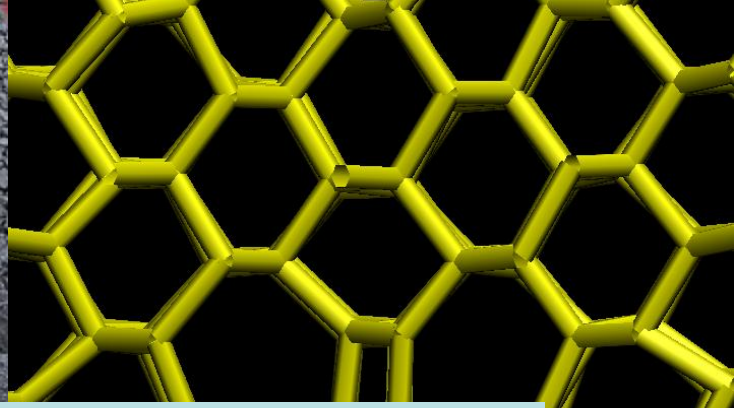
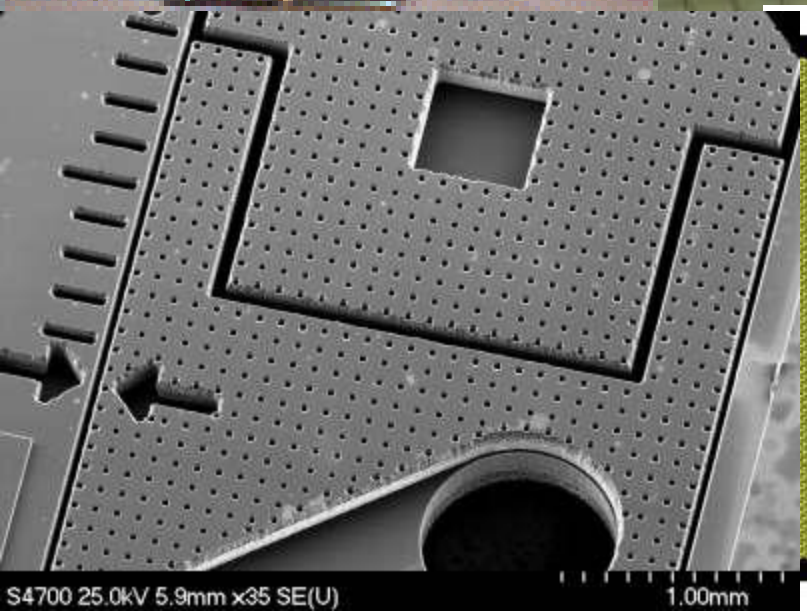
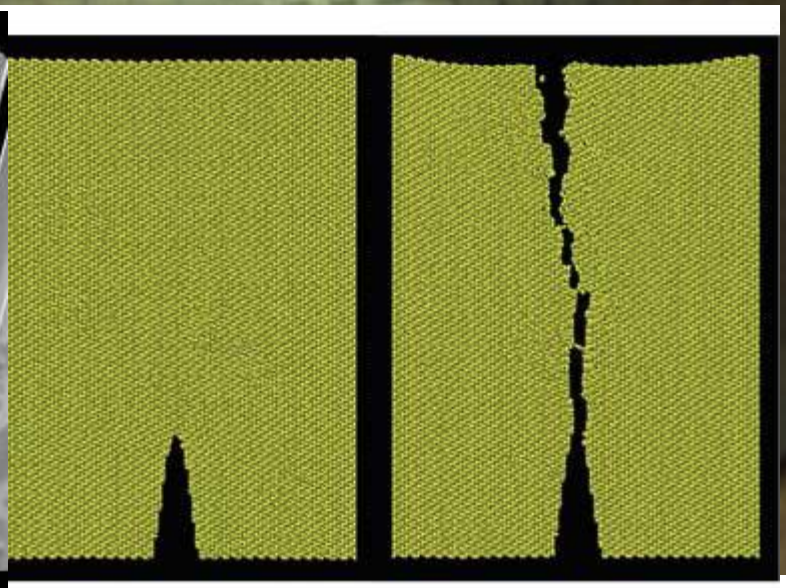


Atomistic- and Multiscale Modeling of Materials Failure

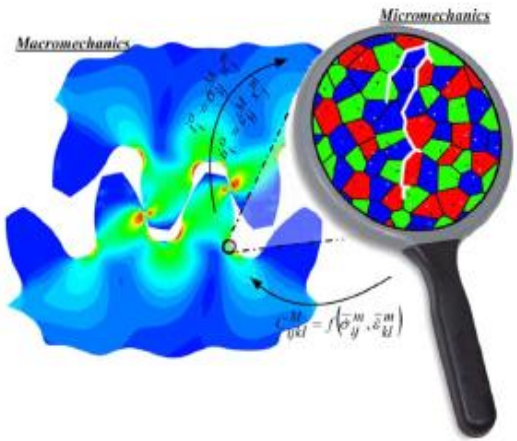
Christian Thaulow,

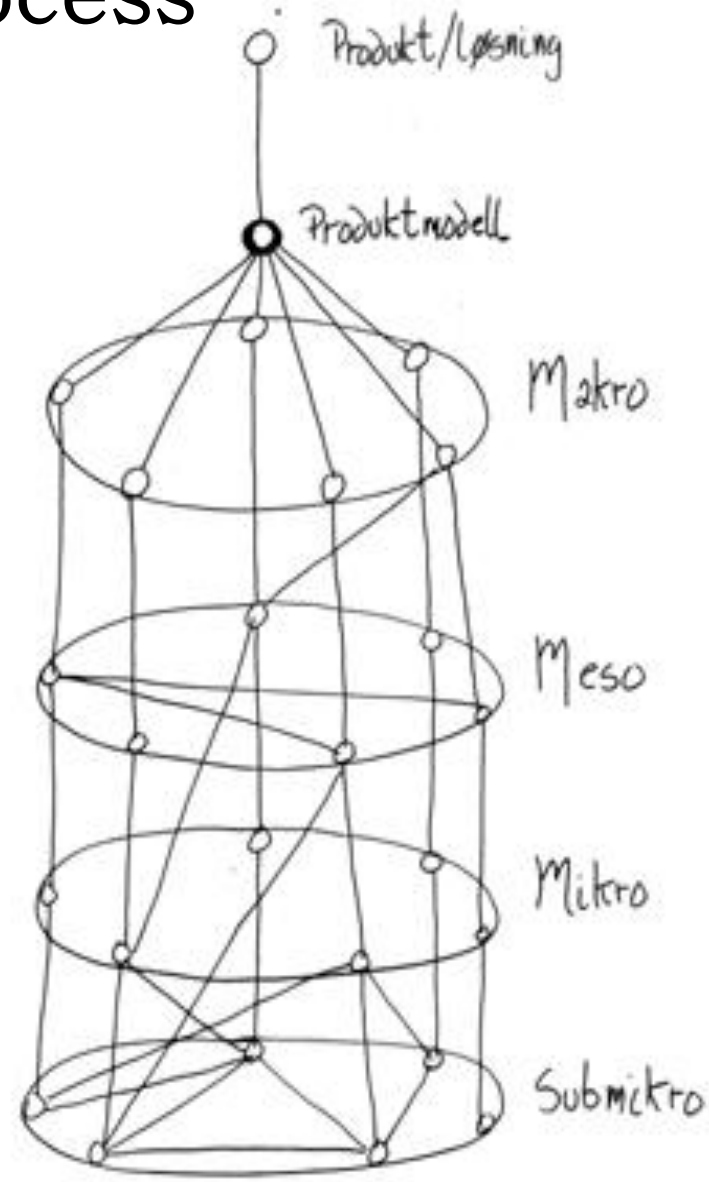
Dept Engineering Design and Materials, NTNU, Norway





Material optimization process





All knowing depends on the structure of the knower

We do not see that we do not see

Fracture Mechanics Historical Development

continuum mechanics → **FEM** → **multiscale modeling**

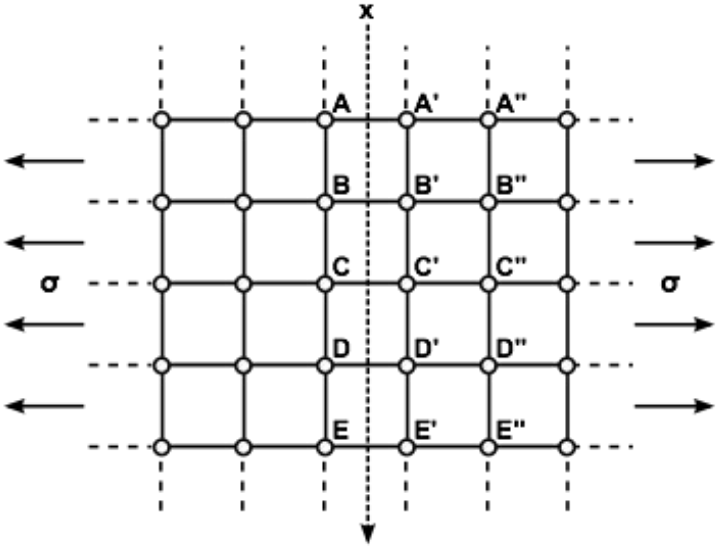
K - CTOD

crack growth **constraint** **nano**

G - J

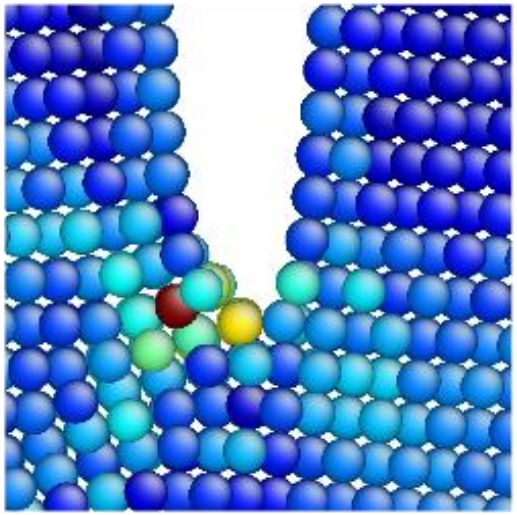
single parameter → **two-parameter** → **many parameters**

from atomistic view



1920

to atomistic modeling



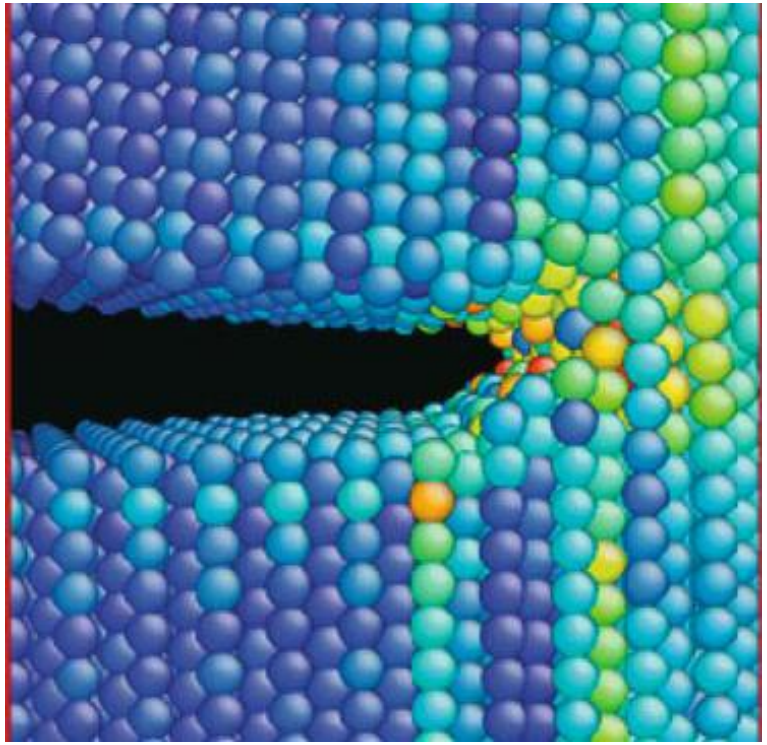
2010

1 000 000 000 000 000 000

From LARGE Scale testing: 100MN and 10 minutes

to

Atomistic Mechanics: 10pN and 1 femtosecond



Laboratory for Atomistic and Molecular Mechanics (LAMM)

Markus J. Buehler

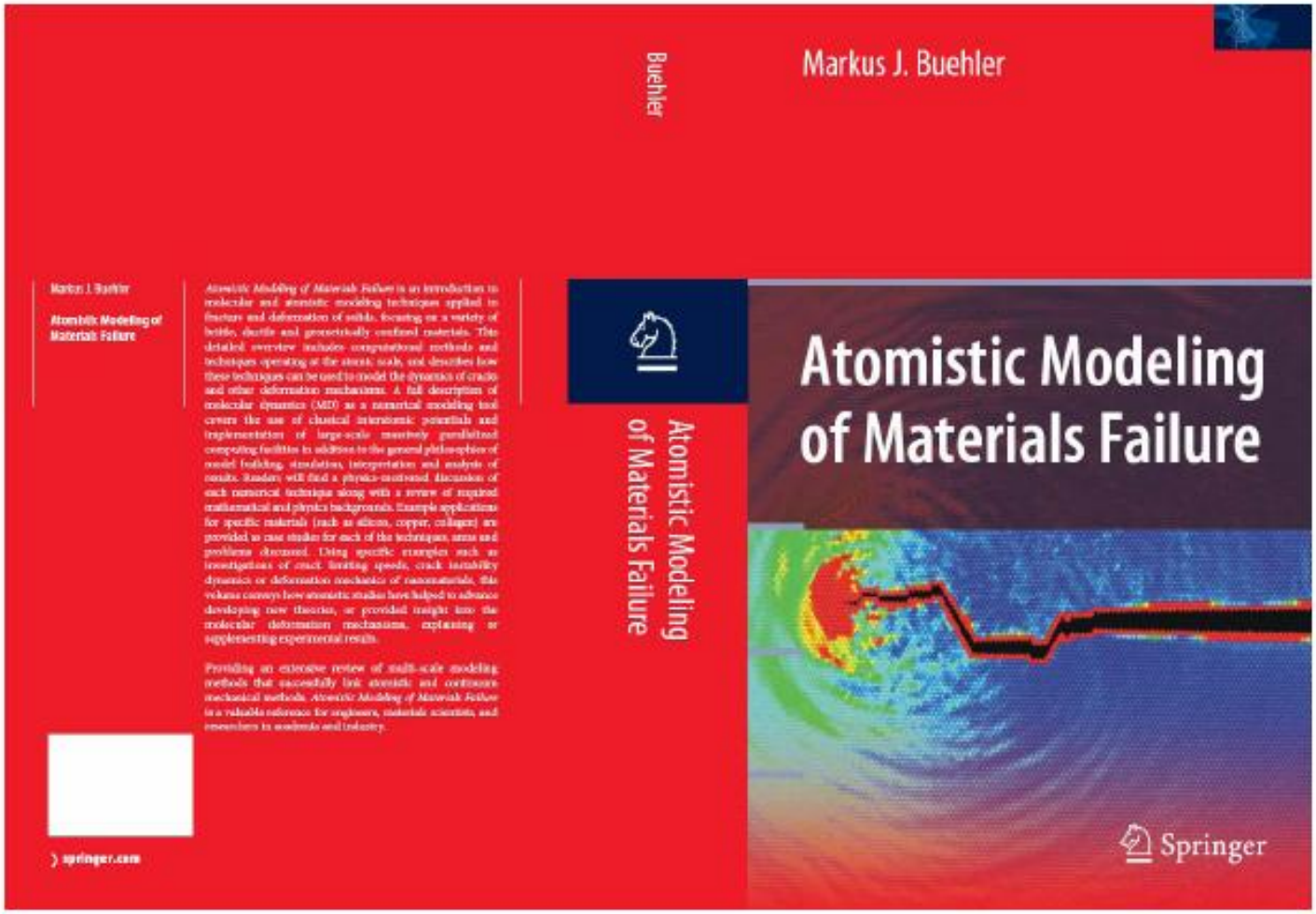
PI, Laboratory for Atomistic and Molecular Mechanics Department of Civil and Environmental Engineering
Massachusetts Institute of Technology

E-mail: mbuehler@MIT.EDU

URL: http://web.mit.edu/mbuehler/www/

Massachusetts Institute of Technology

1.545 – Atomistic Modeling and Simulation of Materials and Structures



Visions for the future…

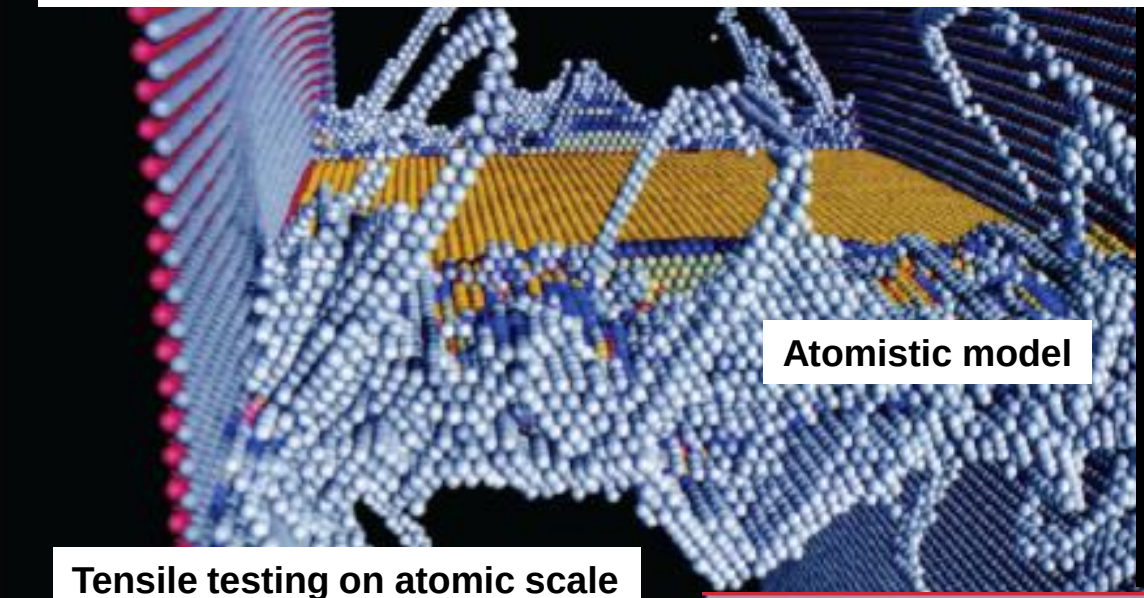
Marcus Buehler

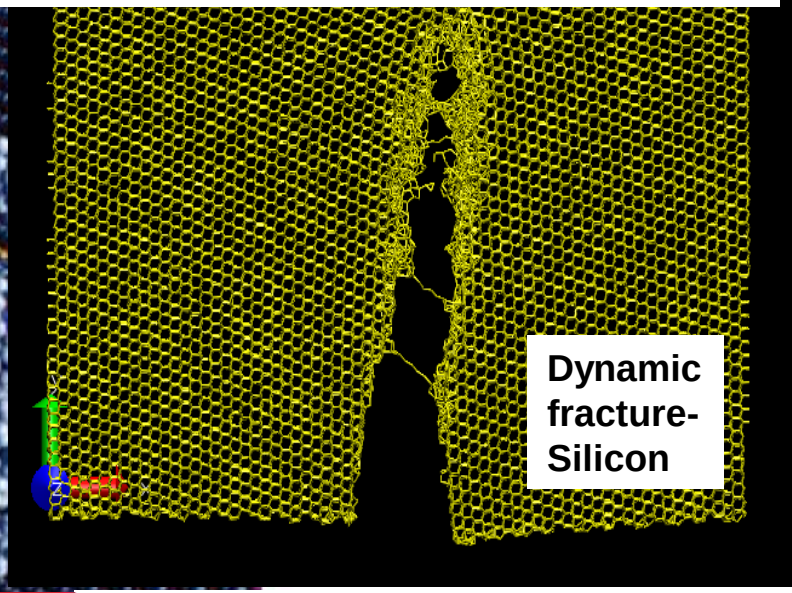
- **Atomistic simulations in material design becomes normal**
- **The next generation of CAE software will integrate nano and micro structures**
- **Concurrent multi-field variational FEM equations that couple nano and micro structures and continuum.**
- **A predictive multiscale constitutive law that bridges nano and micro structures with the continuum concurrently via statistical averaging and monitoring the microstructure/defect evolutions (i.e., manufacturing processes).**
- **Improved methods for the hierarchical and concurrent analyses**
- **Probabilistic simulation-based design techniques enabling even more realistic simulations**
- **..**

Want to learn how to design tomorrows materials?
Did you know that it can be done with nanoscience and a computer?

