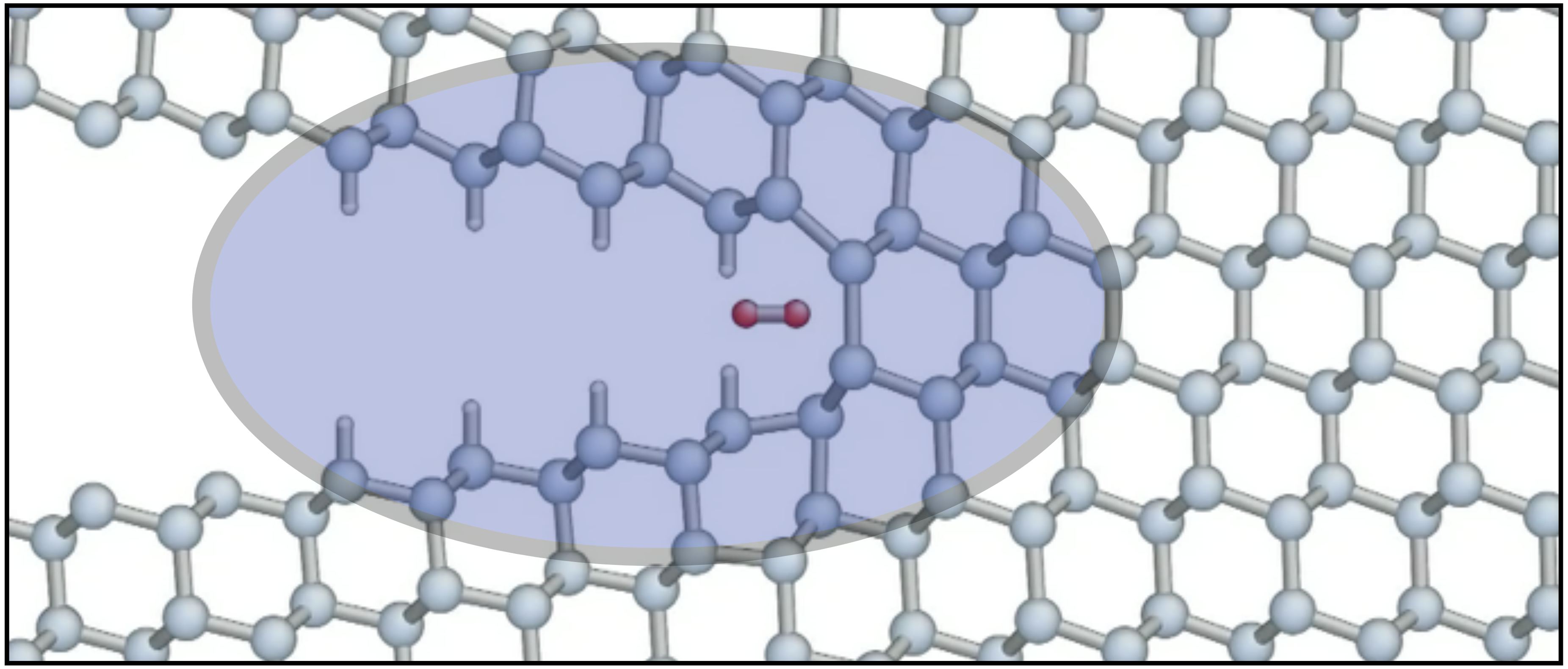


A Glazier, G Peralta, JR Kermode,
A De Vita and D Sherman, Phys. Rev. Lett,
112 **115501 (2014).**

Stress corrosion cracking – silicon (111) surface

- Si(111), sub-critical loading $G = 2.70$ J/m^2 $< G_c = 2.88$ J/m^2
- QM (DFT) region: ~200 atoms
- Crack is lattice trapped at 300 K