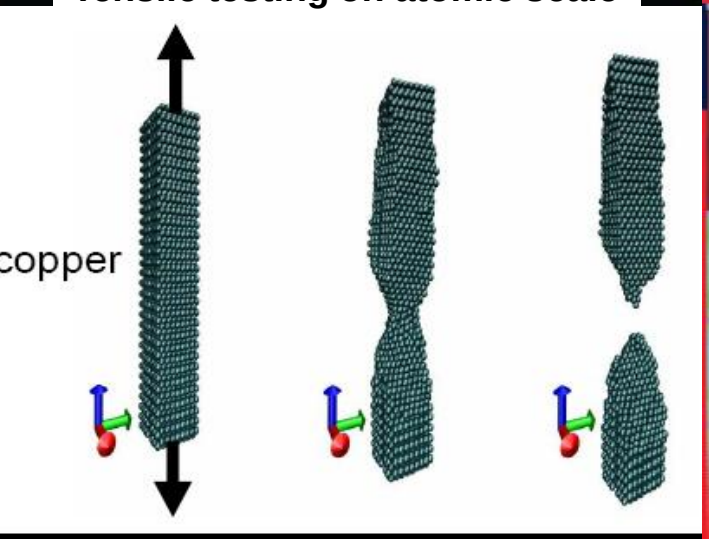
TMM4162/MM8406 - Atomistic Modeling of Materials Failure

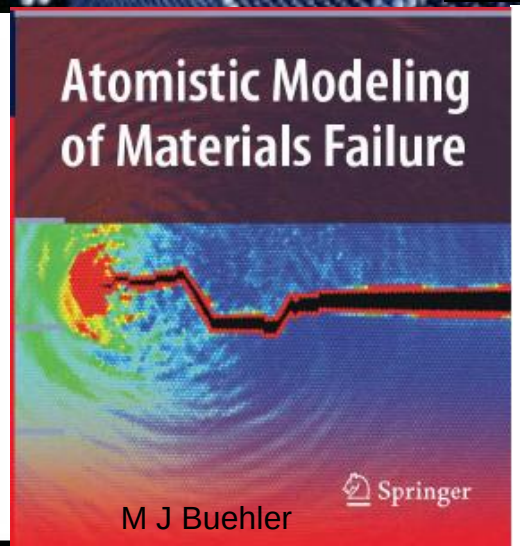
New from spring 2010

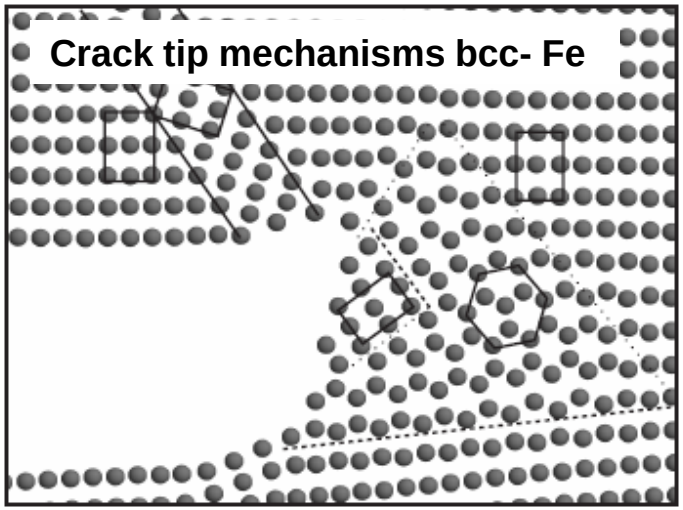




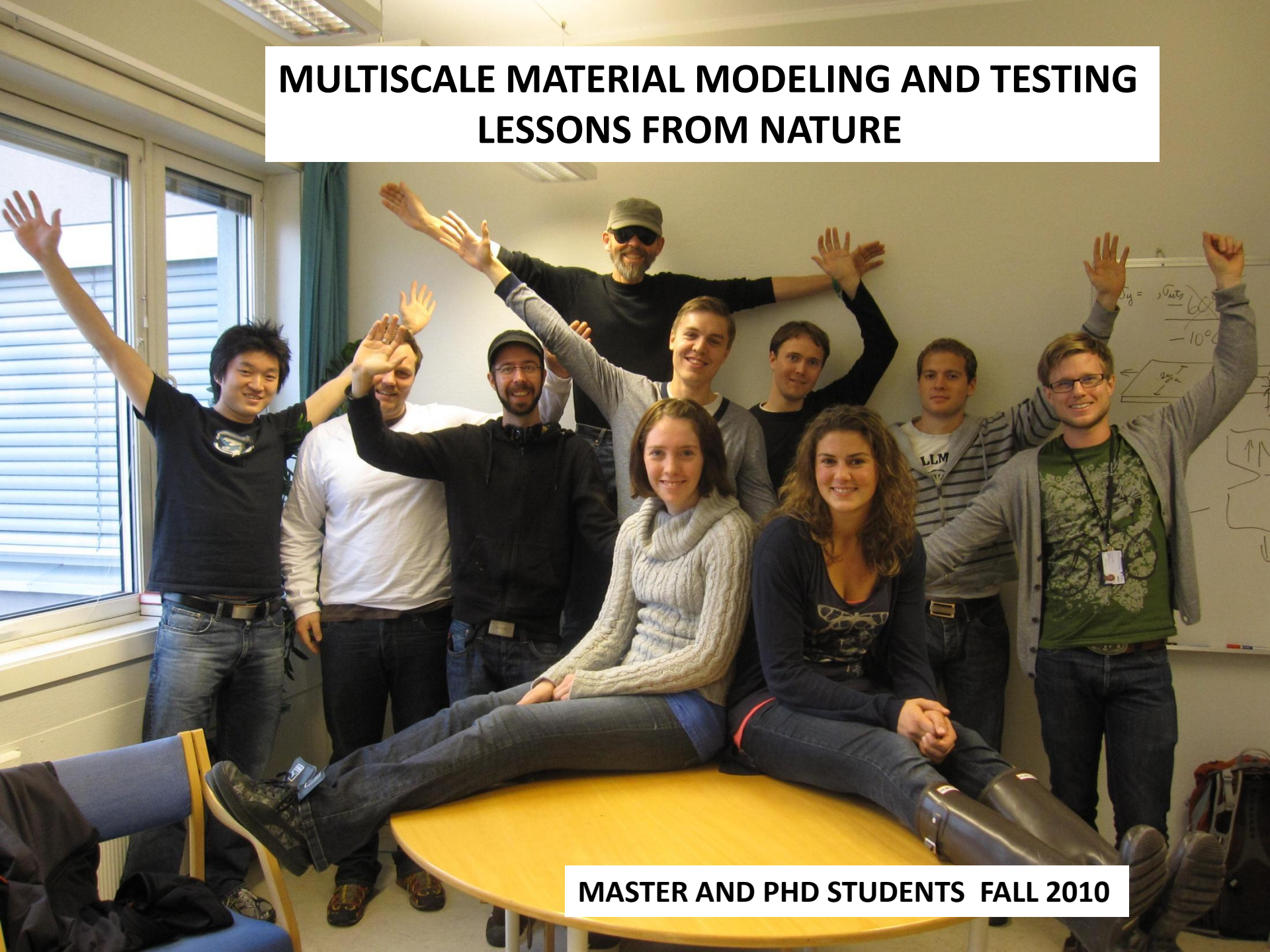
Tensile testing on atomic scale







MULTISCALE MATERIAL MODELING AND TESTING
LESSONS FROM NATURE



MASTER AND PHD STUDENTS FALL 2010

Research group at NTNU

Atomistic and Multiscale Material Modeling and Testing

NTNU Department of Engineering Design and Materials

Christian Thaulow – Atomistic- and Multiscale Material Modeling and Testing

Christer H Ersland, PhD Arctic Materials **-** Atomistic modeling of bcc-Fe

Inga Ringdalen Vatne, PhD Arctic Materials - Multiscale Material Modeling of Fracture in Iron and Steel

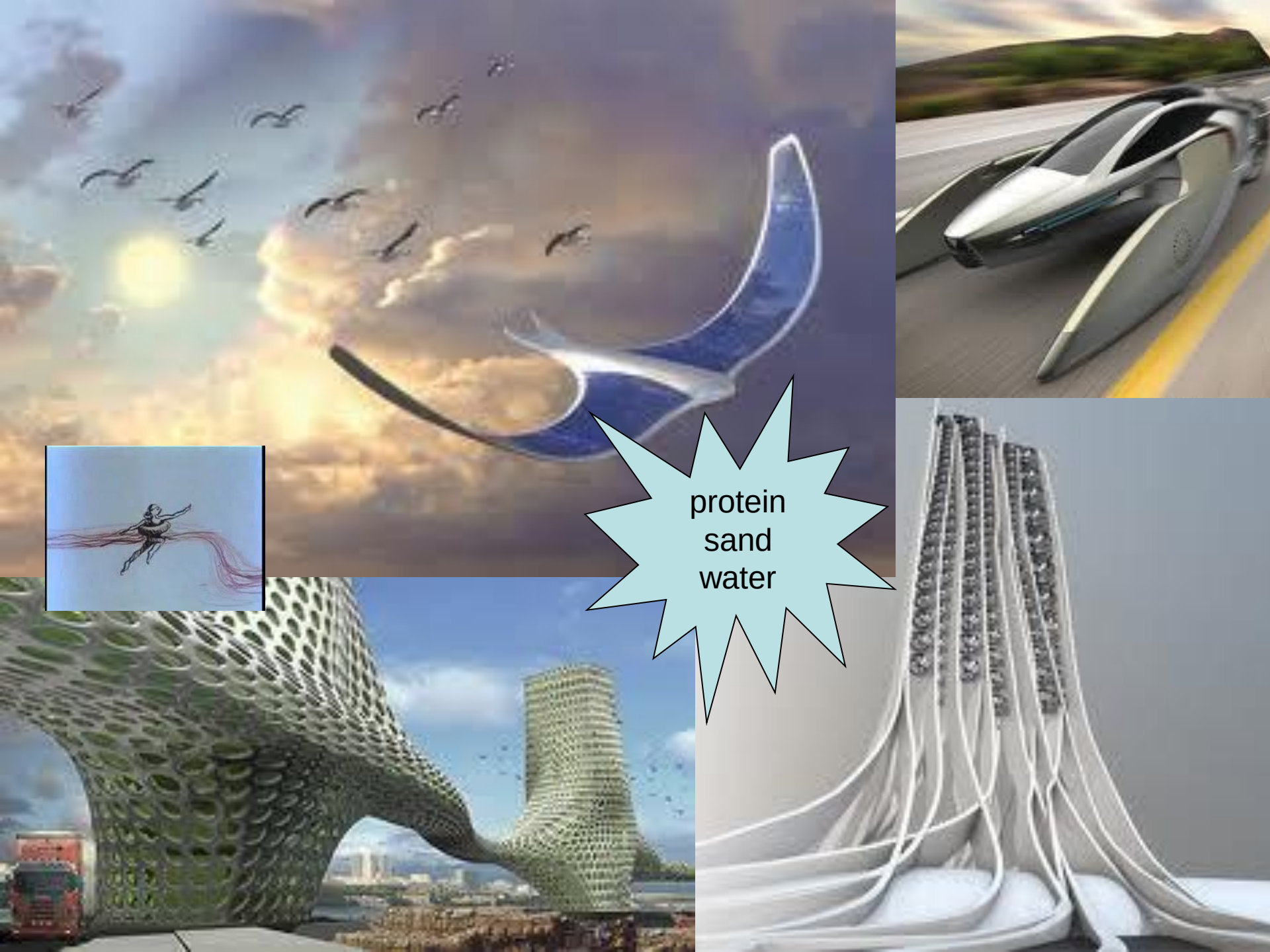
Adina Basa, PhD HISC Petromaks project - Nanoindentation of steels with in situ hydrogen charging

Bjørn Rogne, PhD Nanomechanical testing of steel

5 Masterstudents on nanotechnology, fall 2010

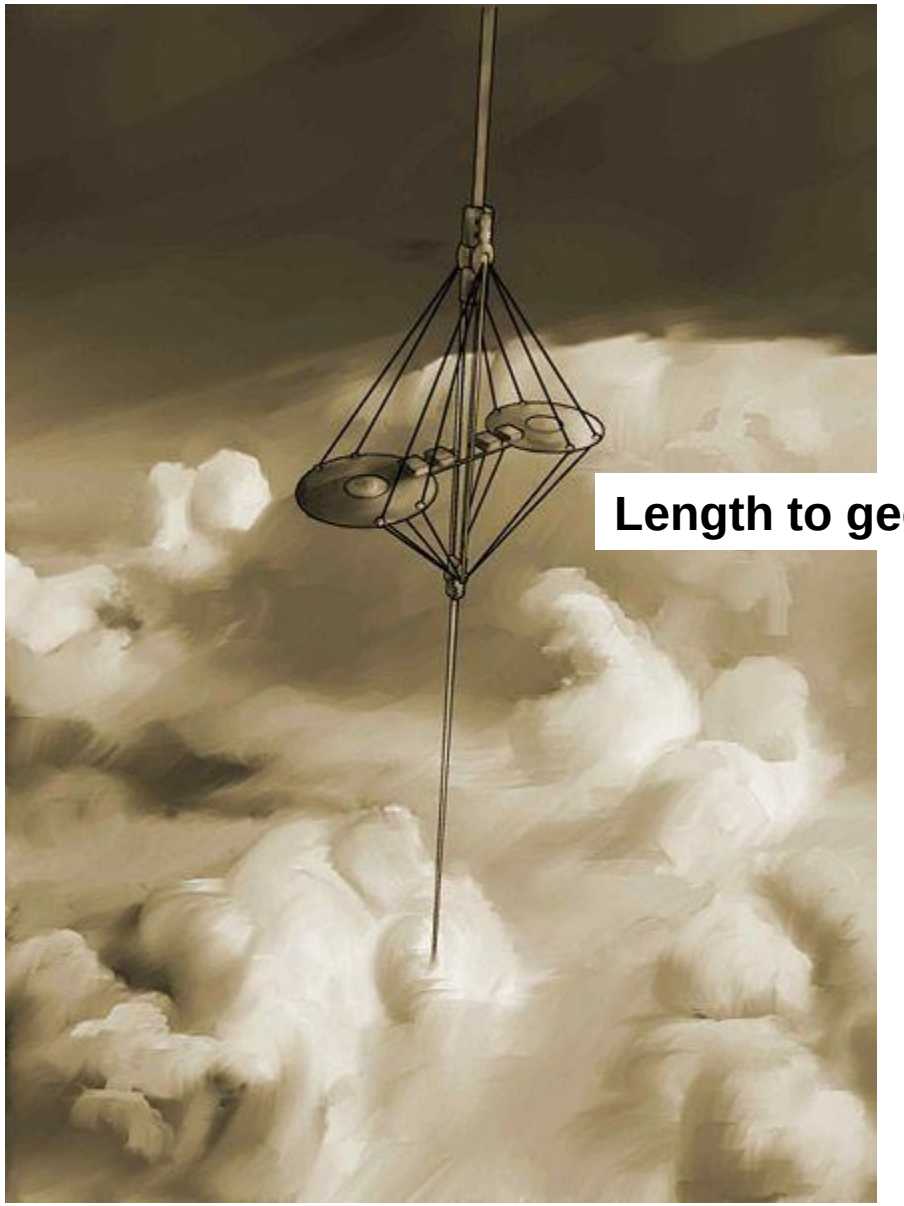
Cooperation:
NTNU NanoLab, NTNU Supercomputer; SINTEF, MIT, Fraunhofer IWM

Natures building blocks

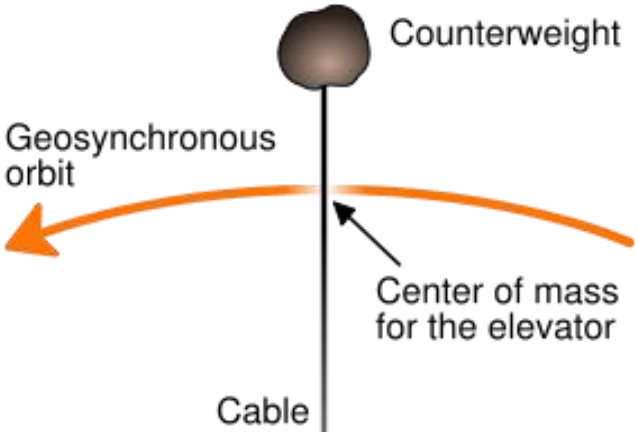

protein
sand
water

The Space Elevator

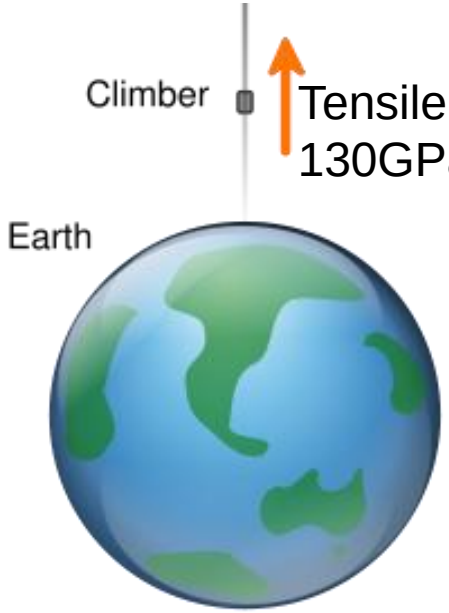
Material for the elevator-project



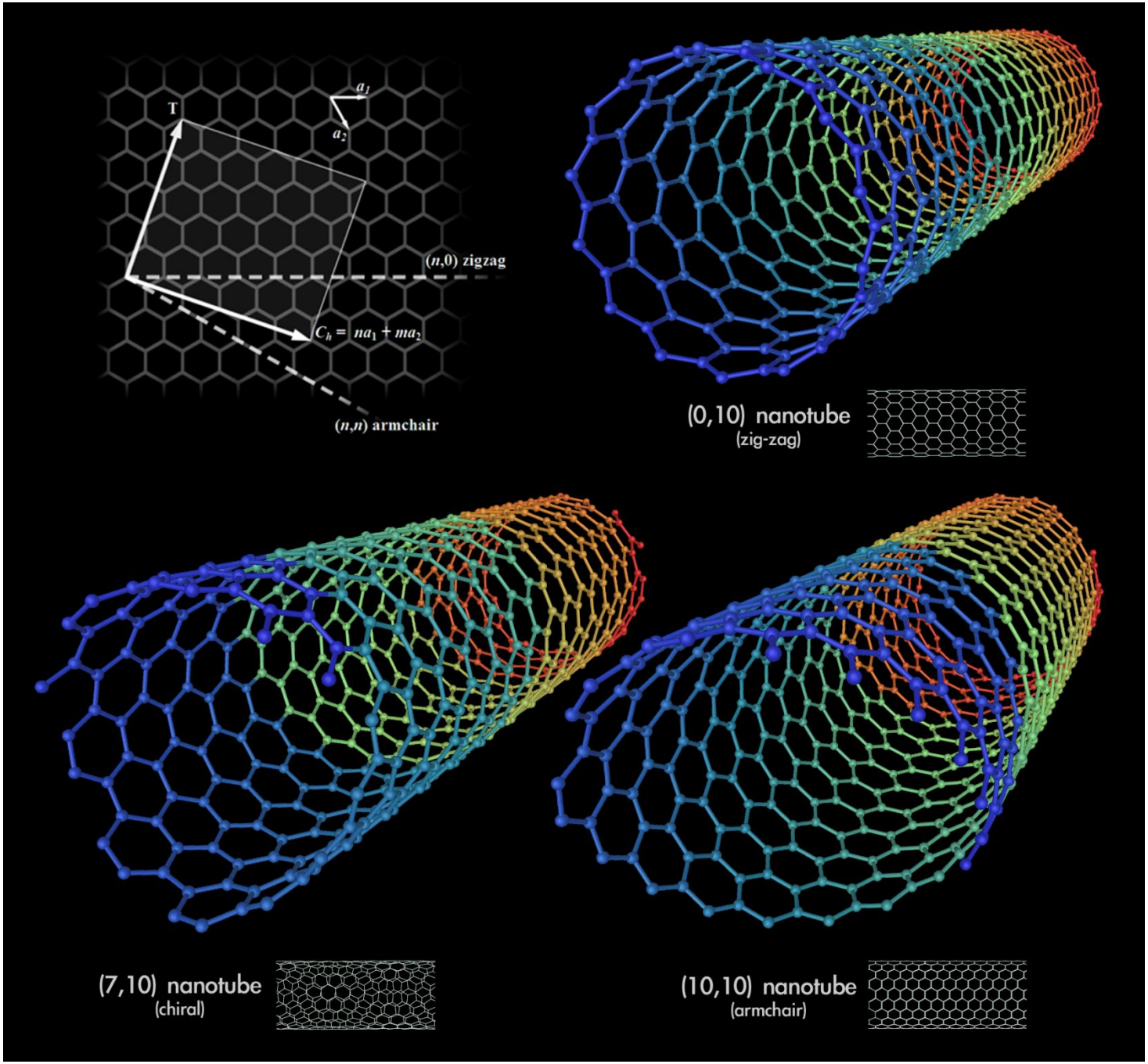
100.000 km
launching into outer space



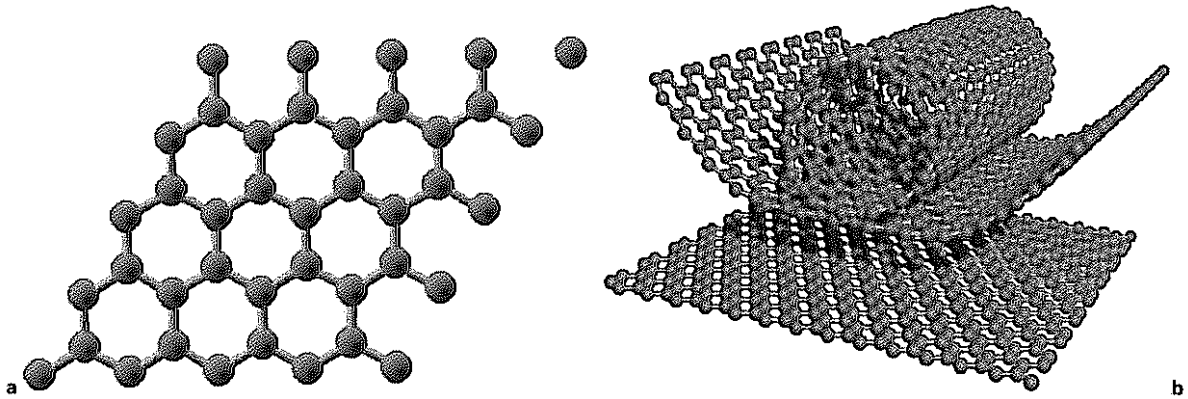
Length to geostationary position: 35.586 km



Tensile strength: 130GPa


T
a_1
a_2
(n,0) zigzag
$C_h = na_1 + ma_2$
(n,n) armchair
(0,10) nanotube
(zig-zag)
(7,10) nanotube
(chiral)
(10,10) nanotube
(armchair)

Carbon nanotubes

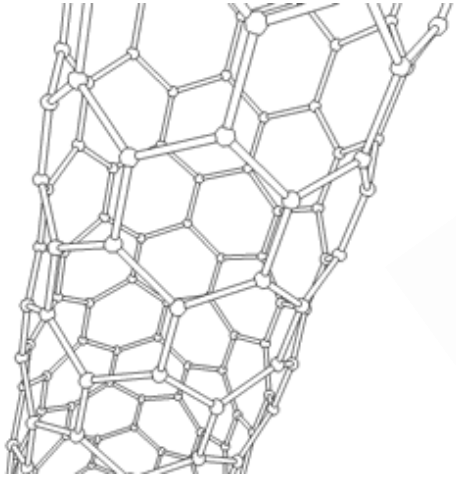


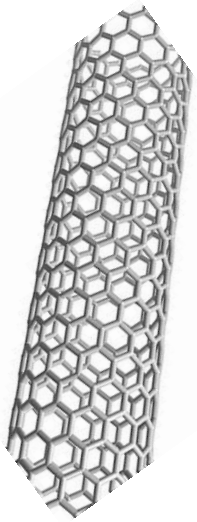
2 *a* Graphene sheet and *b* schematic diagram showing how graphene sheet might be rolled to form tube[16]

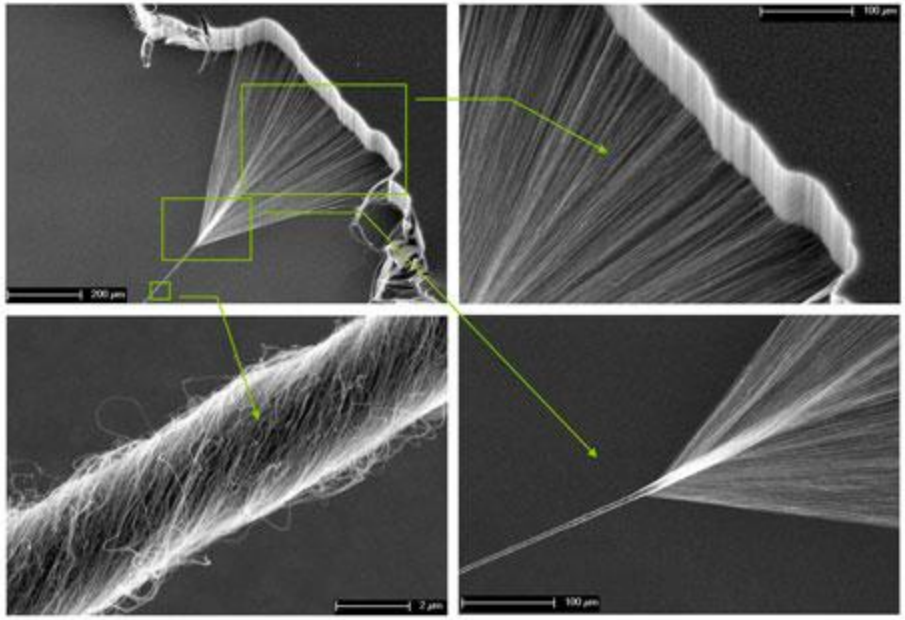
Table 1 Measured strength of carbon nanotube based ropes as function of length

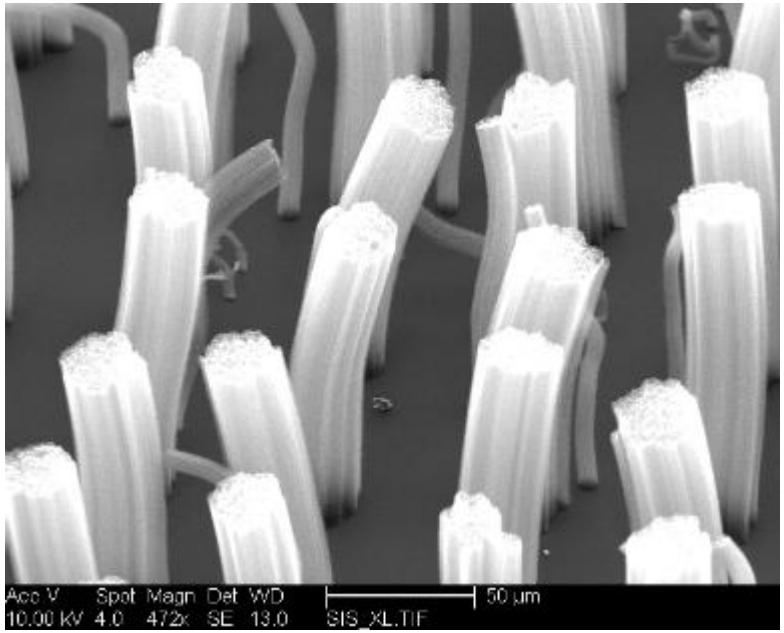
Length	Strength, GPa	Reference
460 nm	150	25
1·8 μm	24	26
2·9 μm	28	26
6·0 μm	39	26
6·5 μm	20	26
6·7 μm	35	26
6·9 μm	63	26
11·0 μm	21	26
1–2 mm	3·6	27
2 mm	1·7	28

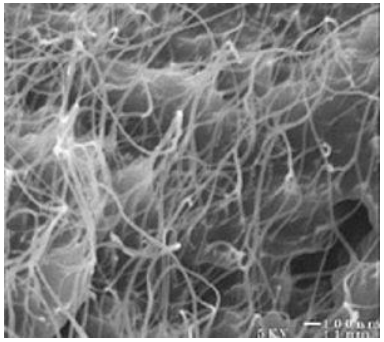
Carbon nanotubes











SUPERHYDROPHOBIC CNT SURFACES

Bouncing Water Droplet on a Superhydrophobic Carbon Nanotube Array

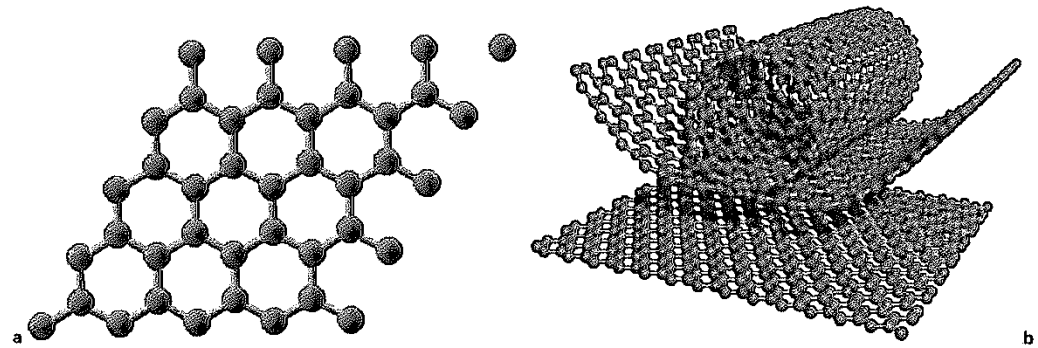
Adrianus I. Aria and Morteza Gharib

Graduate Aeronautical Laboratories,
California Institute of Technology, Pasadena, CA 91125, USA

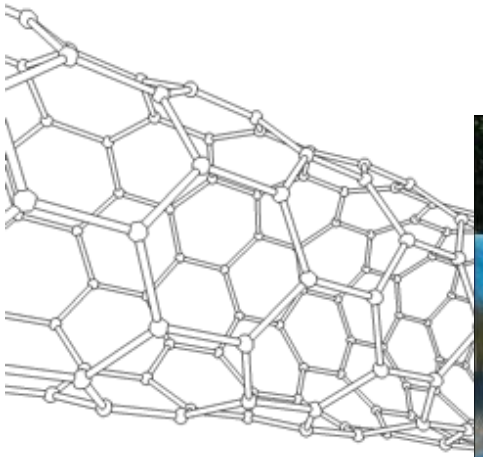
October 8, 2010

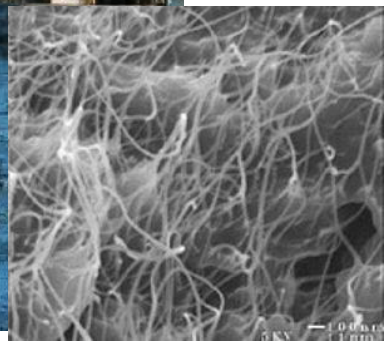
Abstract

Over the past few decades, superhydrophobic materials have attaracted a lot of interests, due to their numerous practical applications. Among various superhydrophobic materials, carbon nanotube arrays have gained enormous attentions simply because of their outstanding properties. The impact dynamics of water droplet on a superhydrophobic carbon nanotube array is shown in this fluid dynamics video.

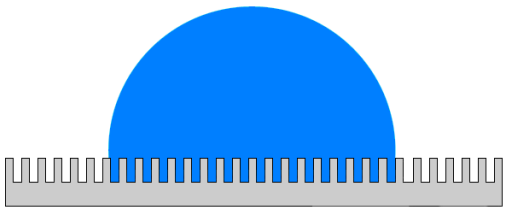


2 *a* Graphene sheet and *b* schematic diagram showing how graphene sheet might be rolled to form tube[16]

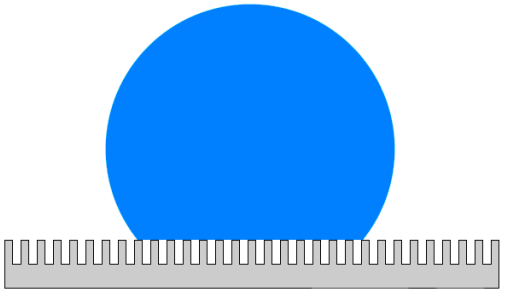


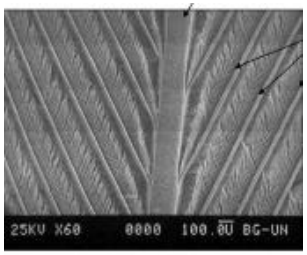


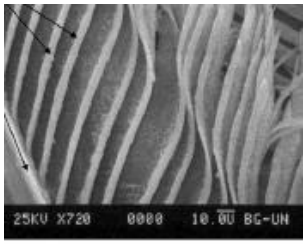
Wenzel

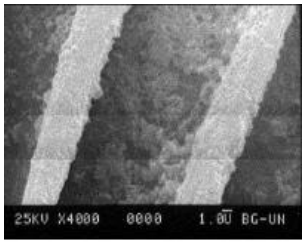


Cassie - Baxter

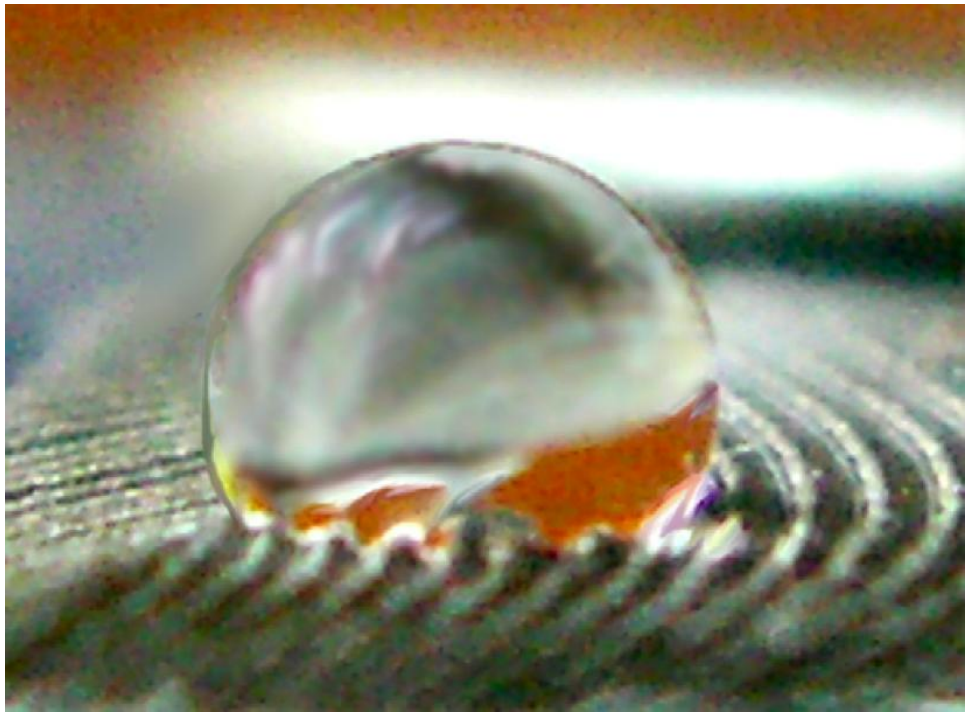




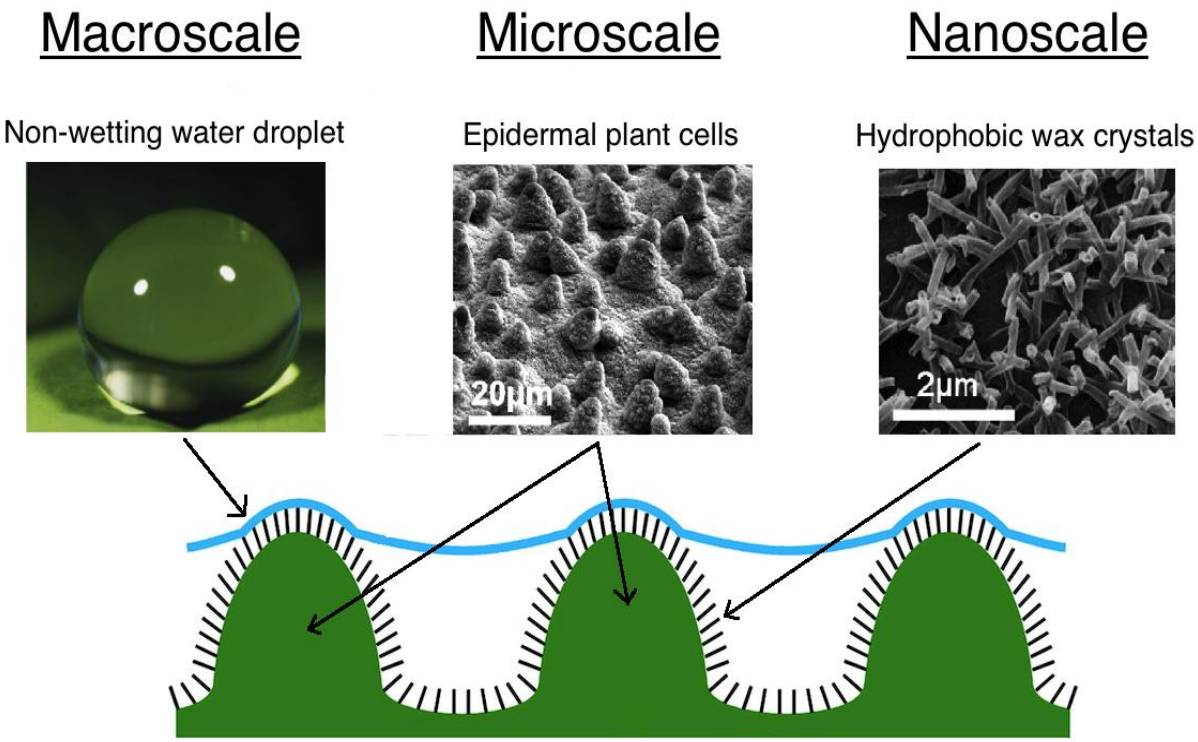




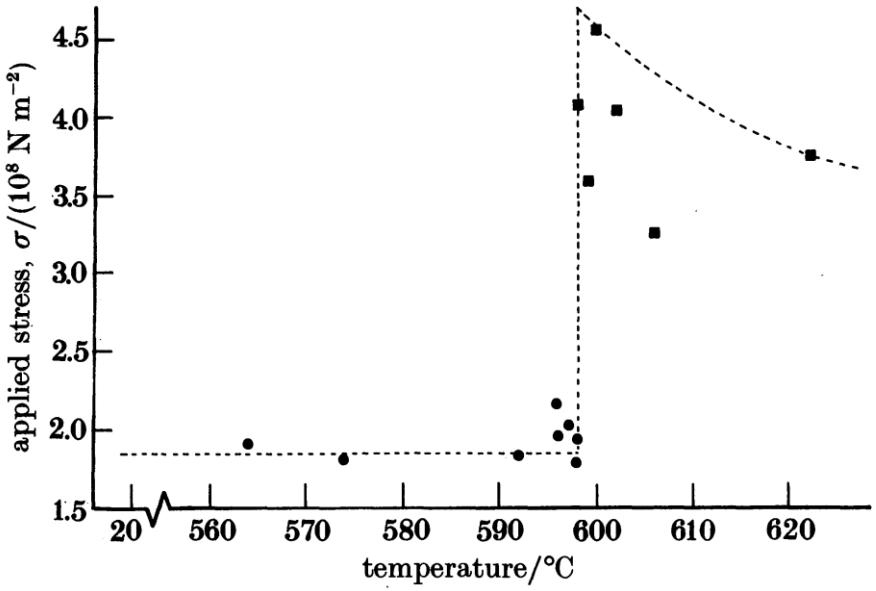
Pigeon feathers



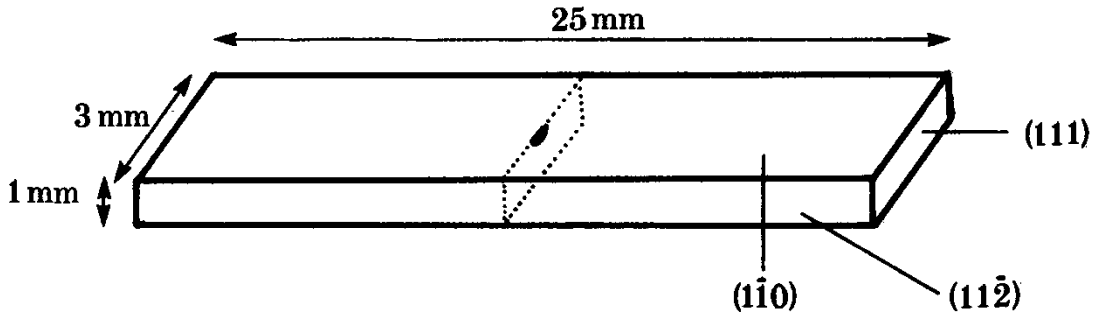
Lotus leaf


Macroscale
Microscale
Nanoscale
Non-wetting water droplet
Epidermal plant cells
Hydrophobic wax crystals
20μm
2μm

Brittle to Ductile Transition (BDT) measurements on single crystals silicon



Sharp transition from brittle to ductile behavior



Samuel and Roberts, 1989

- **Pair potential**: all bonds depend only on pairs of atoms

$$\phi_i = \frac{1}{2} \sum_{j=1..N_{neigh}} \phi(r_{ij})$$

- **EAM potential**: in addition to pairs of atoms have contribution due to environment of atoms, expressed through electron density (which is a pair potential)

$$\phi_i = \sum_{j=1..N_{neigh}} \frac{1}{2} \phi(r_{ij}) + F(\rho_i(r_{ij}))$$

depends on all neighbors of i (multi-body)

- **MEAM potential**: electron density itself is also a multi-body potential (depends on bond angles)

$$\phi_i = \sum_{j=1..N_{neigh}} \frac{1}{2} \phi(r_{ij}) + F(\rho_i(r_{ij}, \theta_{ijk}))$$

Modeling of silicon: Interatomic Potential

Several empirical potentials fitted to experimental data:

Stillinger-Weber [1]

Tersoff [2]

EDIP (Environment dependent Interatomic Potential)[3]

Problems:

1. Inaccurate description of silicon bonds close to fracture
2. Incorrect predictions of fracture modes (ductility and crack opening instead of brittle).

Coupling Tight-Binding or QM with empirical potentials

1. TB/EDIP and TB/Tersoff coupling [4,5]
2. DFT/Stillinger-Weber coupling[6]

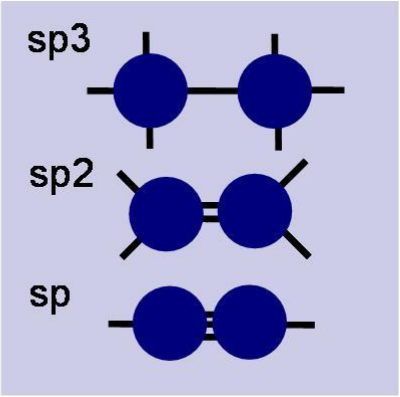
Can model brittle fracture well but too small reactive regions for dislocation emission and plasticity.

1. Stillinger and Weber, PRB **31**(8), 5262 (1985); 2. Tersoff, PRL **56**(6), 632 (1986); 3. Justo et al, PRB **58**(5), 2539 (1998); 4. Abraham et al, Europhys. Lett. **44**, 783 (1998); 5. Bernstein and Hess, PRL **91**(2), 025501 (2003); 6.Csanyi et al, PRL **93**(17), 175503 (2004).