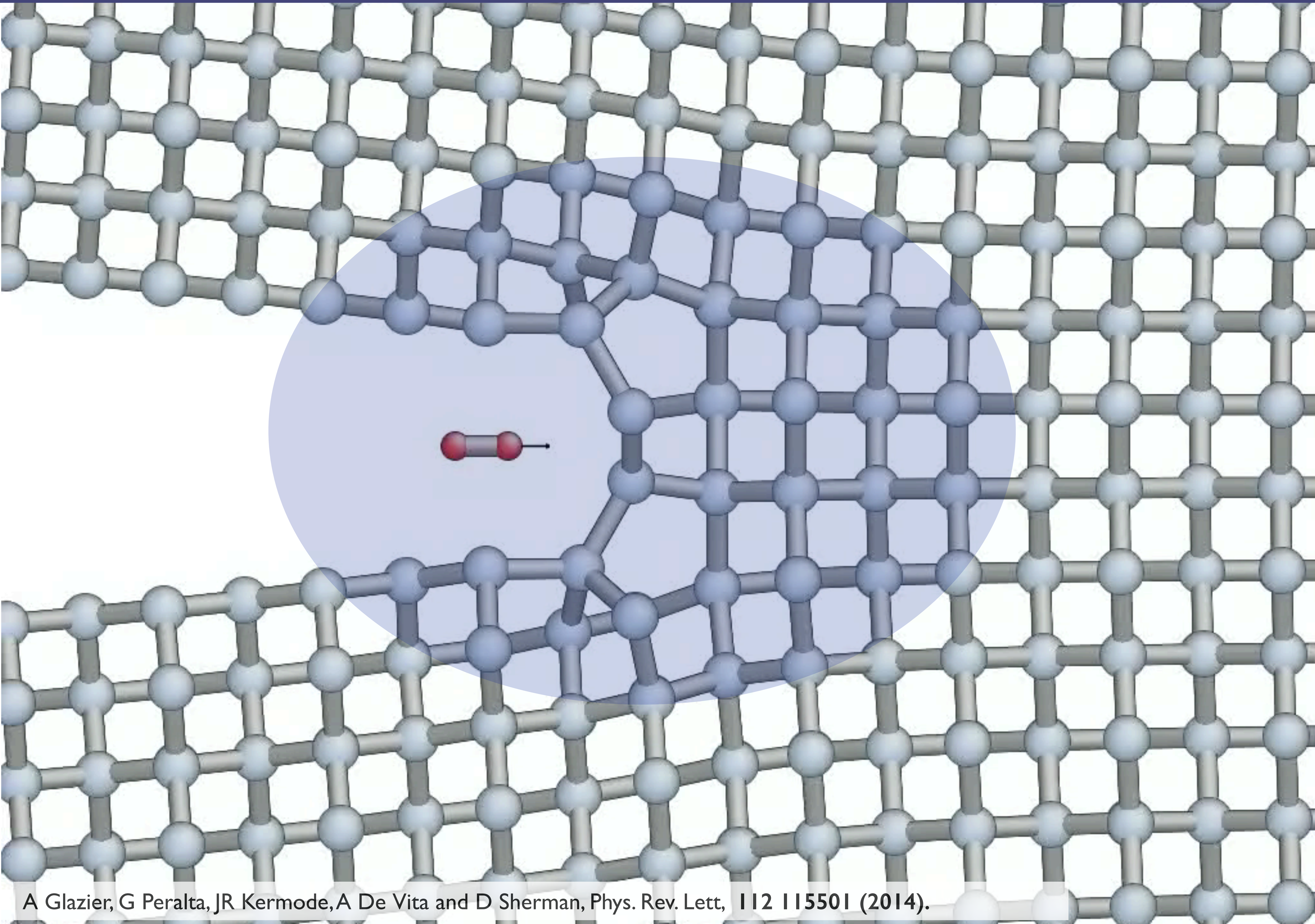




- Add O_2: dissociates, providing enough heat to break one Si–Si bond
- Diffusion limited regime: oxygen supply controls crack speed