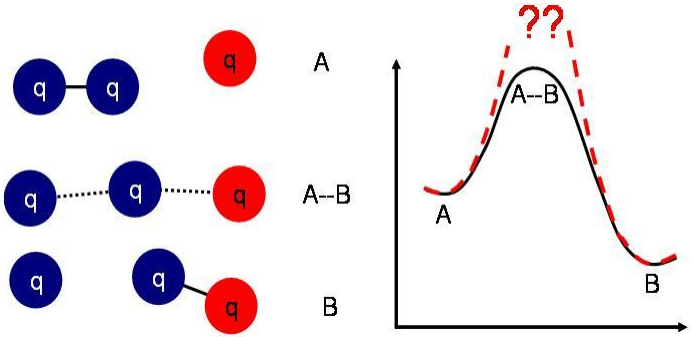
Reactive force field (ReaxFF)[1]

$$E_{system} = \underbrace{E_{bond} + E_{vdWaals} + E_{Coulomb}}_{\text{2-body}} + \underbrace{E_{val}}_{\text{3-body}} + \underbrace{E_{tors}}_{\text{4-body}}$$

$$+ \underbrace{E_{over} + E_{under}}_{\text{multi-body}}$$



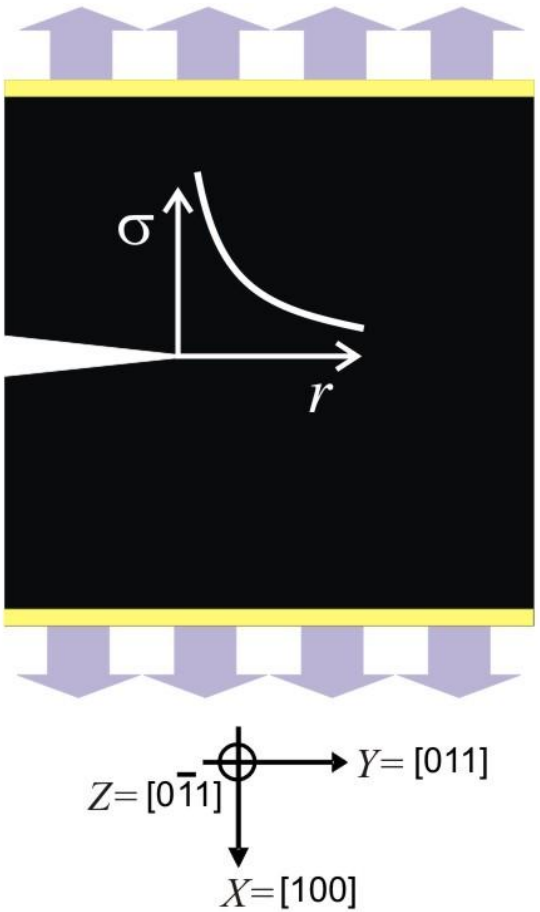
	Nonreactive FFs	Reactive FFs ReaxFF
Ground state energies (e.g. distinguish sp3-sp2-sp…)	Yes (few states)	Yes
Excited / transition states (go from one to another ground state; see also Figure 4)	No	Yes
Breaking of bonds and continuous energies during reactions	No (sometimes: Morse functions for bond breaking but energetics are typically wrong)	Yes
Formation of bonds	No	Yes
Charge flow during reactions	No	Yes
Organic-Inorganic interfaces (or between other materials)	No (mostly)	Yes (bridging FFs)
Retyping necessary after reaction	Yes (have C2,C3 etc. for different hybridization)	No (atom types are element types)

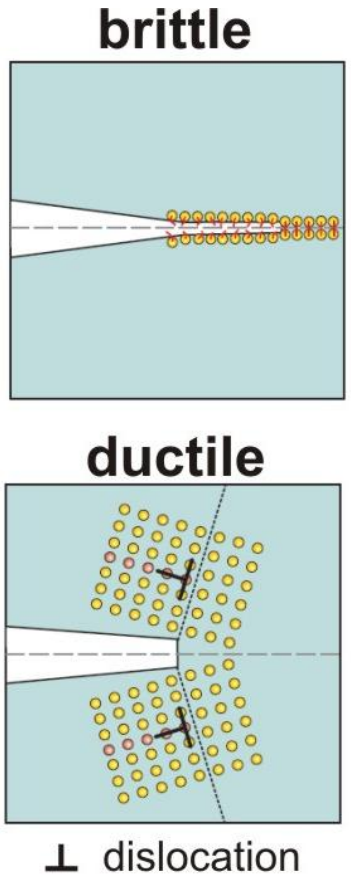


A **bond length/bond order relationship** is used to obtain smooth transition from **non-bonded to single, double, and triple bonded systems**.

1. A.C.T. van Duin et al, J Phys Chem A **105(41)**, pp. 9396 (2001).

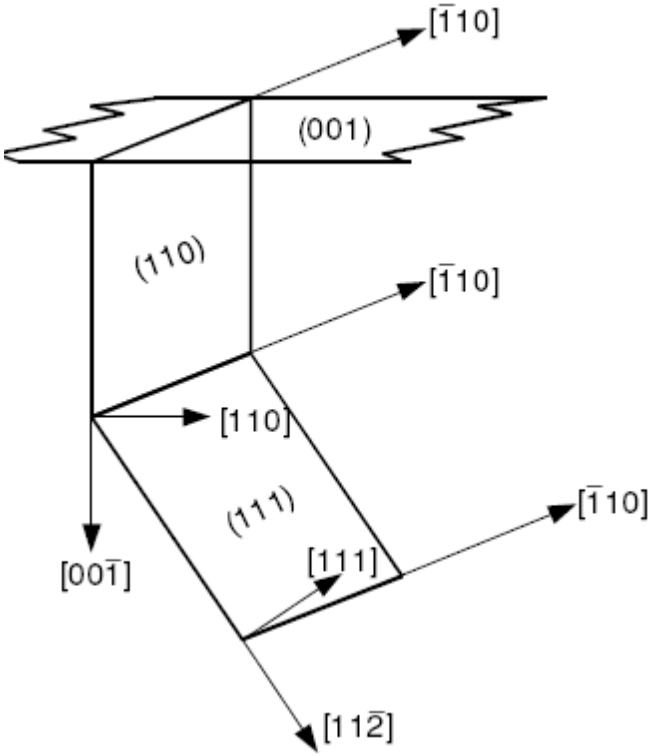
Fracture model





•Use of parallelized code with entire system (30.000-200.000 atoms) modeled by ReaxFF.

•Mode I loading of a crack in single crystal silicon. Notch in [011] direction on a (100) plane. Periodic boundary conditions in x- and z direction

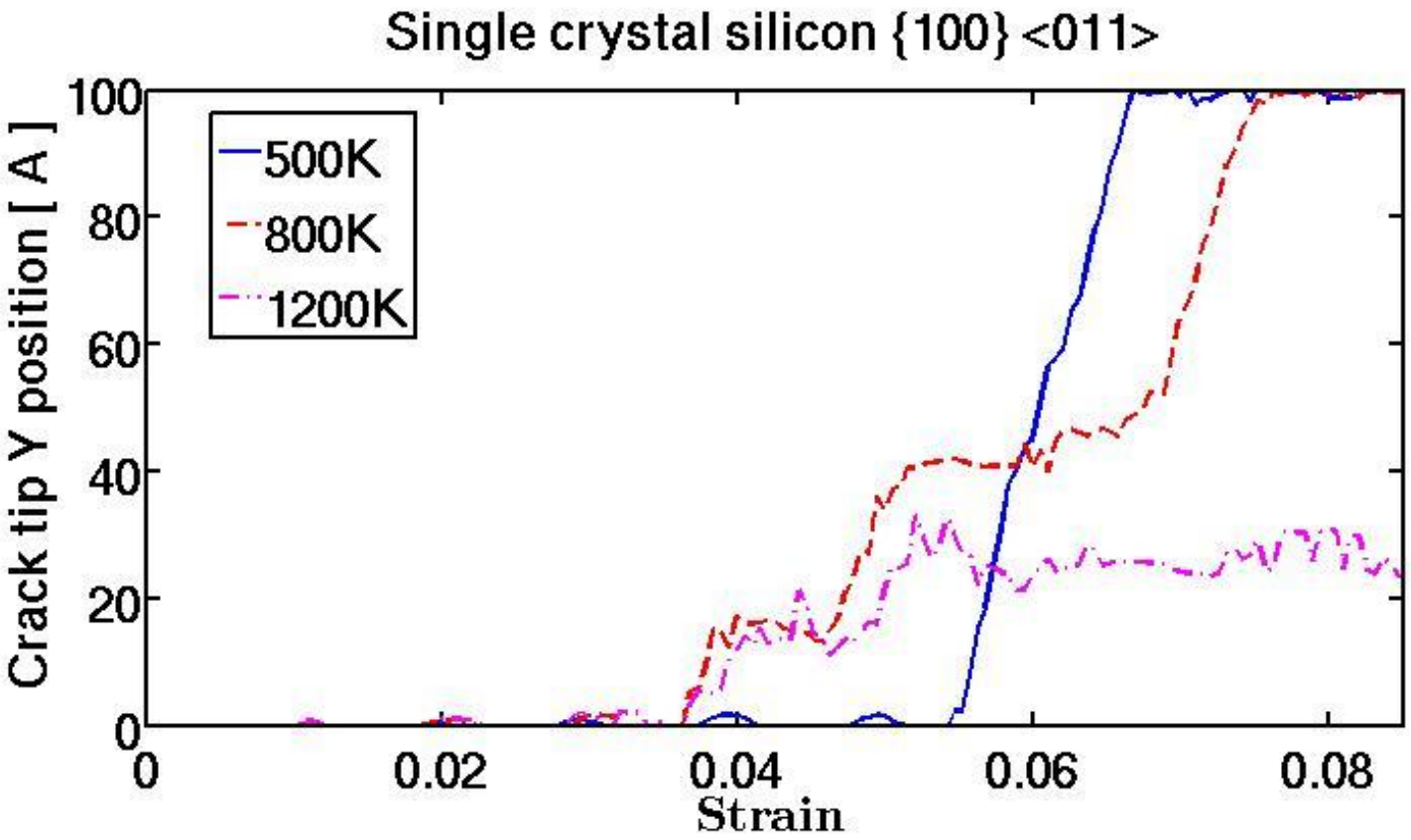


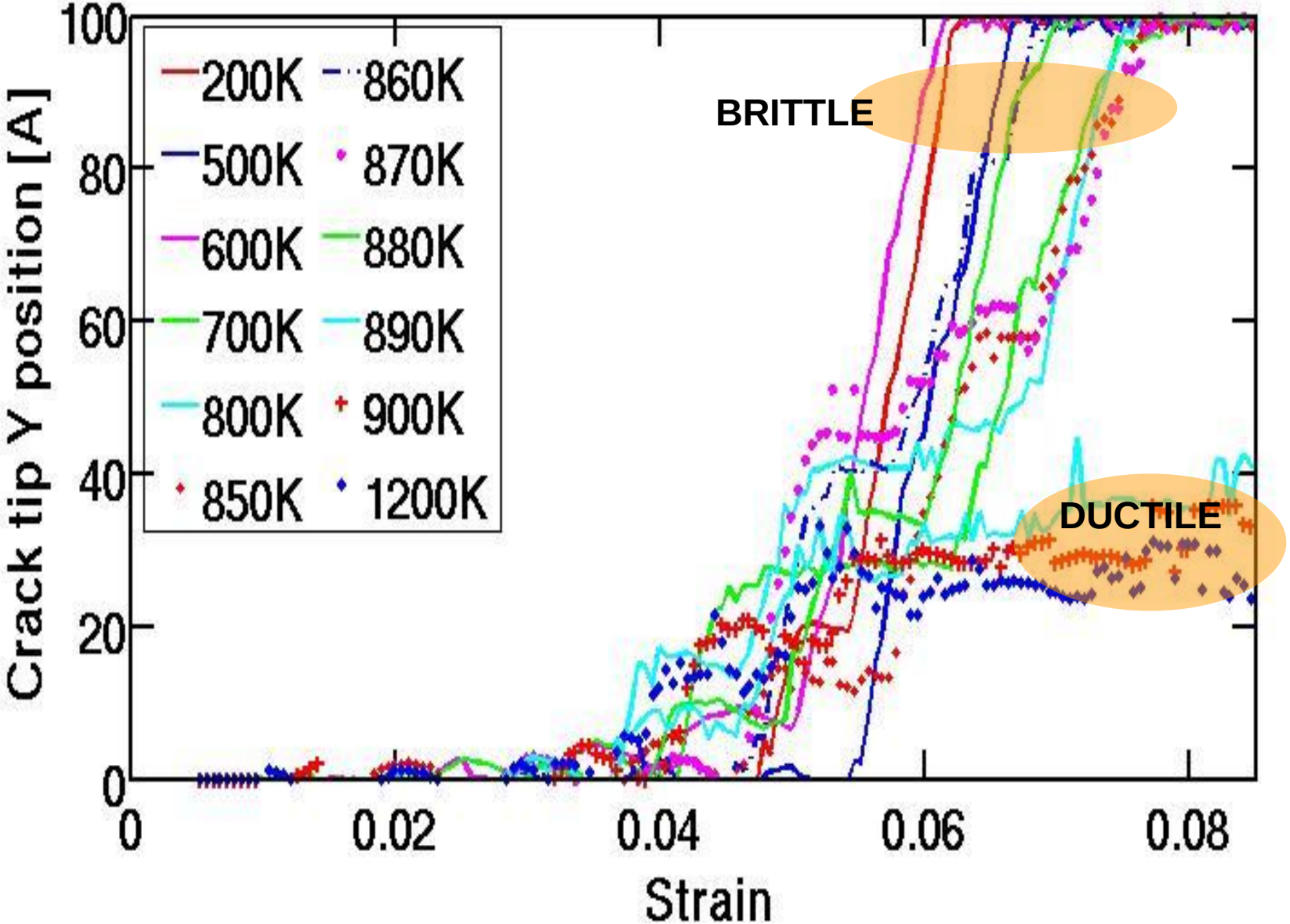
Case 1: {110} cleavage fracture plane
in the <100> and <110> directions.
Semiconductors, MEMS devices

Case 2: {111} cleavage fracture plane
in the <110> and <112> directions.
Fundamental studies

Case 3: {100} cleavage fracture plane
In the <011> direction.
Not observed in practice

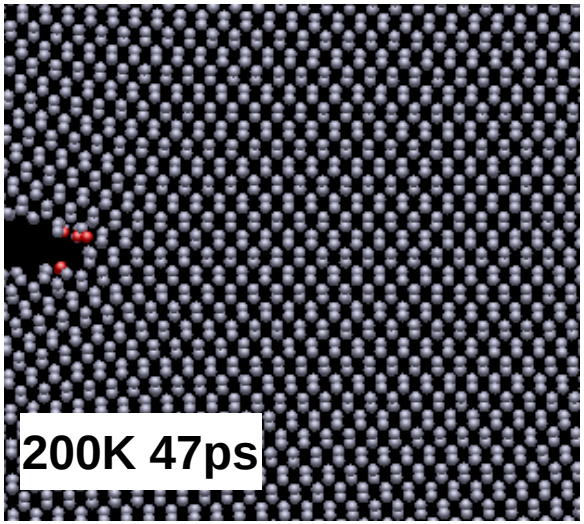
Small Model:
27.000 atoms, 200Å long and wide, thickness 15Å

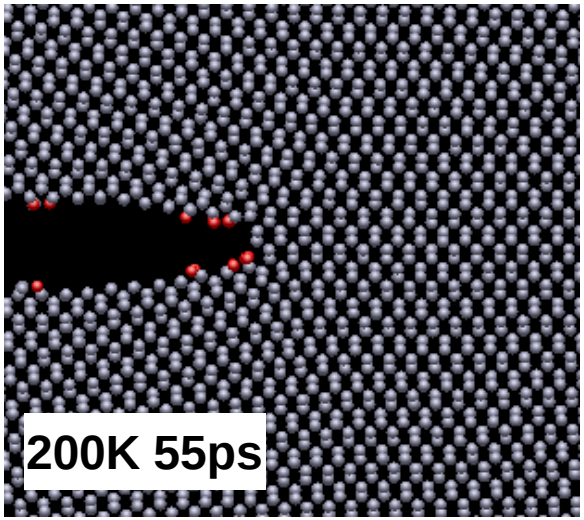


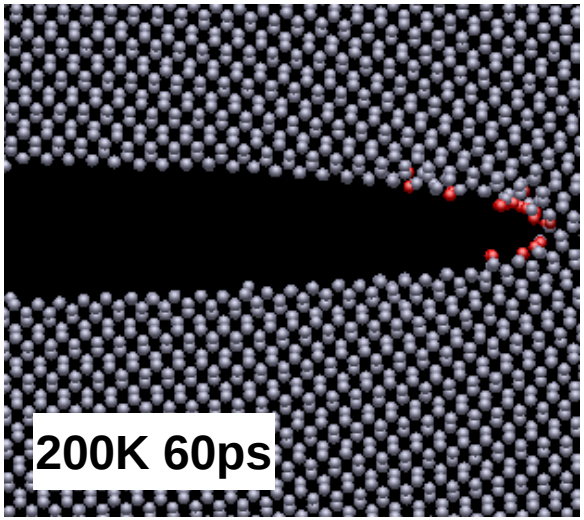


Atomistic Study of Crack-Tip Cleavage to Dislocation Emission Transition in Silicon Single Crystal
Dipanjan Sen,Christian Thaulow Stella V. Schieffer Alan Cohen and Markus J. Buehler
PRL 104, 235502 (2010)

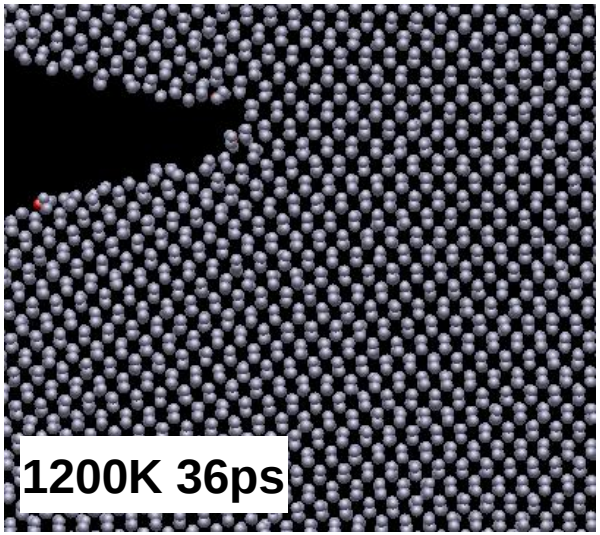
Crack motion at different temperatures

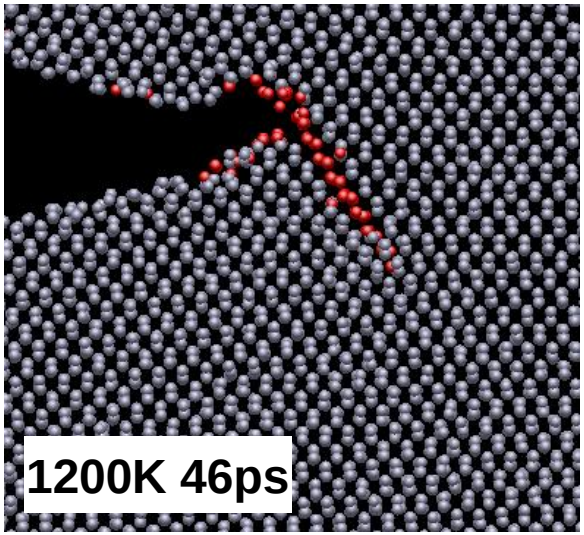


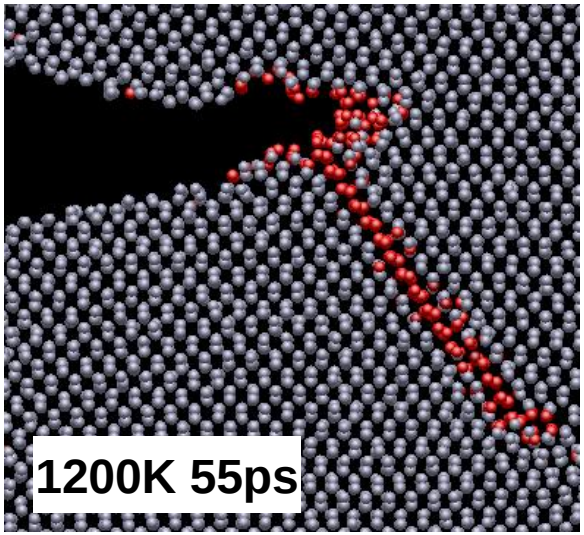




Crack propagation snapshots at low Temp- brittle fracture



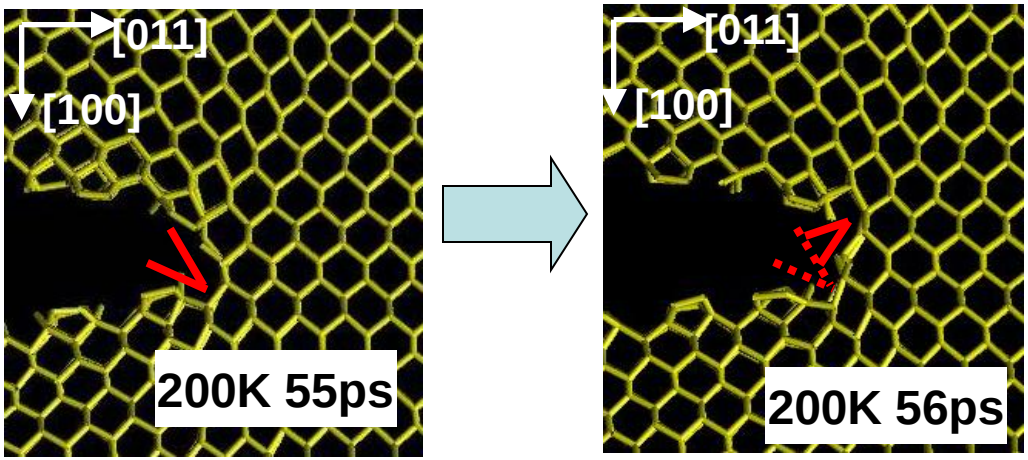




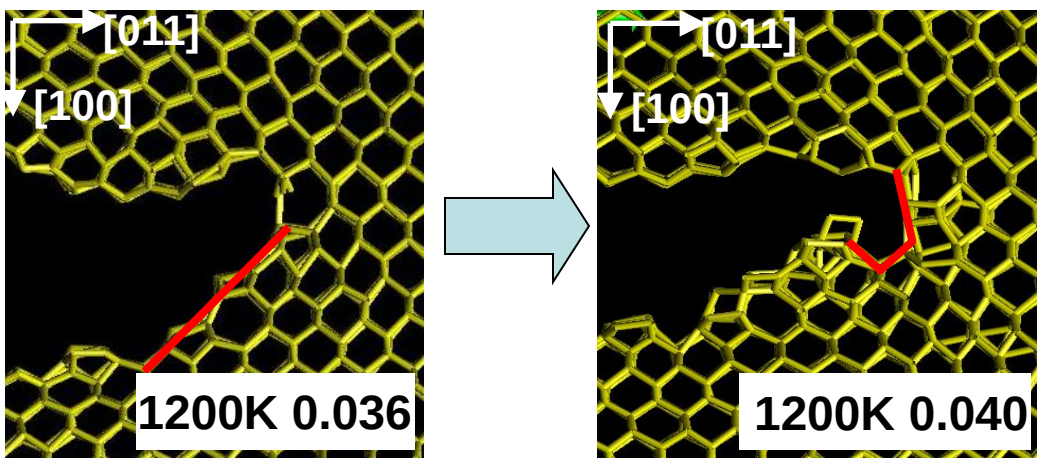
Crack propagation snapshots at high Temp- ductile fracture (slip vector analysis)[1]

1. Zimmermann et al, PRL **87**, 165507 (2001).

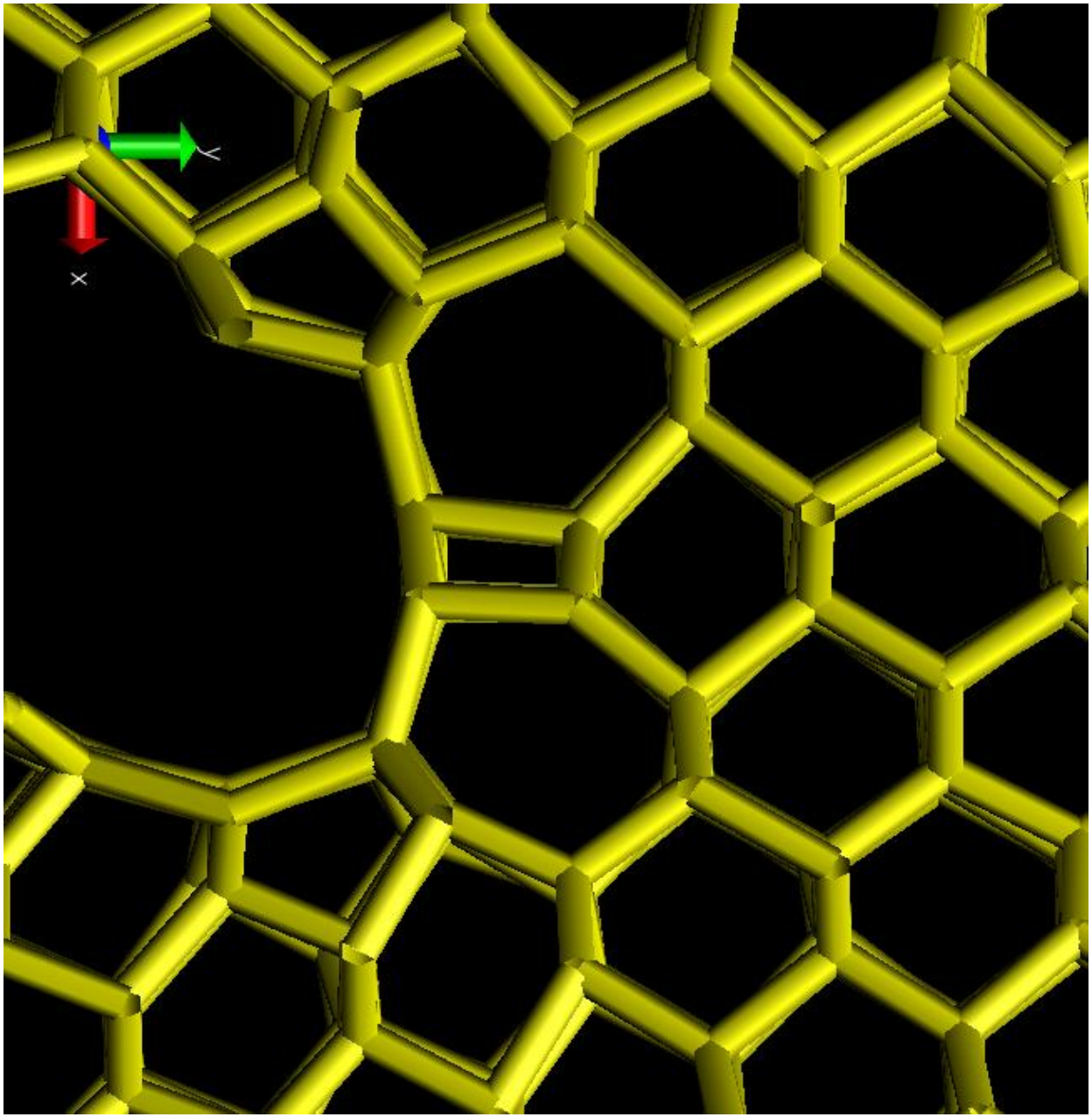
Details of crack tip motion at low and high temperature



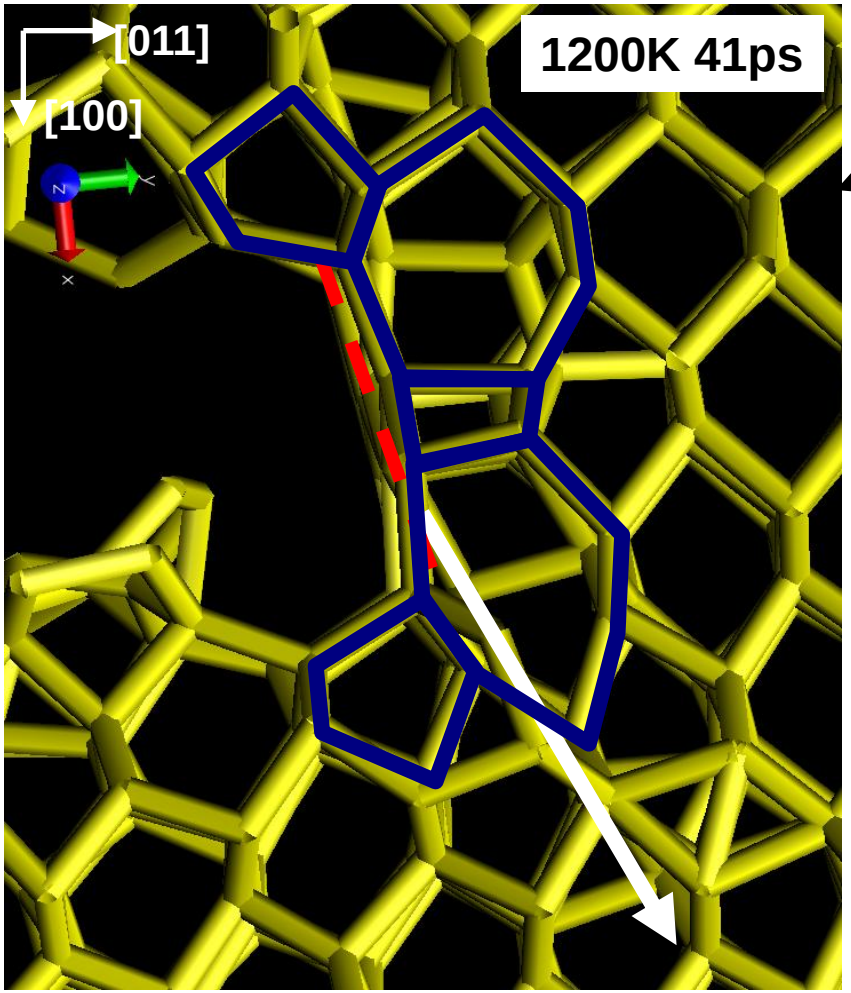
200 K: Crack proceeds in a jagged manner by small steps along (111) planes

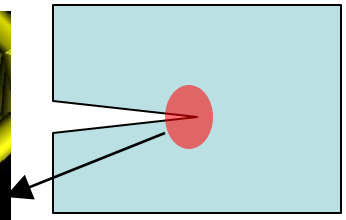


1200 K: Crack forms ledges and small amorphous zones consisting of 5-7 defects


Y
X

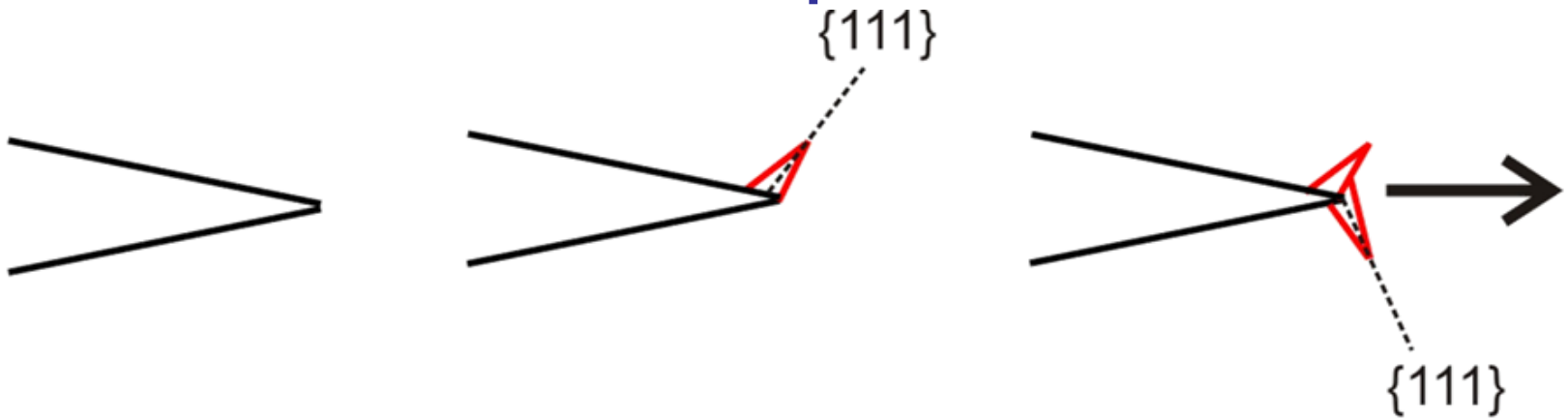
Atomistic mechanism at the crack tip at time of dislocation emission



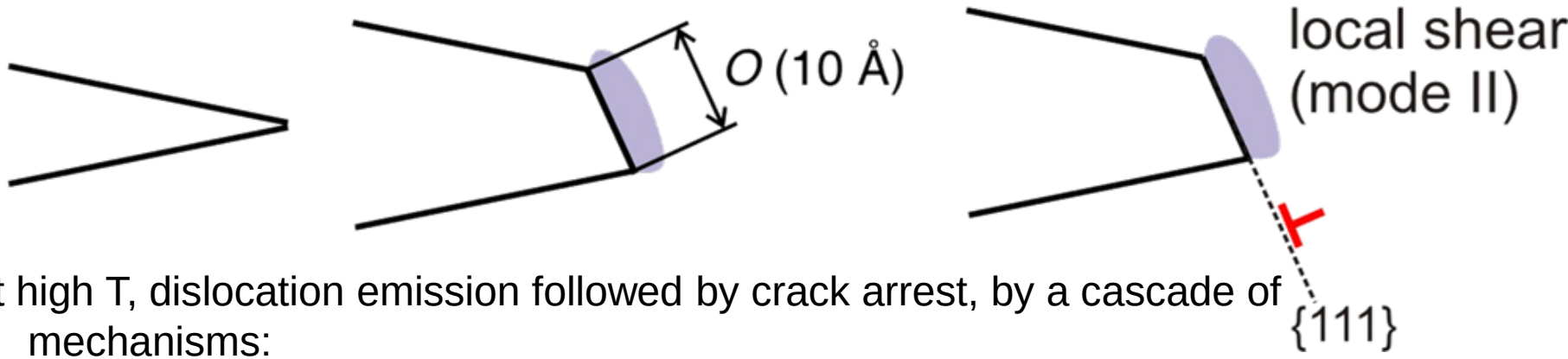


- Ledge formation
- 5-7 ring cluster formation around crack tip

Schematic of crack tip mechanisms observed



At low T, brittle fracture by small crack steps on (111) plane, expected as (111) surface energies are lower.



At high T, dislocation emission followed by crack arrest, by a cascade of mechanisms:

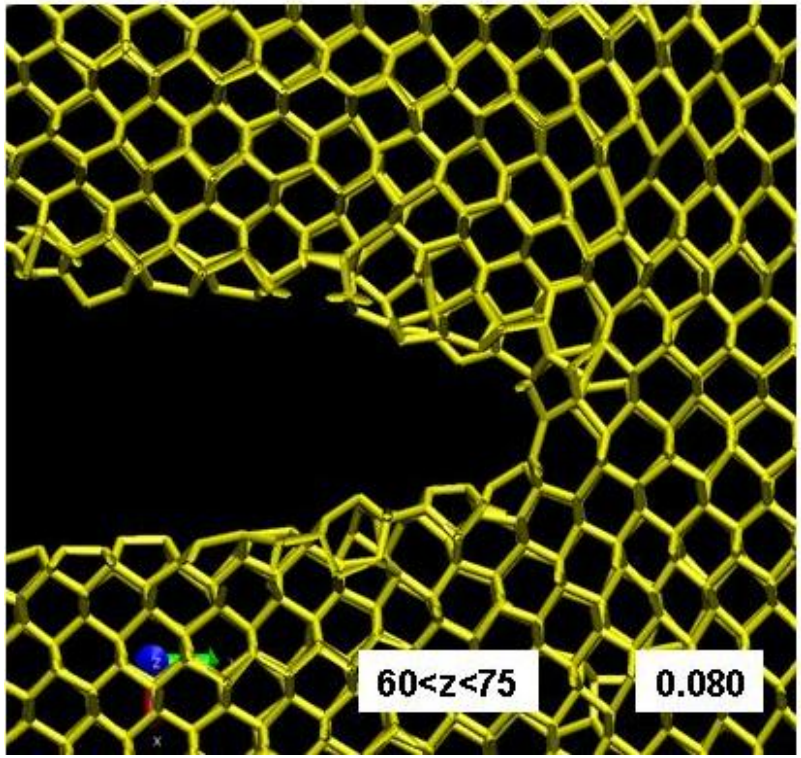
a) small (≈10 Å) disordered zone formed consisting of 5-7 rings at crack tip reducing mode I stress intensity at the tip

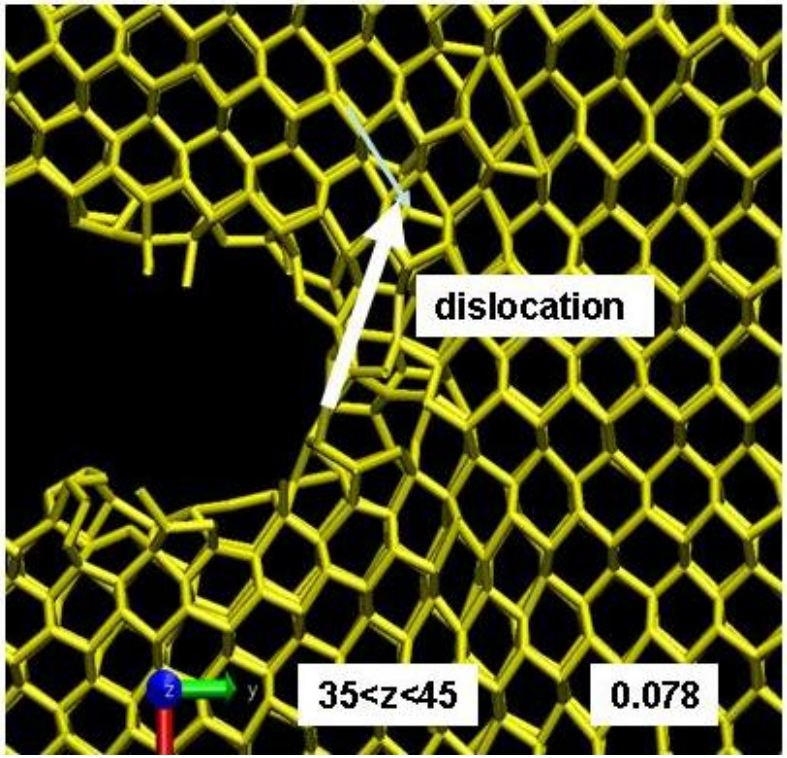
b) ledge formation on (111) planes

c) dislocation emission at the ledge due to increased mode II loading

Large model

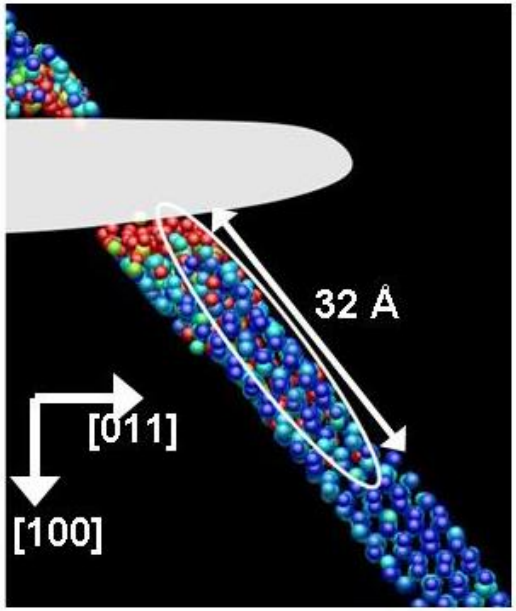
Increase the thickness of the model, 200.000 atoms, 100Å thickness



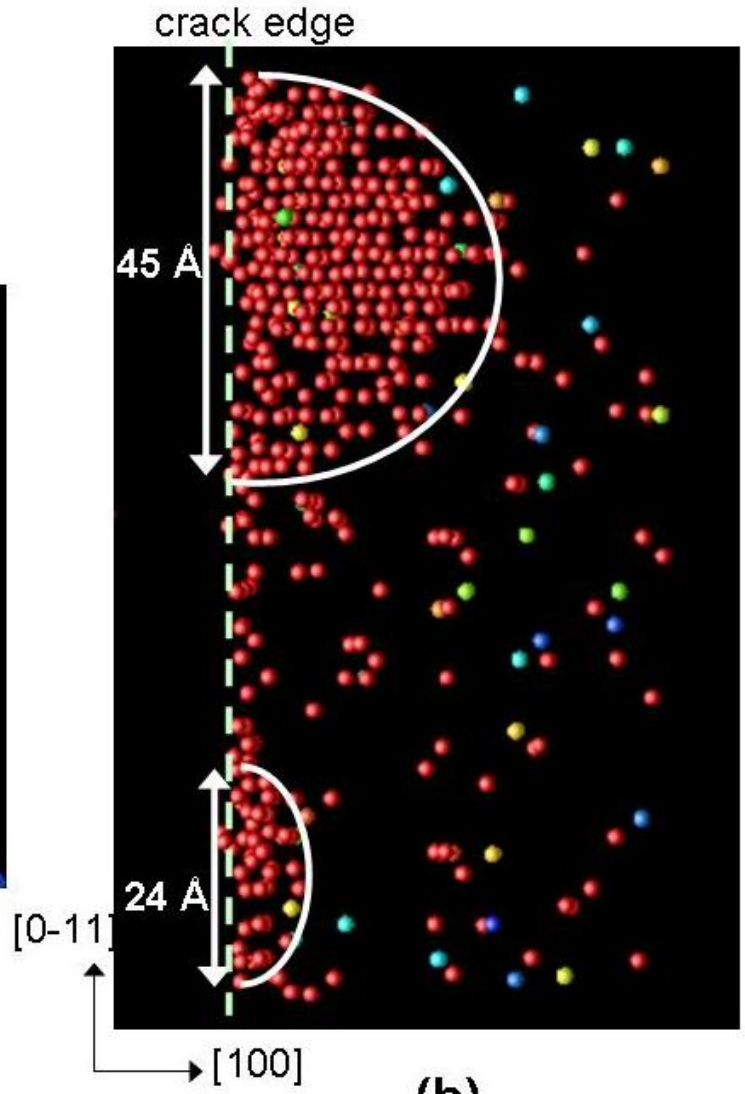


Example of crack front structure at two positions along the crack front.

Analysis of the partial dislocation loop emission at the crack tip on the lower crack surface

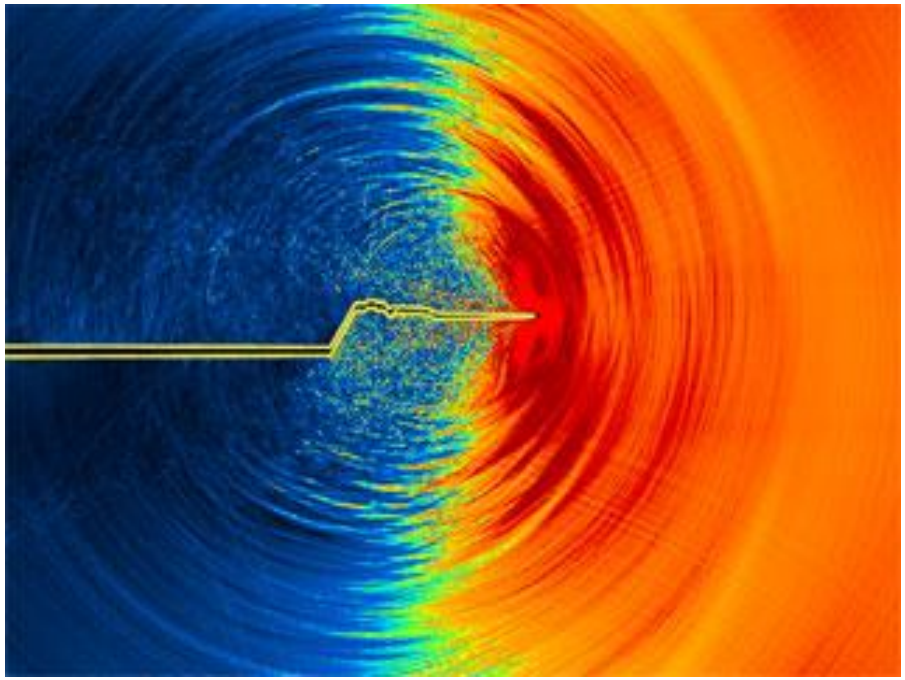


(a)



(b)

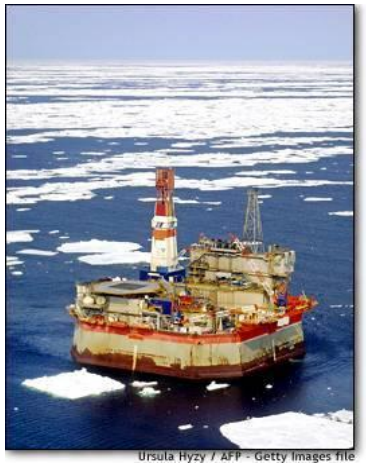
Must the ledges be formed as an integrated part of the dynamic crack front events?