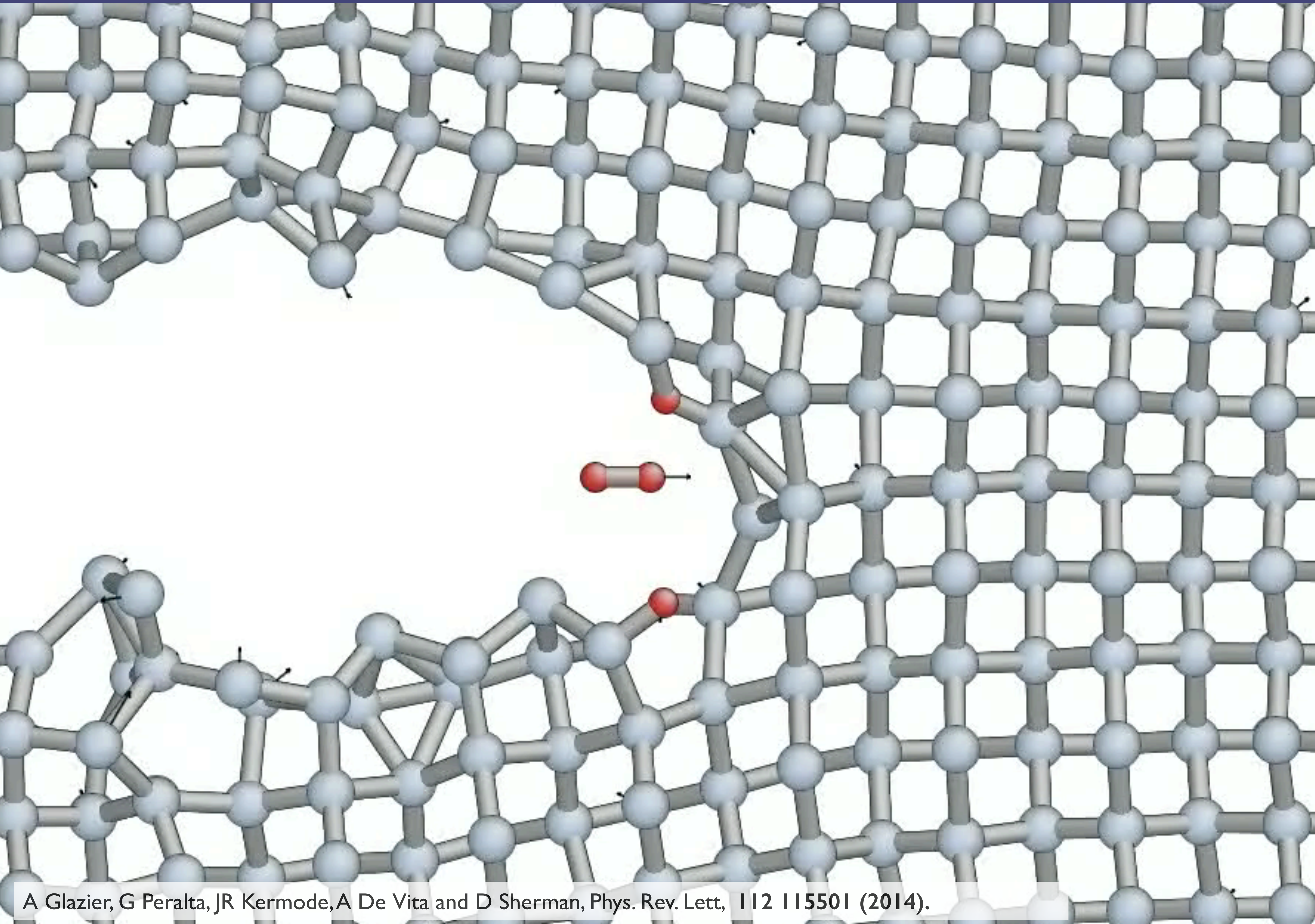
A Glazier, G Peralta, JR Kermode, A De Vita and D Sherman, Phys. Rev. Lett, **112 115501 (2014).**