Dynamic instability occurring on the crack tip. As the crack velocity increases, its forward motion becomes more and more unstable: the crack changes direction and leaves behind an increasingly irregular surface. M J Buehler

f02n02io.301605.0	forecast	6/4	19:51	R	50	forecast	f01n11
f05n02io.301592.0	forecast	6/4	19:51	R	50	forecast	f03n08
f02n02io.301606.0	forecast	6/4	19:51	R	50	forecast	f04n11
f05n02io.301593.0	forecast	6/4	19:51	R	50	forecast	f06n05
f02n02io.301607.0	forecast	6/4	19:51	R	50	forecast	f05n04
f05n02io.301594.0	forecast	6/4	19:51	R	50	forecast	f06n04
f02n02io.301608.0	forecast	6/4	19:51	R	50	forecast	f06n11
f05n02io.301595.0	forecast	6/4	19:51	R	50	forecast	f06n10
f02n02io.301609.0	forecast	6/4	19:51	R	50	forecast	f06n08
f05n02io.301596.0	forecast	6/4	19:51	R	50	forecast	f06n03
f02n02io.301610.0	forecast	6/4	19:51	R	50	forecast	f01n06
f05n02io.301597.0	forecast	6/4	19:51	R	50	forecast	f06n12
f02n02io.301611.0	forecast	6/4	19:51	R	50	forecast	f06n09
f05n02io.301598.0	forecast	6/4	19:52	R	50	forecast	f05n06
f02n02io.301612.0	forecast	6/4	19:52	R	50	forecast	f06n01
f05n02io.301599.0	forecast	6/4	19:52	R	50	forecast	f04n09
f02n02io.301613.0	forecast	6/4	19:52	R	50	forecast	f04n06
f05n02io.301600.0	forecast	6/4	19:52	R	50	forecast	f03n12
f02n02io.301614.0	forecast	6/4	19:52	R	50	forecast	f04n08
f05n02io.301601.0	forecast	6/4	19:52	R	50	forecast	f01n12
f02n02io.301615.0	forecast	6/4	19:52	R	50	forecast	f03n01
f05n02io.301602.0	forecast	6/4	19:52	R	50	forecast	f03n09
f02n02io.301616.0	forecast	6/4	19:52	R	50	forecast	f04n04
f05n02io.301603.0	forecast	6/4	19:52	R	50	forecast	f01n10
f02n02io.301617.0	forecast	6/4	19:52	R	50	forecast	f02n03
f05n02io.301604.0	forecast	6/4	19:52	R	50	forecast	f03n04
f02n02io.300916.0	christth	6/2	22:22	E	50	large	

Arctic Challenges

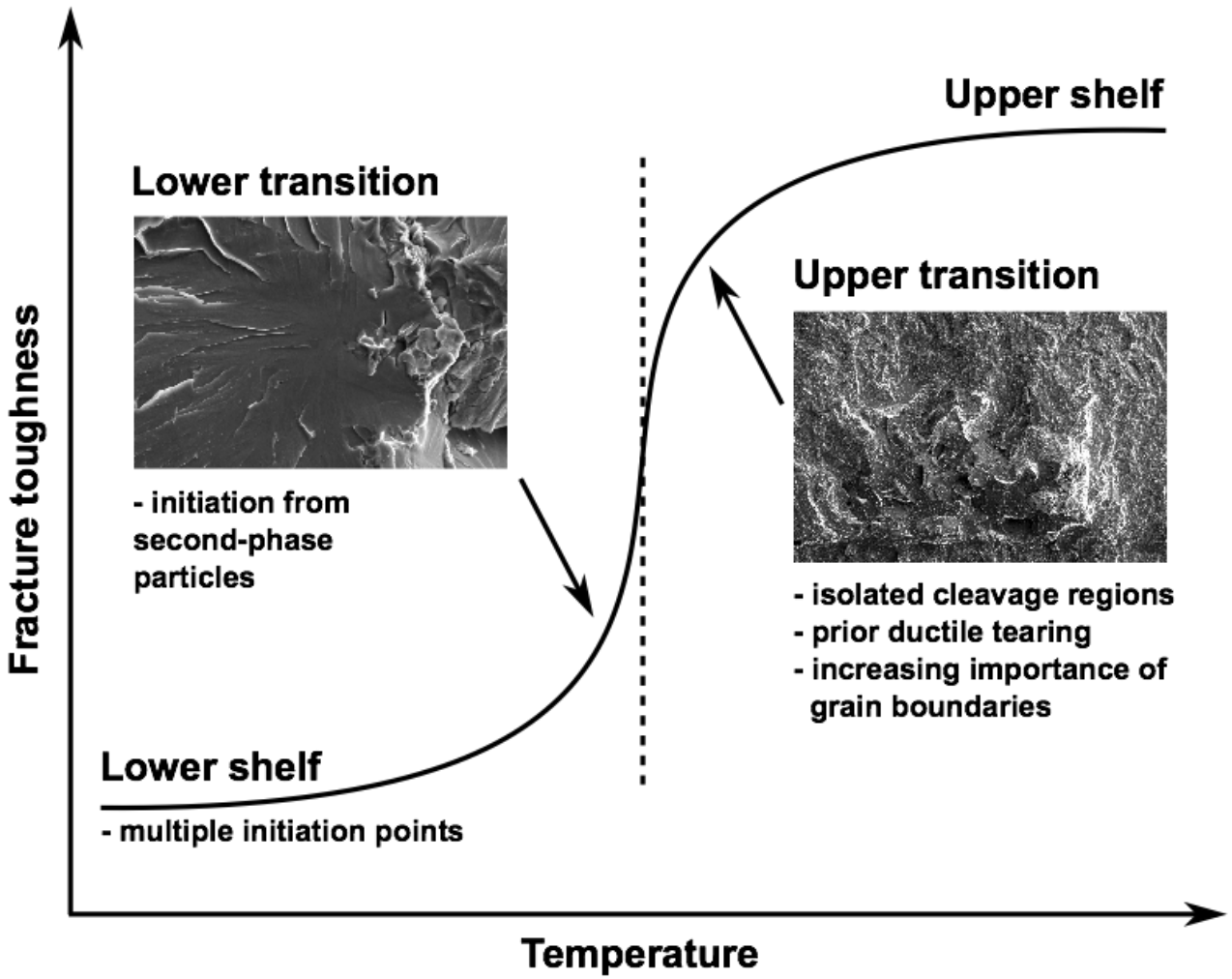


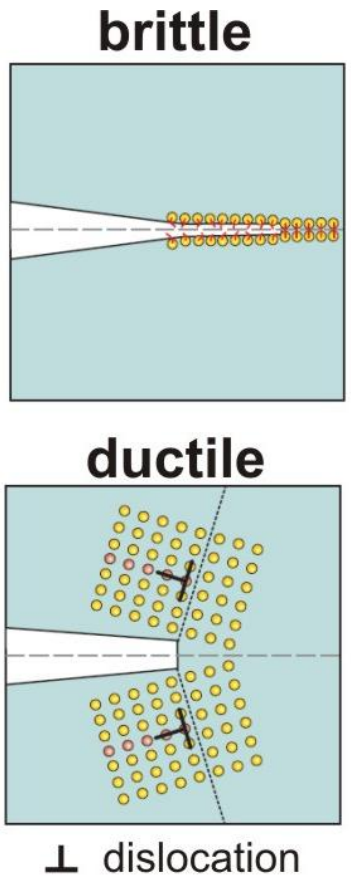
- Design temperature minus 60˚C
- Icebergs
- Ice loads
- Thaw settlement
- Landslides

There is a strong motivation to understand the mechanisms of the BDT

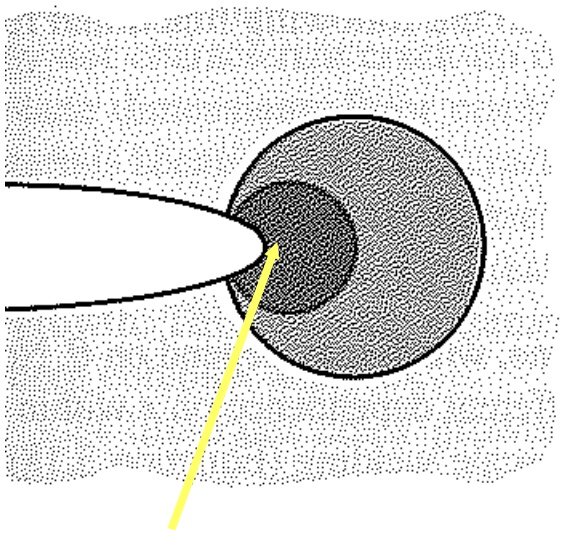
Brittle to Ductile Transition (in Steel)

BRITTLE – DUCTILE TRANSITION

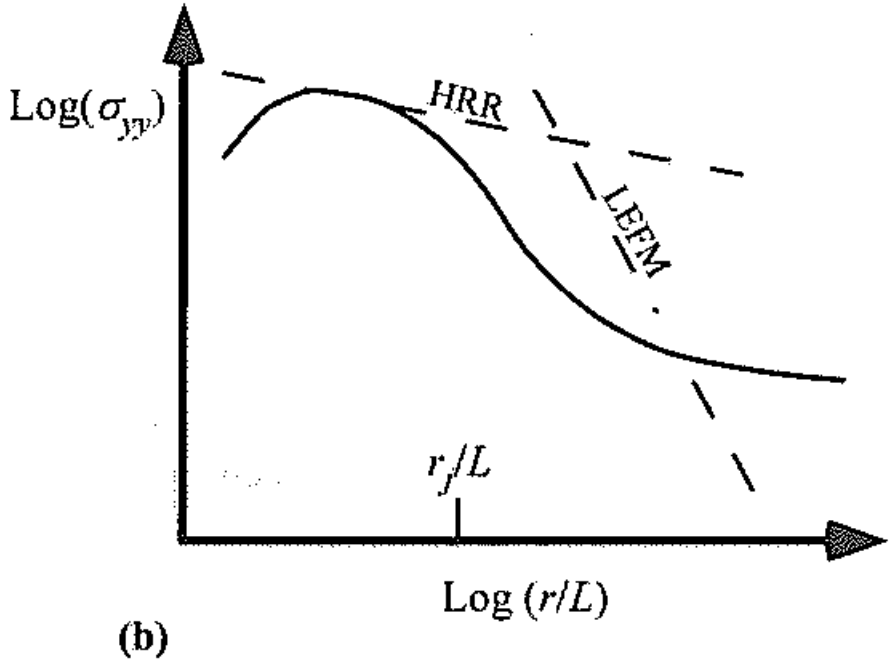


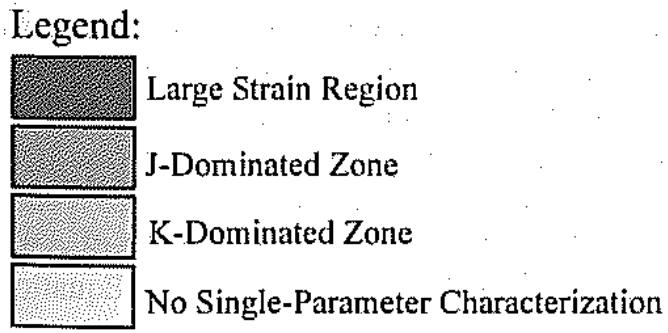


J and CTOD charcterizes crack-tip conditions

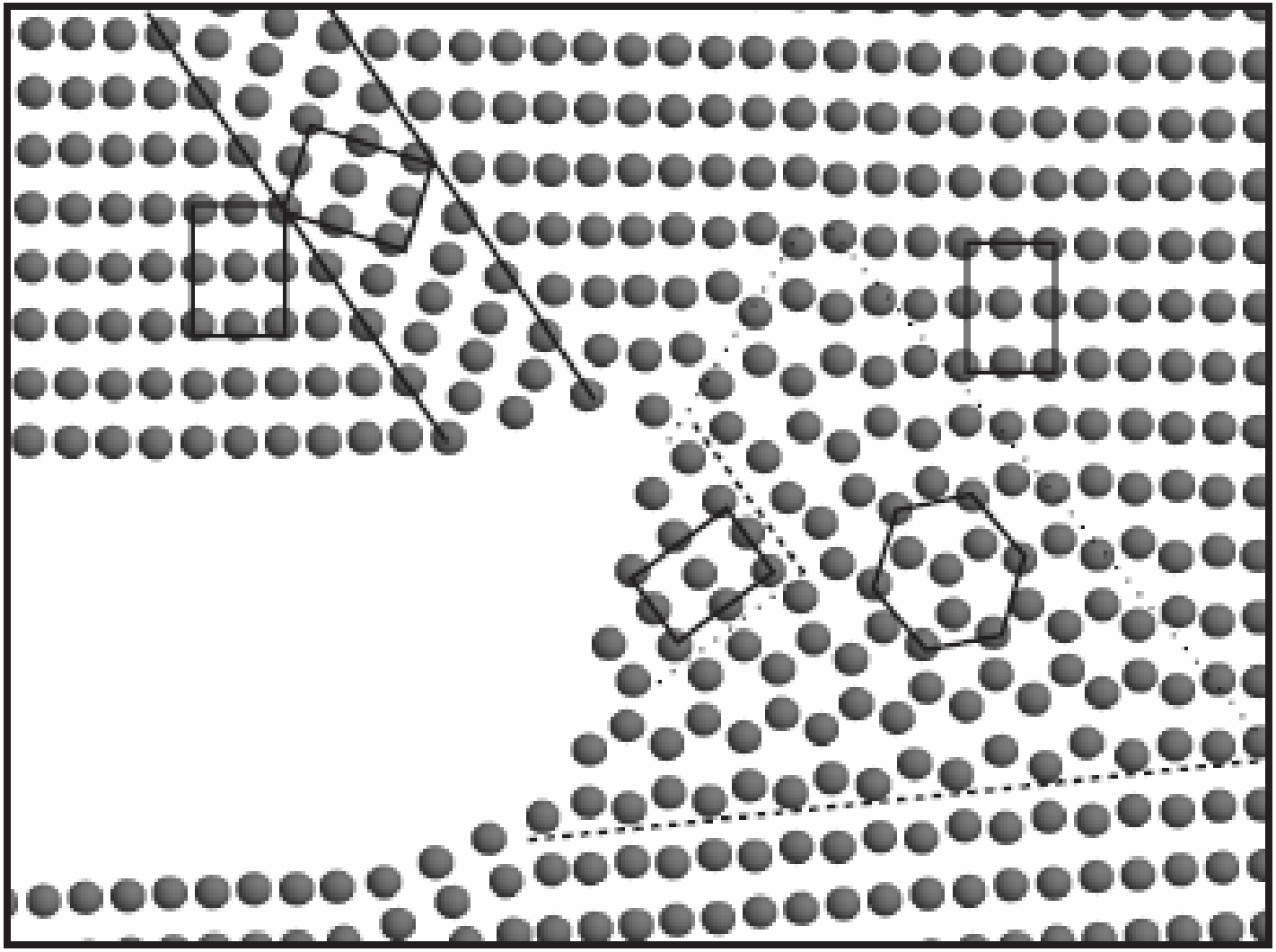


Crack Tip Prosess Zone



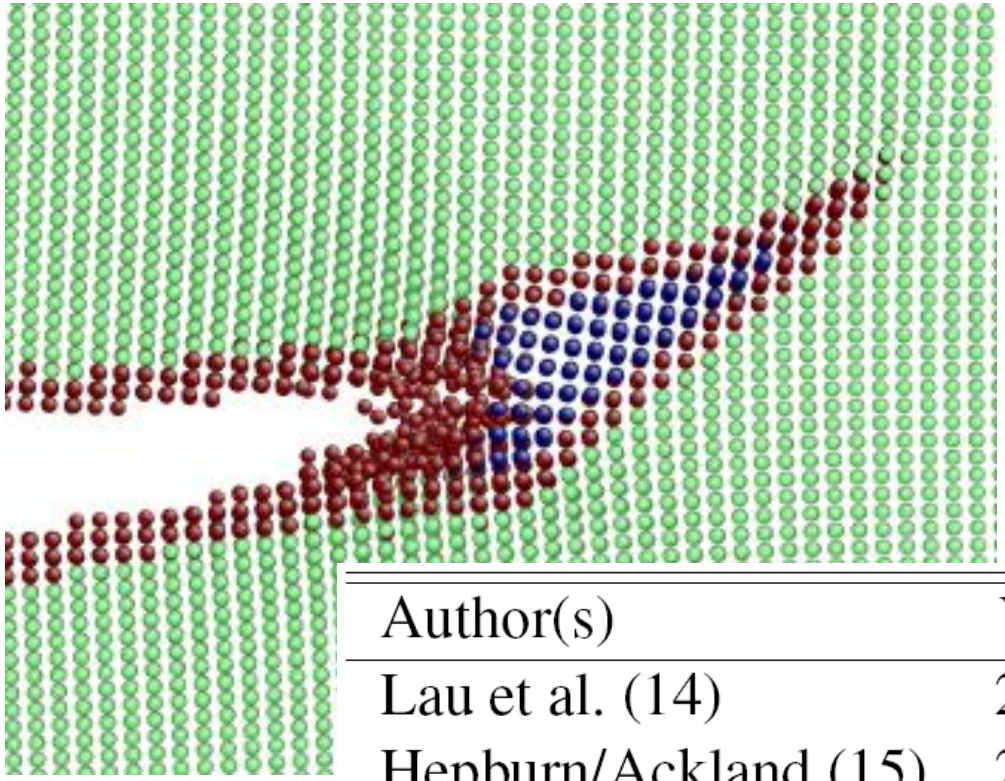


Crack tip mechanisms:



Farkas, 2005

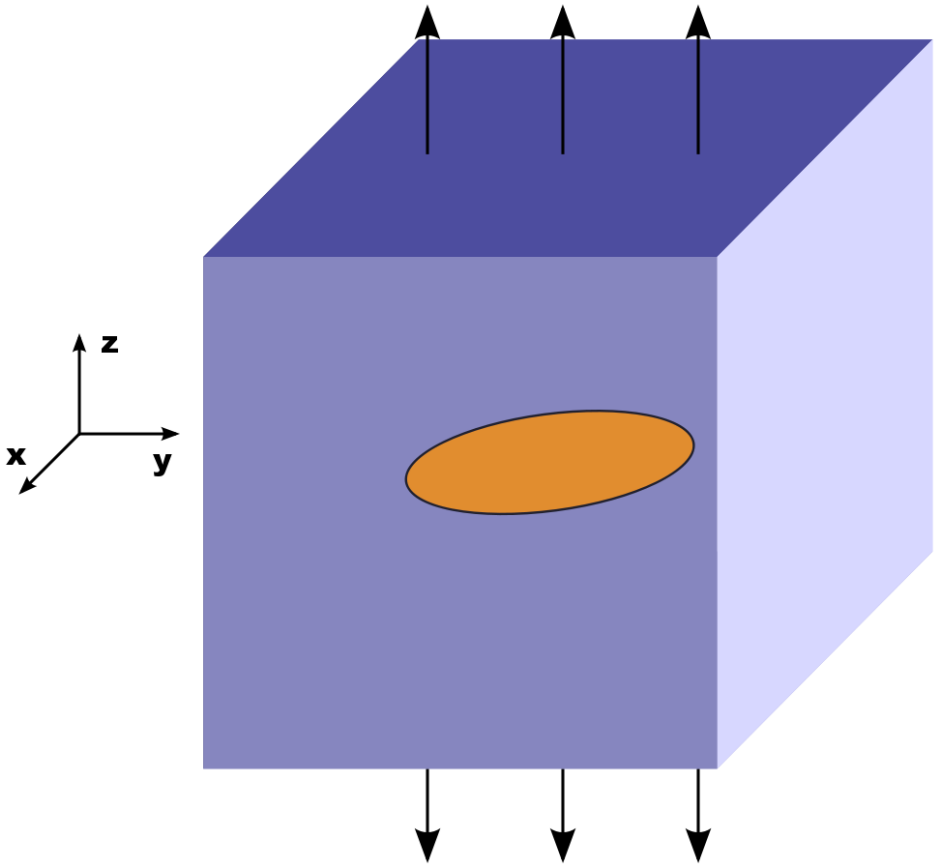
Christer H Ersland, PhD Arctic Materials
Atomistic modeling of bcc-Fe

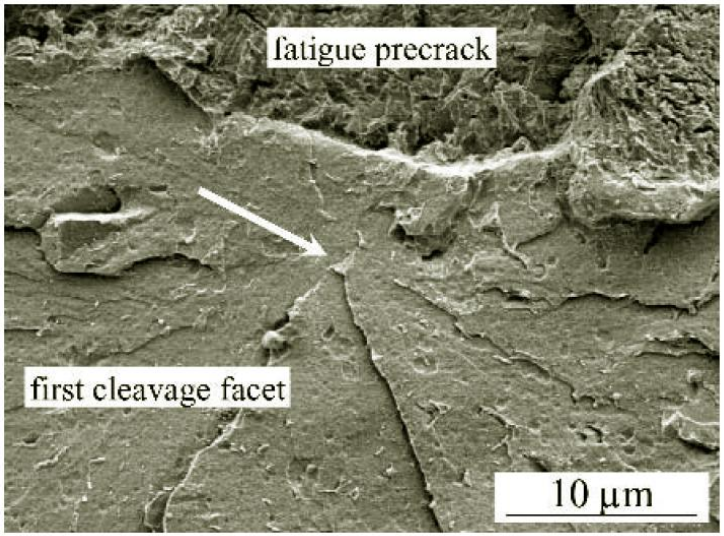


C H Ersland, C Thaulow, D Farkas and E Østby, “Atomistic studies and comparison of α-Fe potentials in mode I fracture” Presented at ECF18, Dresden, Germany, Sept 2010.