Stress corrosion cracking – simulations



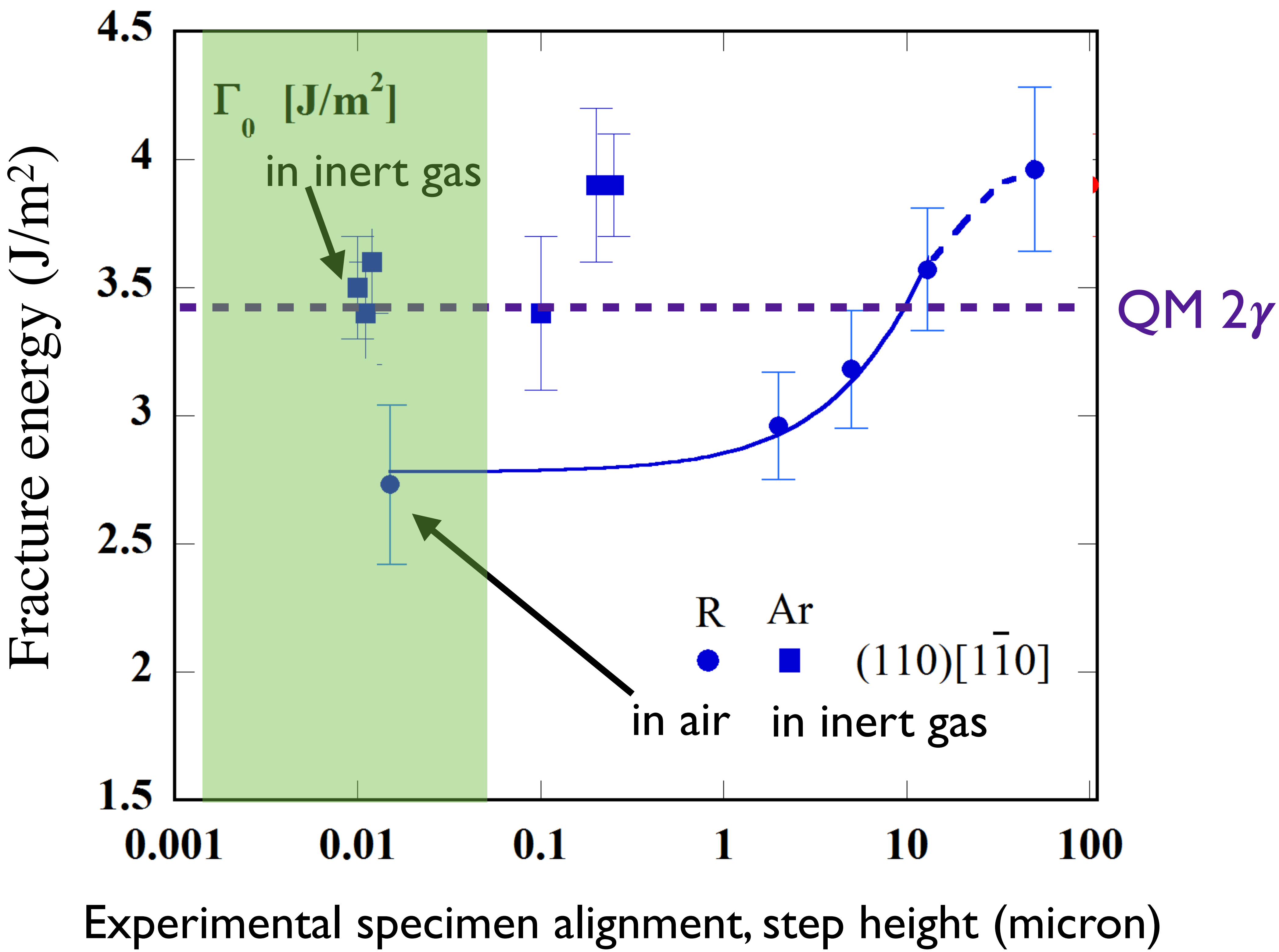
A Glazier, G Peralta, JR Kermode, A De Vita and D Sherman, Phys. Rev. Lett, **112 115501 (2014).**

Stress corrosion cracking – simulations



A Glazier, G Peralta, JR Kermode, A De Vita and D Sherman, Phys. Rev. Lett, **112 115501 (2014).**

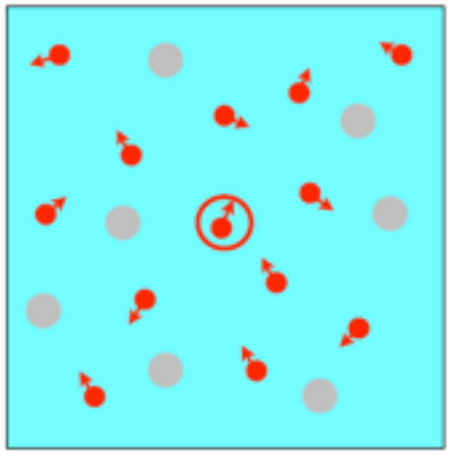
Stress corrosion cracking – experiments



A Glazier, G Peralta, JR Kermode, A De Vita and D Sherman, Phys. Rev. Lett, **112 115501 (2014).**

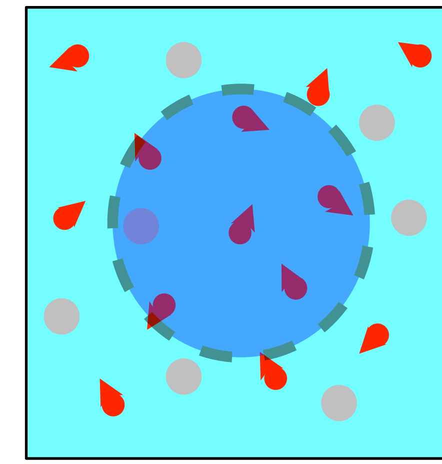
Fracture of quartz – polarisable potential and QM/MM

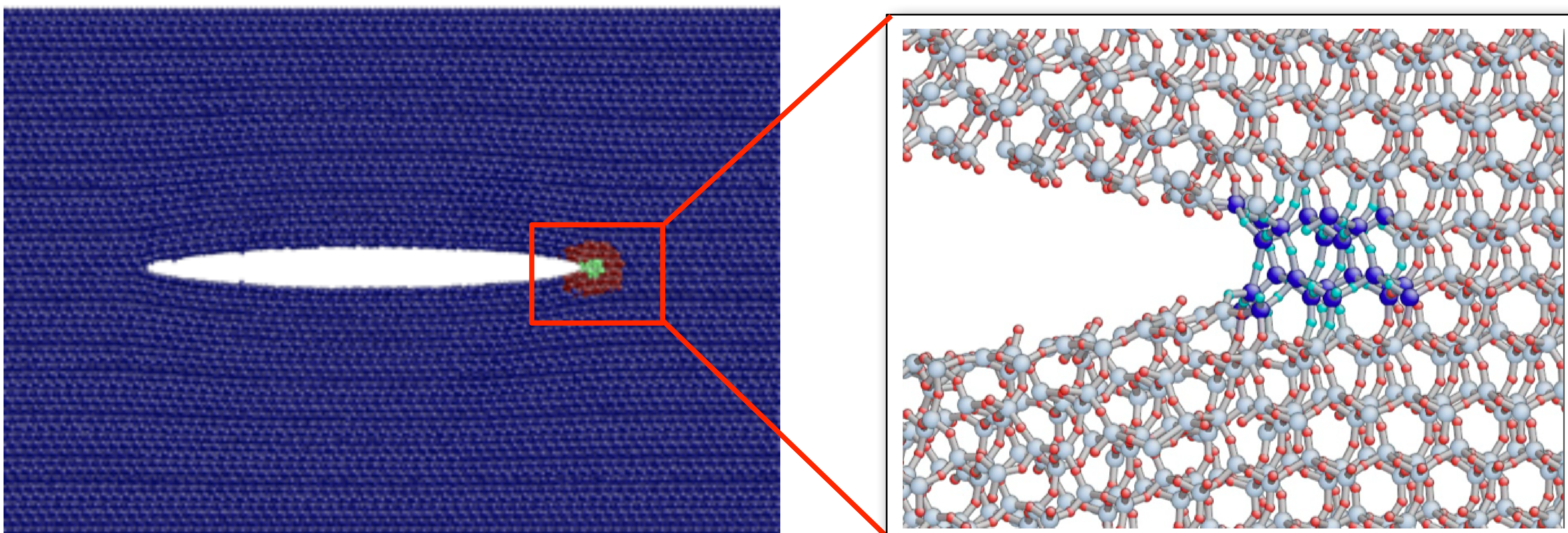
Starting point: Tangney-Scandolo interatomic potential with self-consistent dipoles



$$\mathbf{p}_i = \alpha_i \mathbf{E}_i \left(\{\mathbf{r}_j\}, \{\mathbf{p}_j\} \right)$$

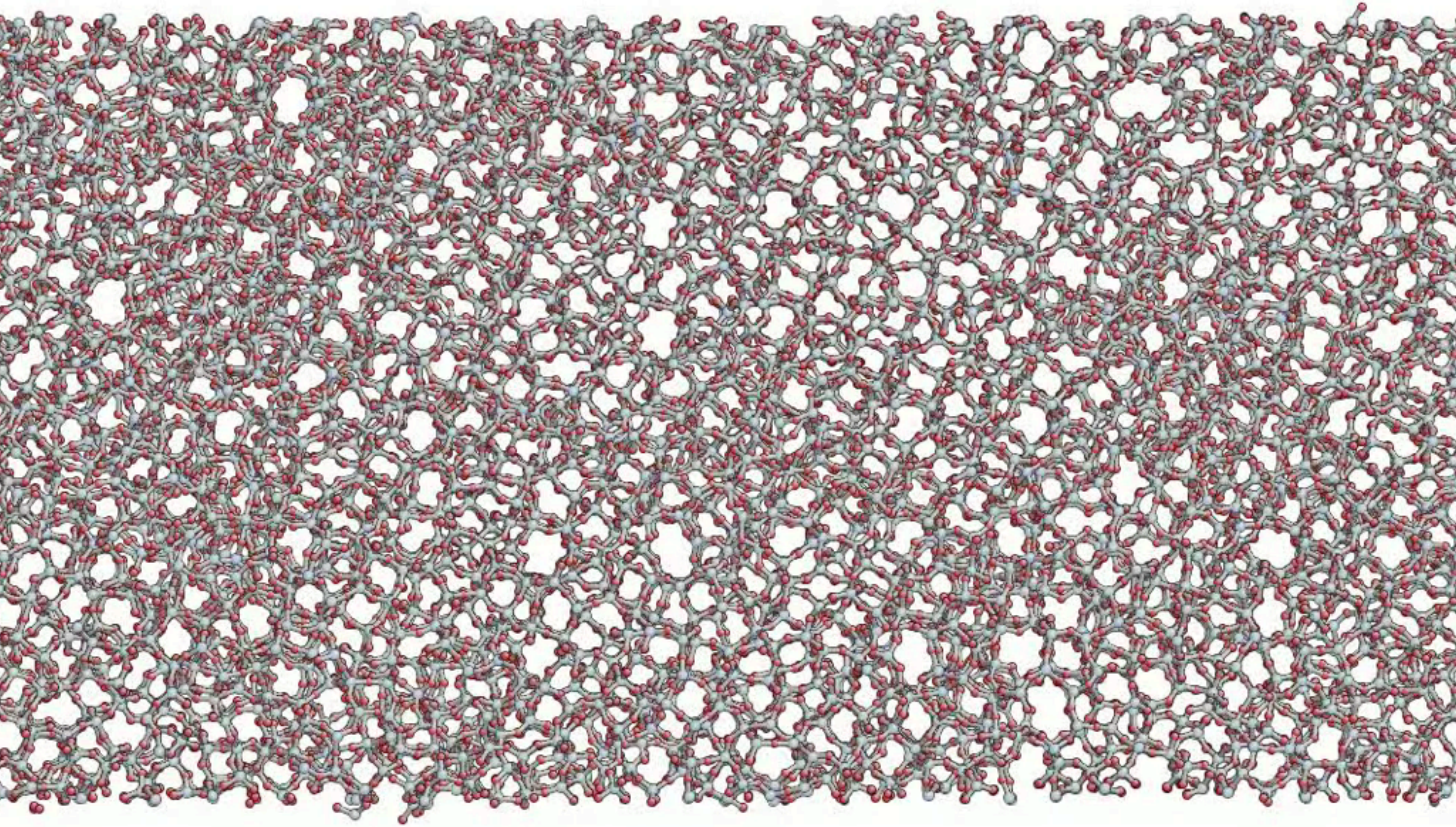
Short range (Yukawa): $\frac{q_i q_j}{r_{ij}} \rightarrow \frac{q_i q_j}{r_{ij}} e^{-\alpha r}$