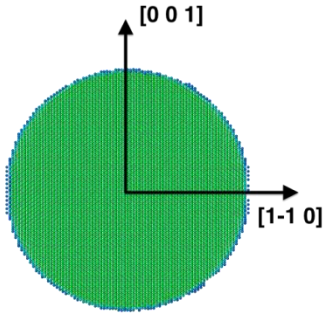
Author(s)	Year	Element(s)	Type
Lau et al. (14)	2007	Fe, C	EAM-FS
Hepburn/Ackland (15)	2008	Fe, C	EAM
Ruda et al. (16)	2009	Fe, C	EAM
Mendelev (17)	-	Fe	EAM
Müller et al. (19)	2007	Fe	ABOP

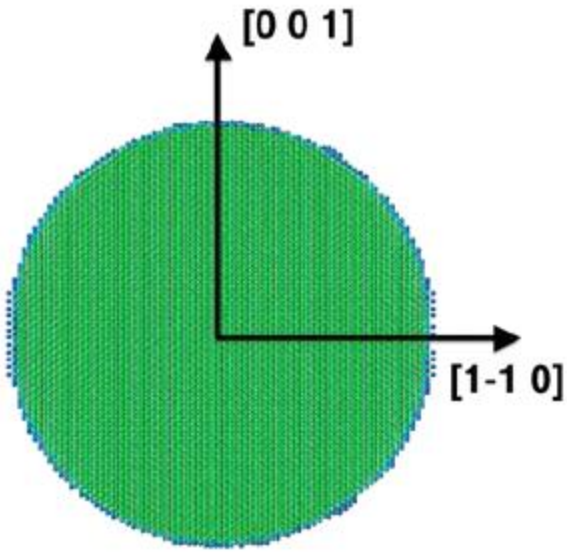
Penny shaped crack



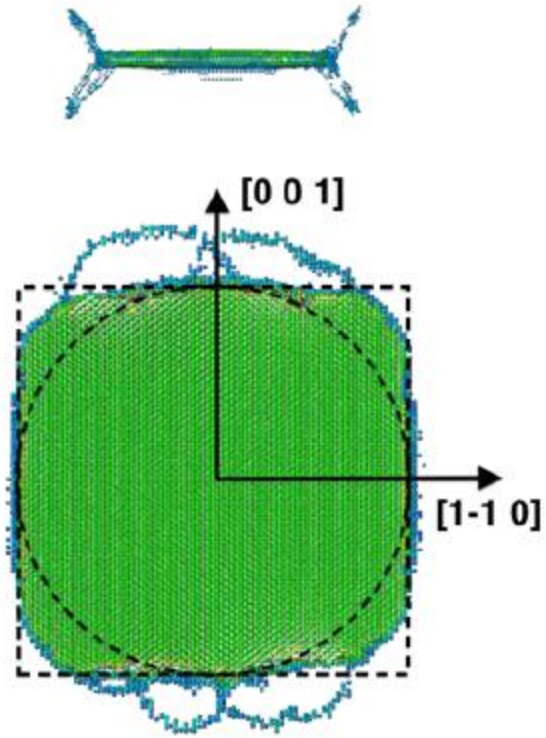


Example: Crack located on the {110} plane

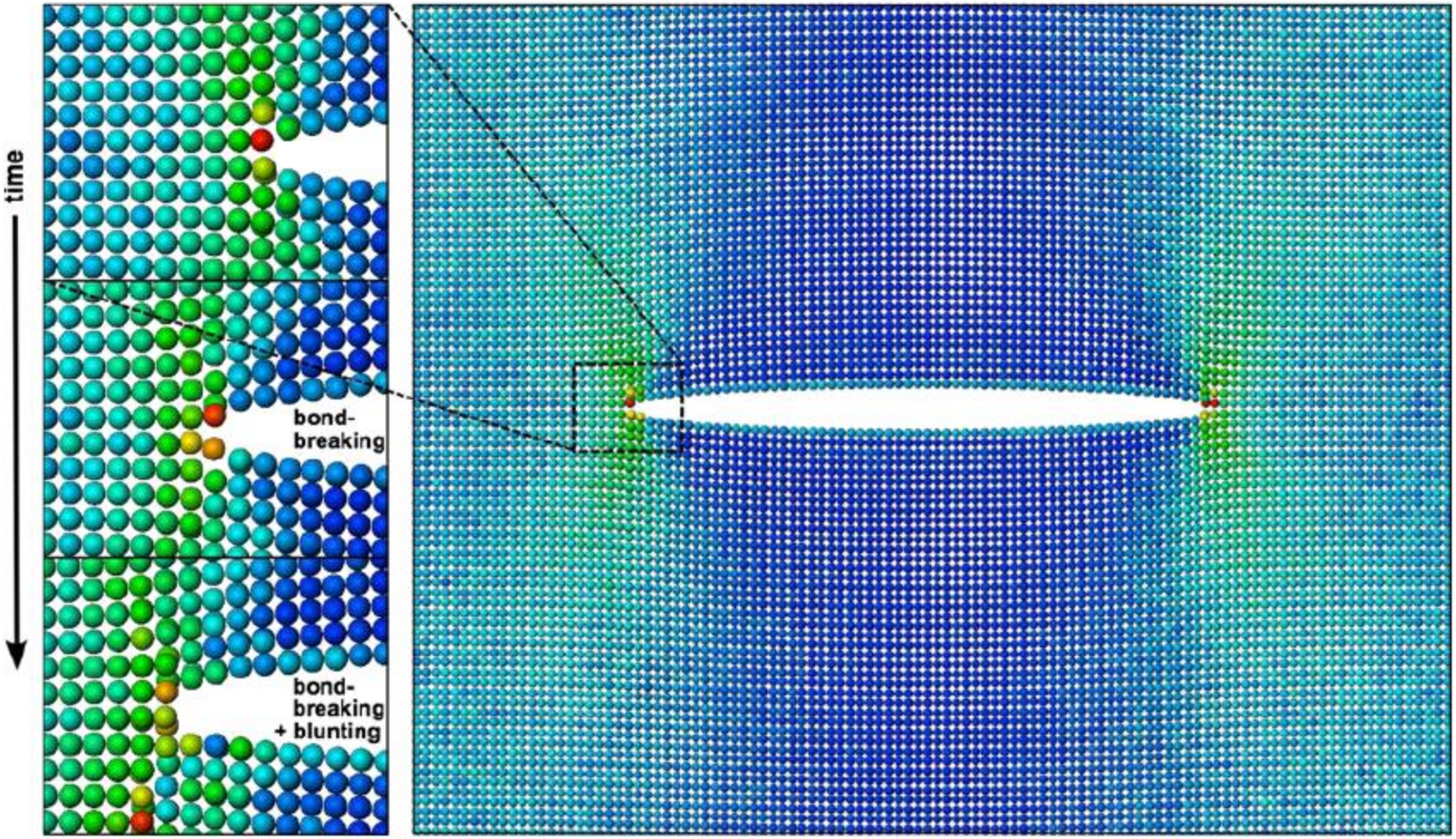


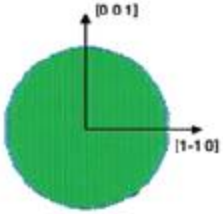


Step 1

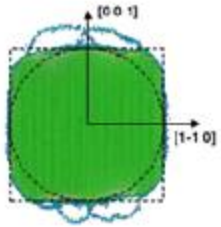


Step 2

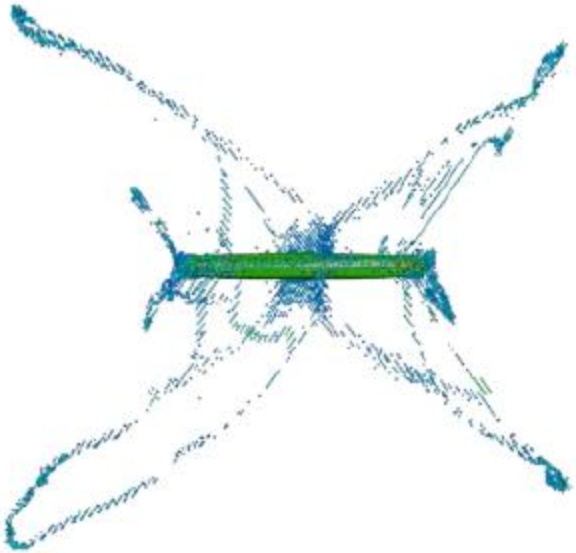

time
bond-
breaking
bond-
breaking
+ blunting

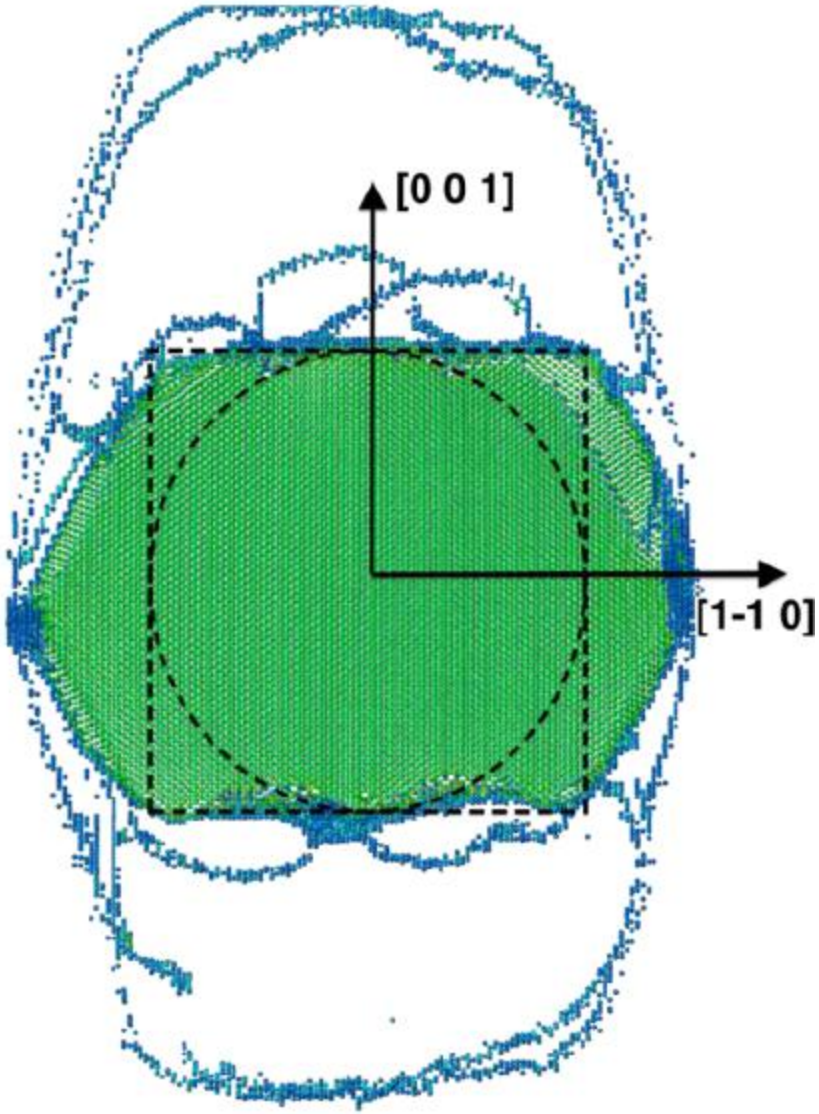


Step 1



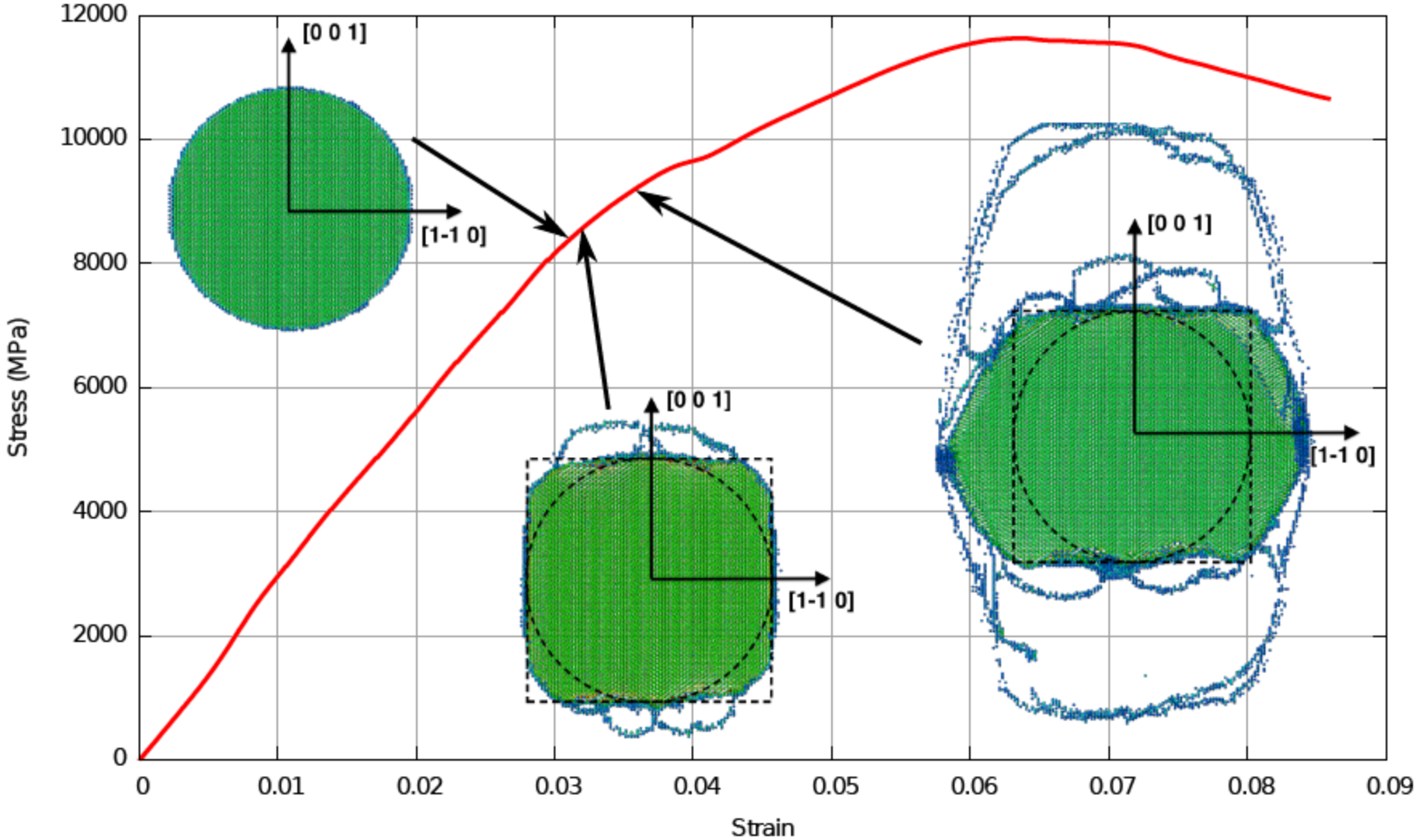
Step 2

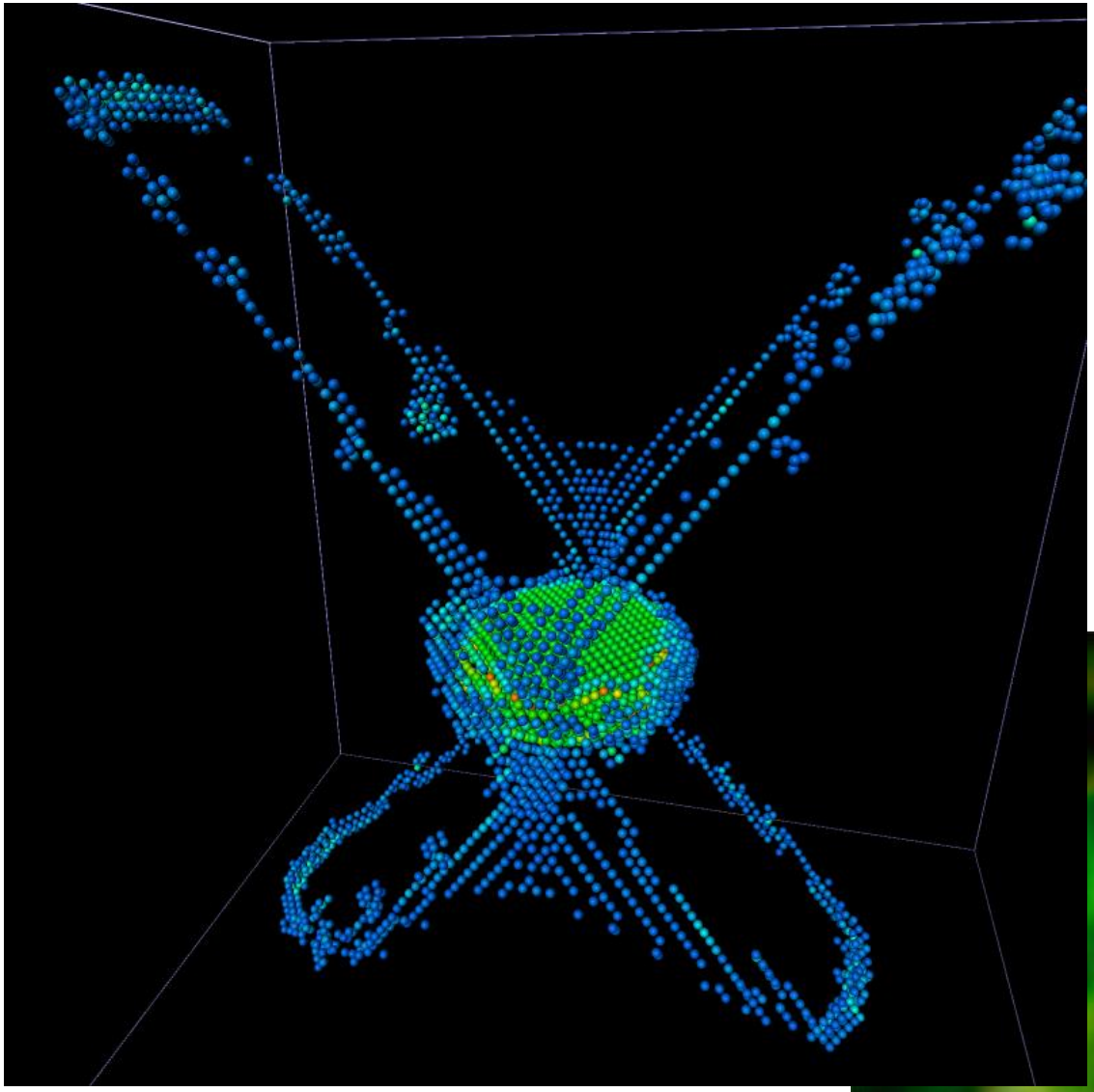




Step 3

Evolution of a penny-shaped crack in the (110)-plane of a pure bcc iron crystal loaded in mode I