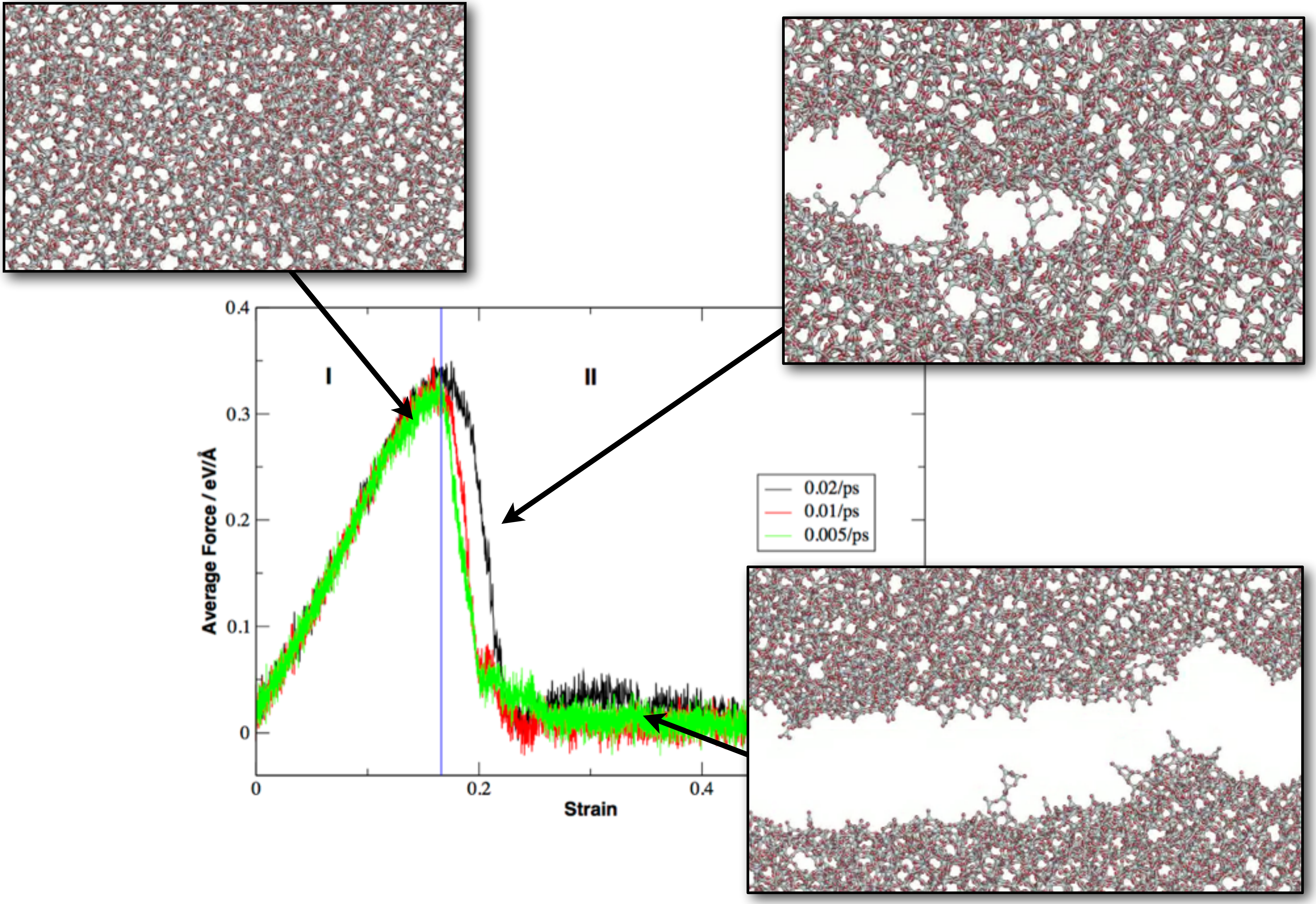


JR Kermode *et al*, J. Chem. Phys. **133** 094102 (2010)

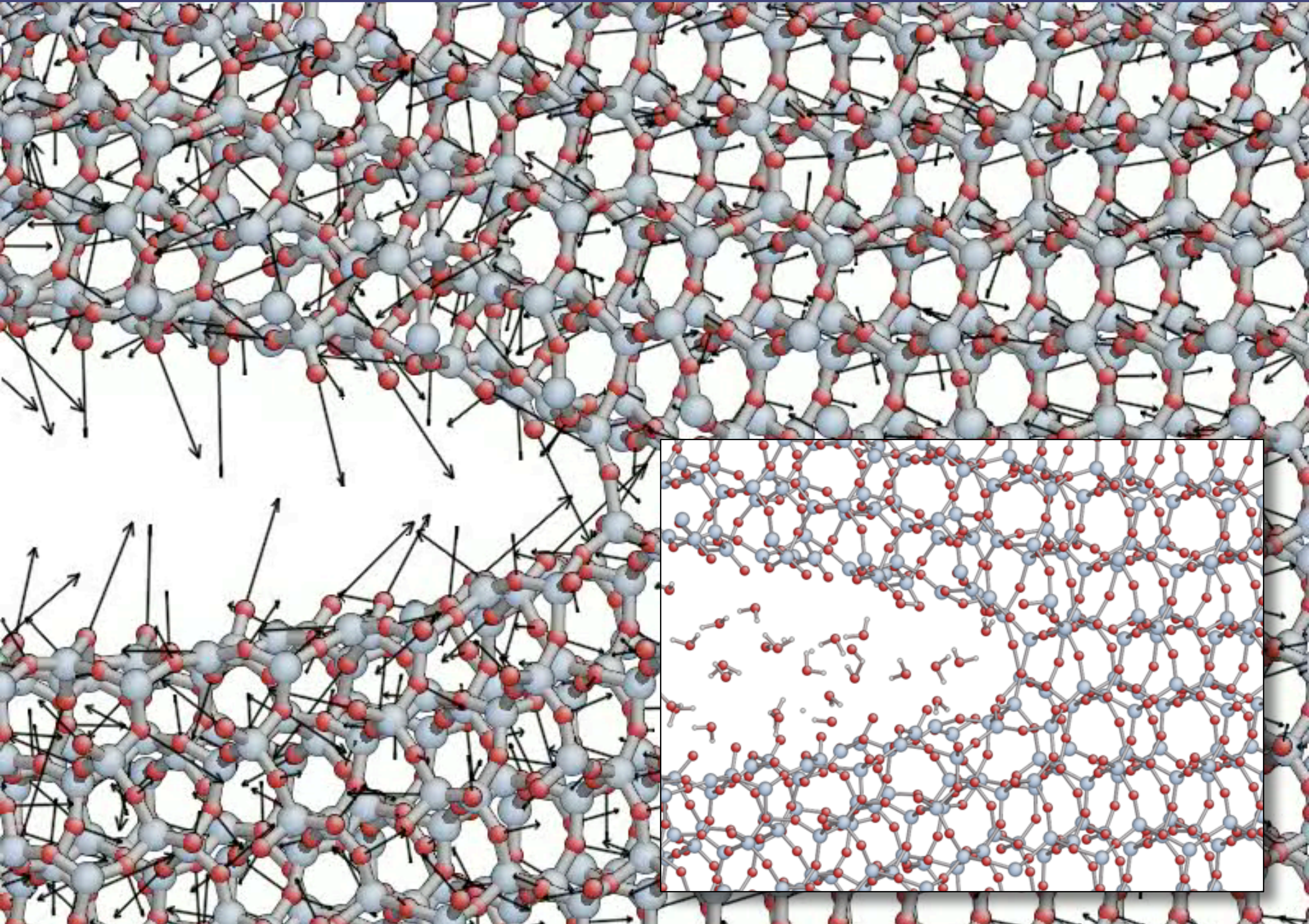
Stress response of amorphous silica to applied strain



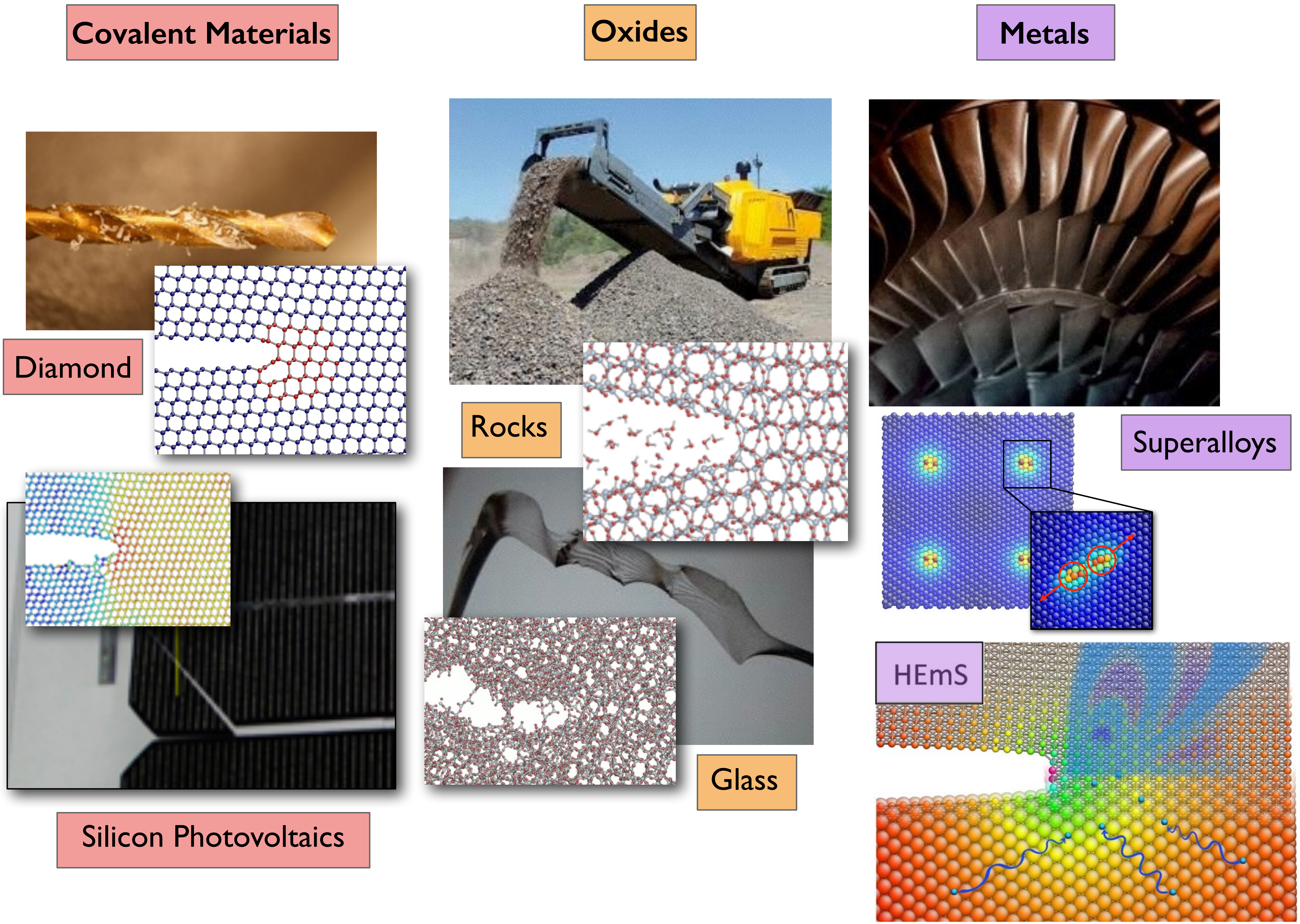
Stress response of amorphous silica to applied strain



QM-based simulations of brittle fracture in quartz



Multiscale Modelling of "Chemomechanical" Materials Failure Processes



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Fouad Atrash, Liron Ben Bashat, Anna Glazier and Dov Sherman

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Noam Bernstein

Tristan Albaret

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