Smoke-rings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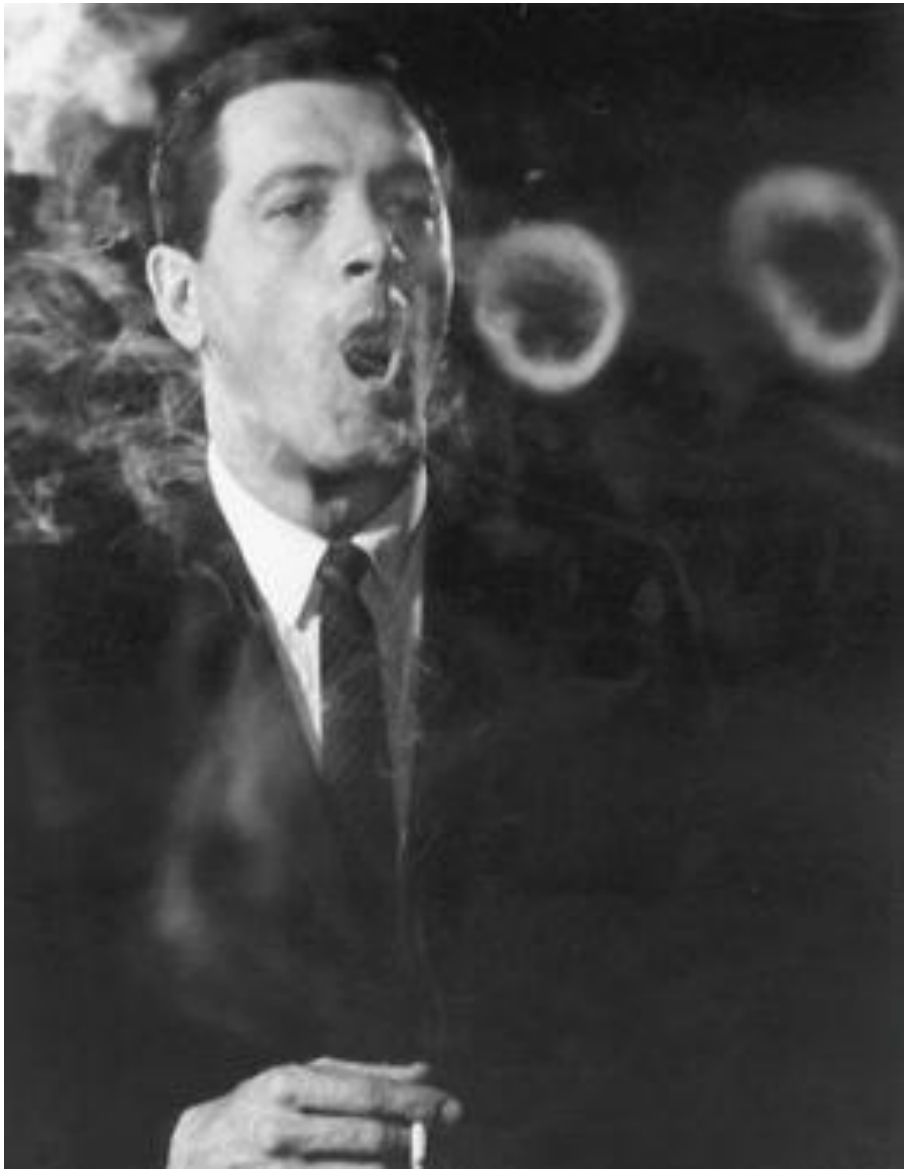
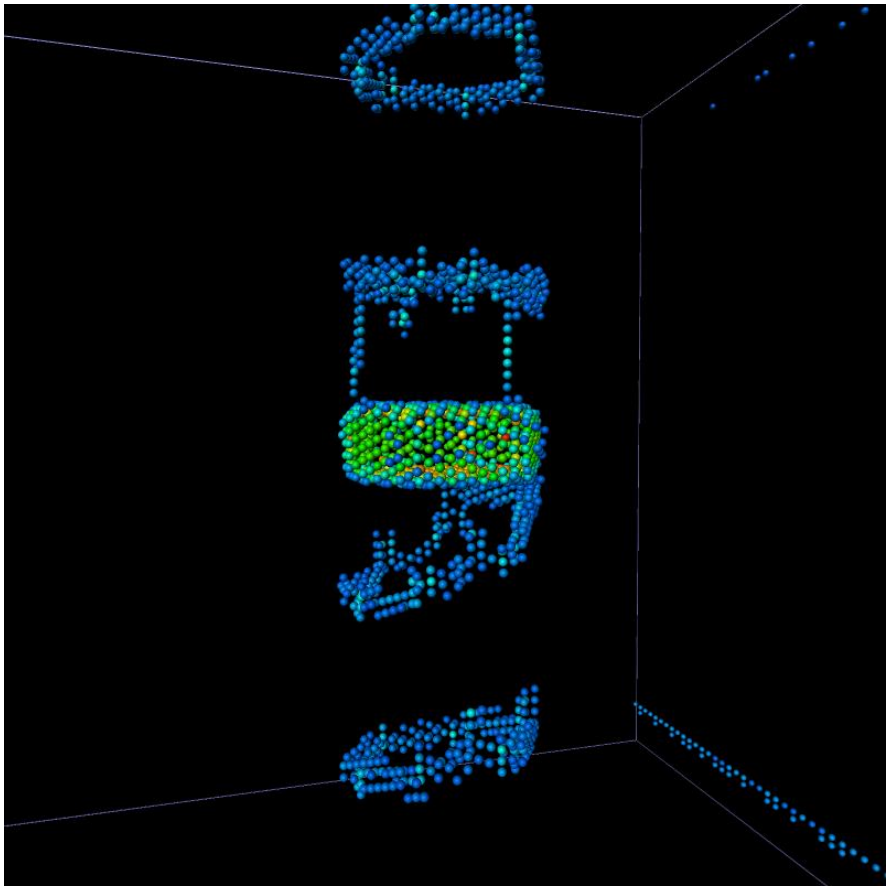
search ID: ena0181





Dual-beam FIB-SEM instrument

FEI COMPANY™
Tools for Nanotech™

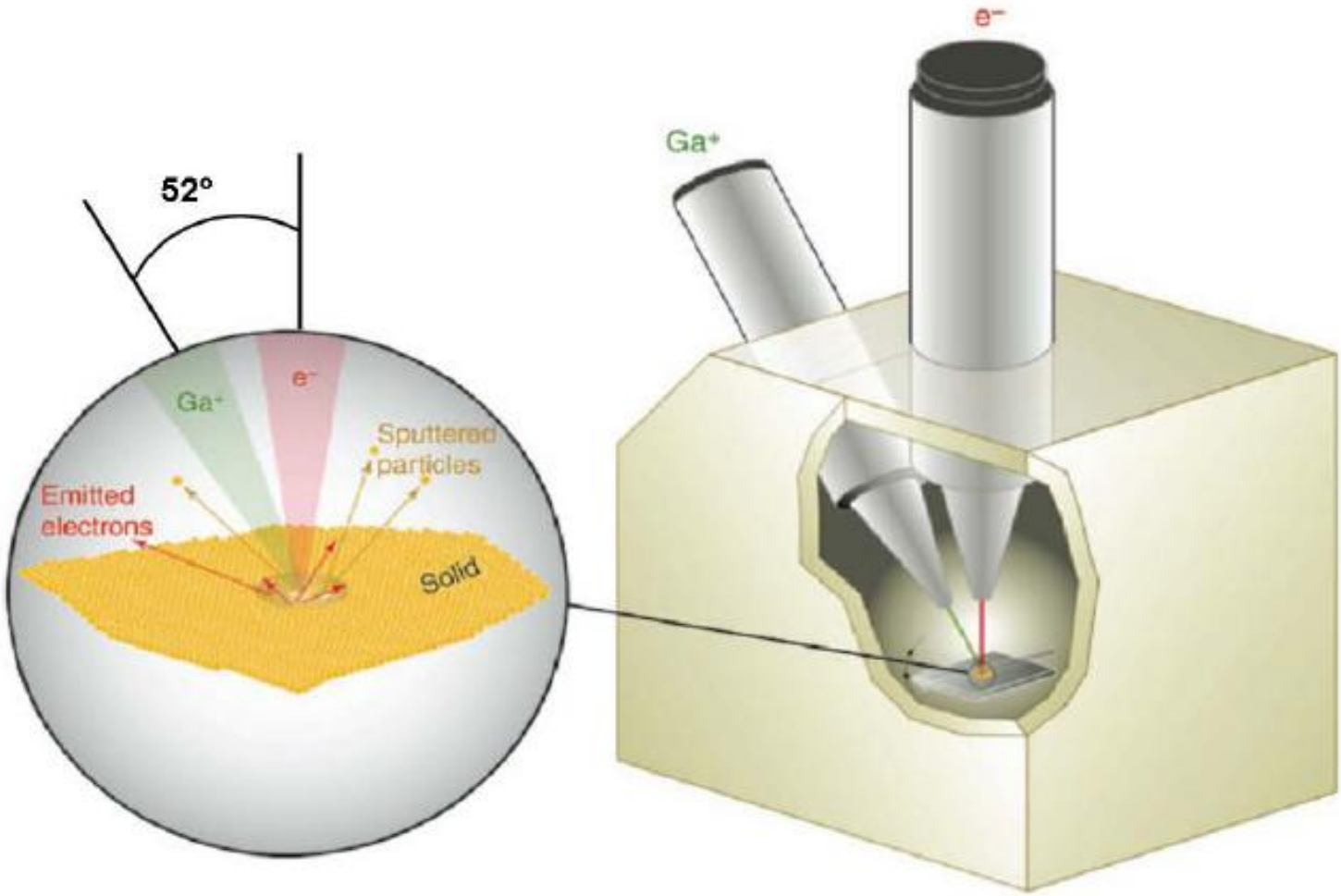
Helios NanoLab

PhD student
Bjørn Rune Sørås Rogne
Nanomechanical testing

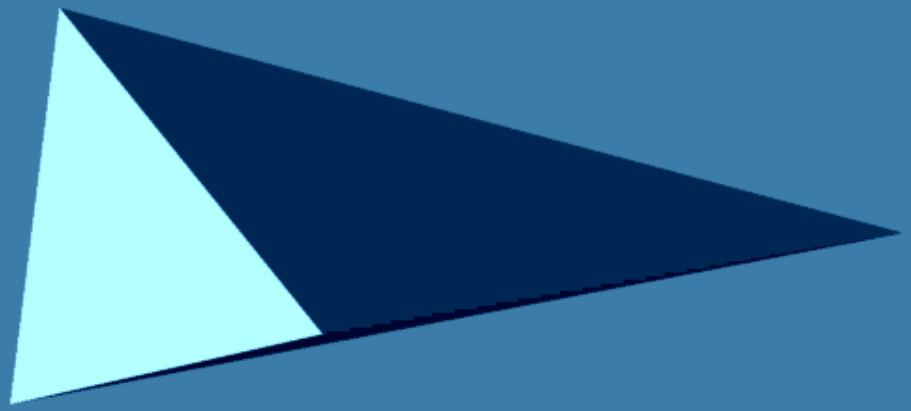
FIB:

Beam Current	Best Use
1.5 - 9.7 pA	High resolution
28 - 48 pA	Standard imaging
>93 pA	Milling

Dual-beam FIB-SEM instrument

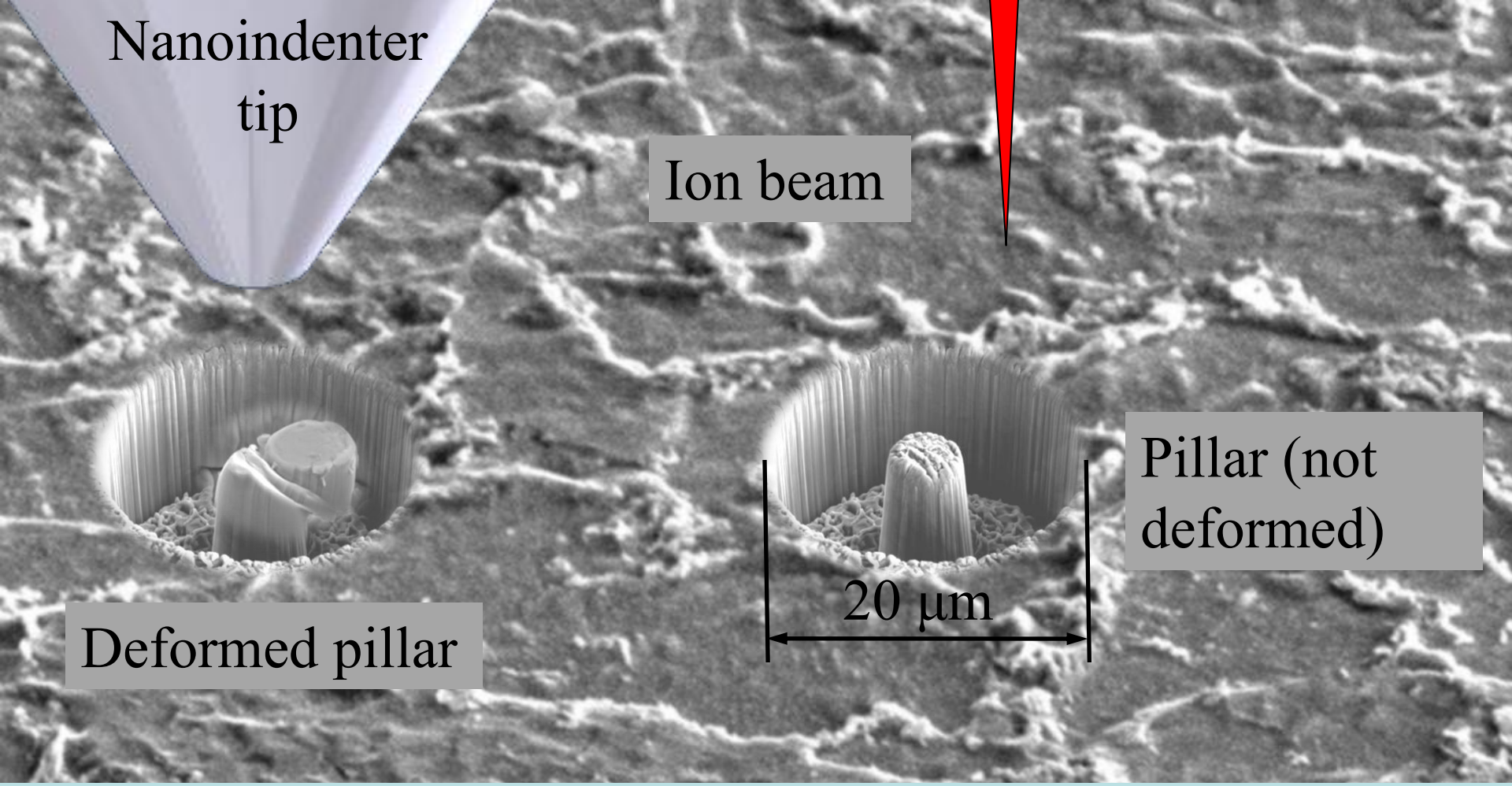


Indentation into the surface



Nanoindentation test – Local hardness test

Material properties:
→Hardness (H)
→Young's modulus (E)

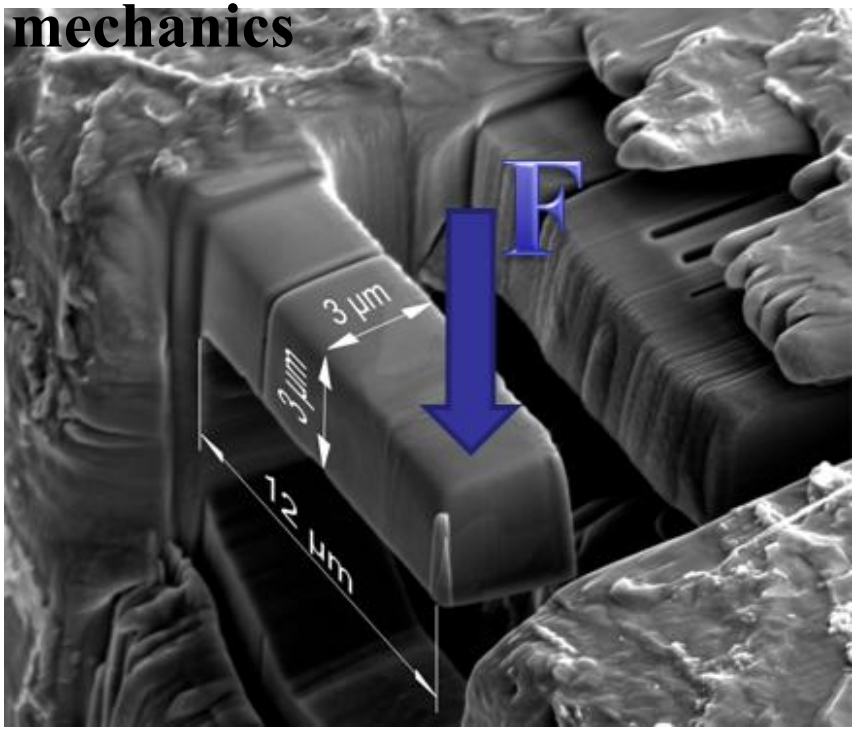


1. Machine out specimens by using a Focused Ion Beam (Ga^+) (NTNU NanoLab).
2. Load the specimens with a flat ended nanoindentation tip (Nanomekanisk lab)

→ Additional material properties can be calculated.

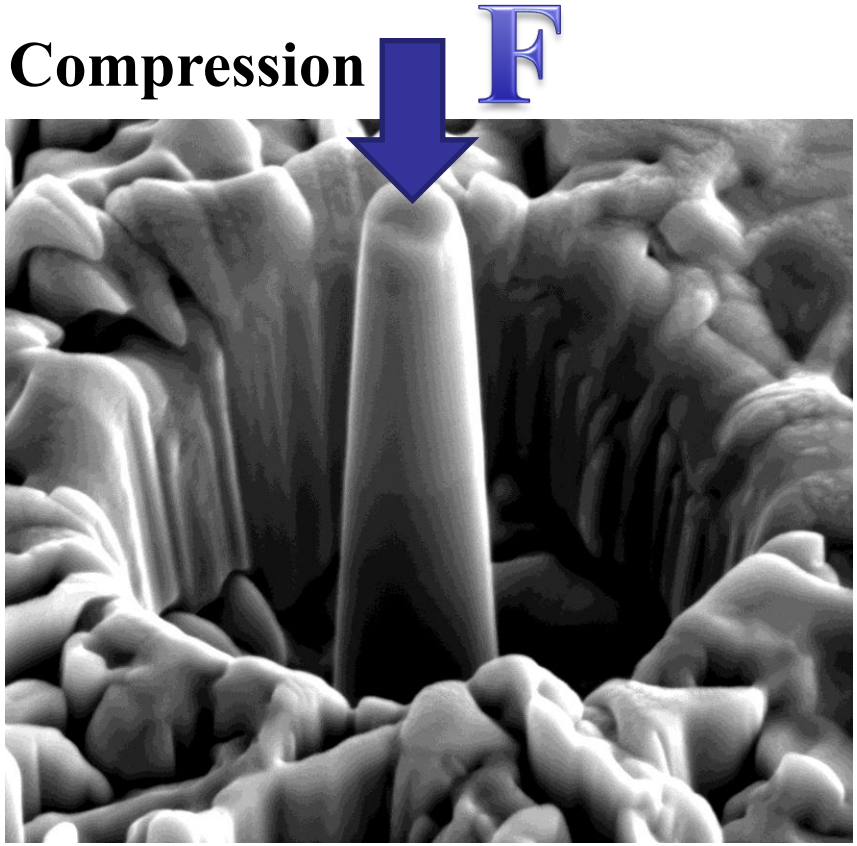
Test specimens

Fracture mechanics



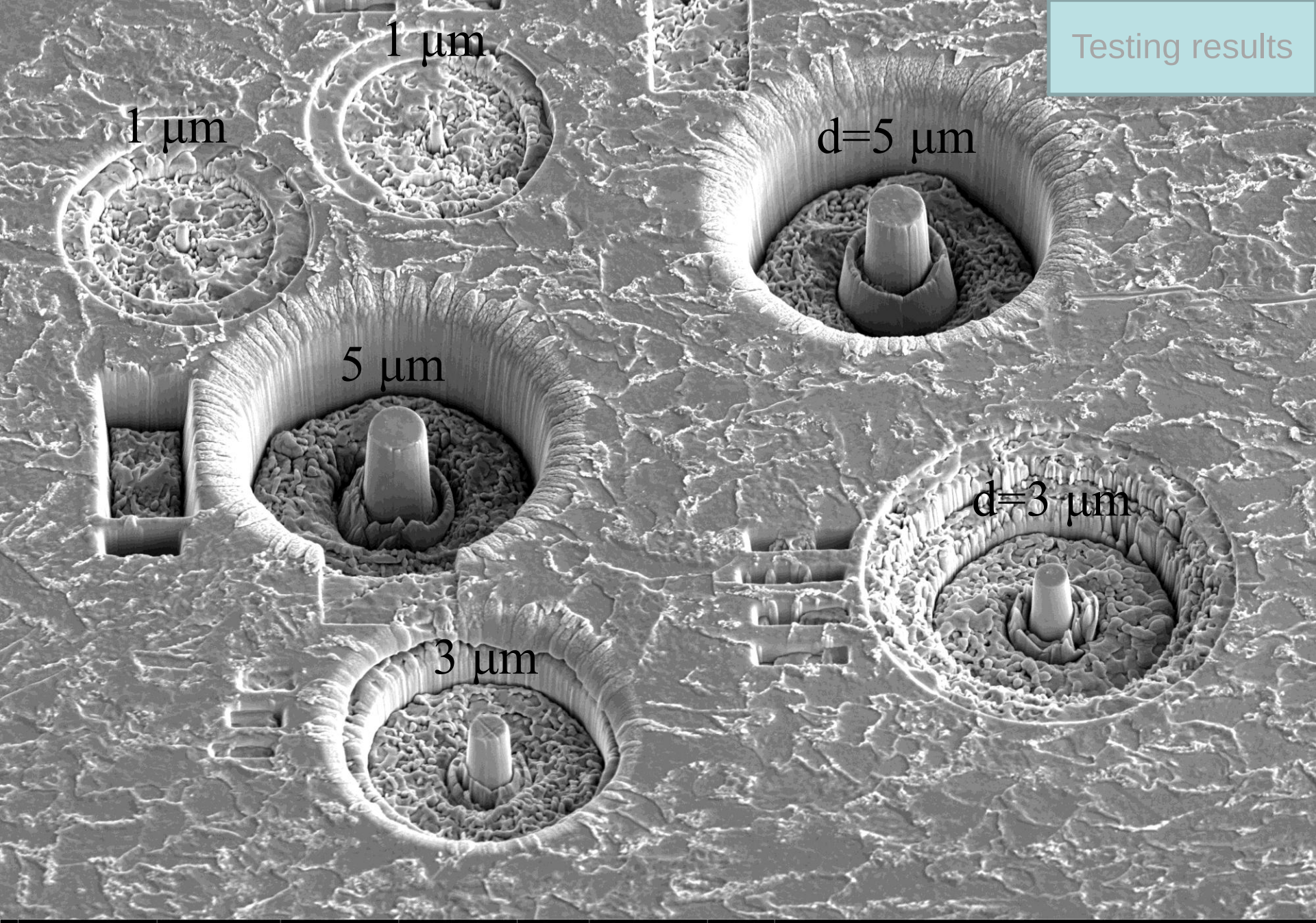
→**Fracture toughness (K_c)**

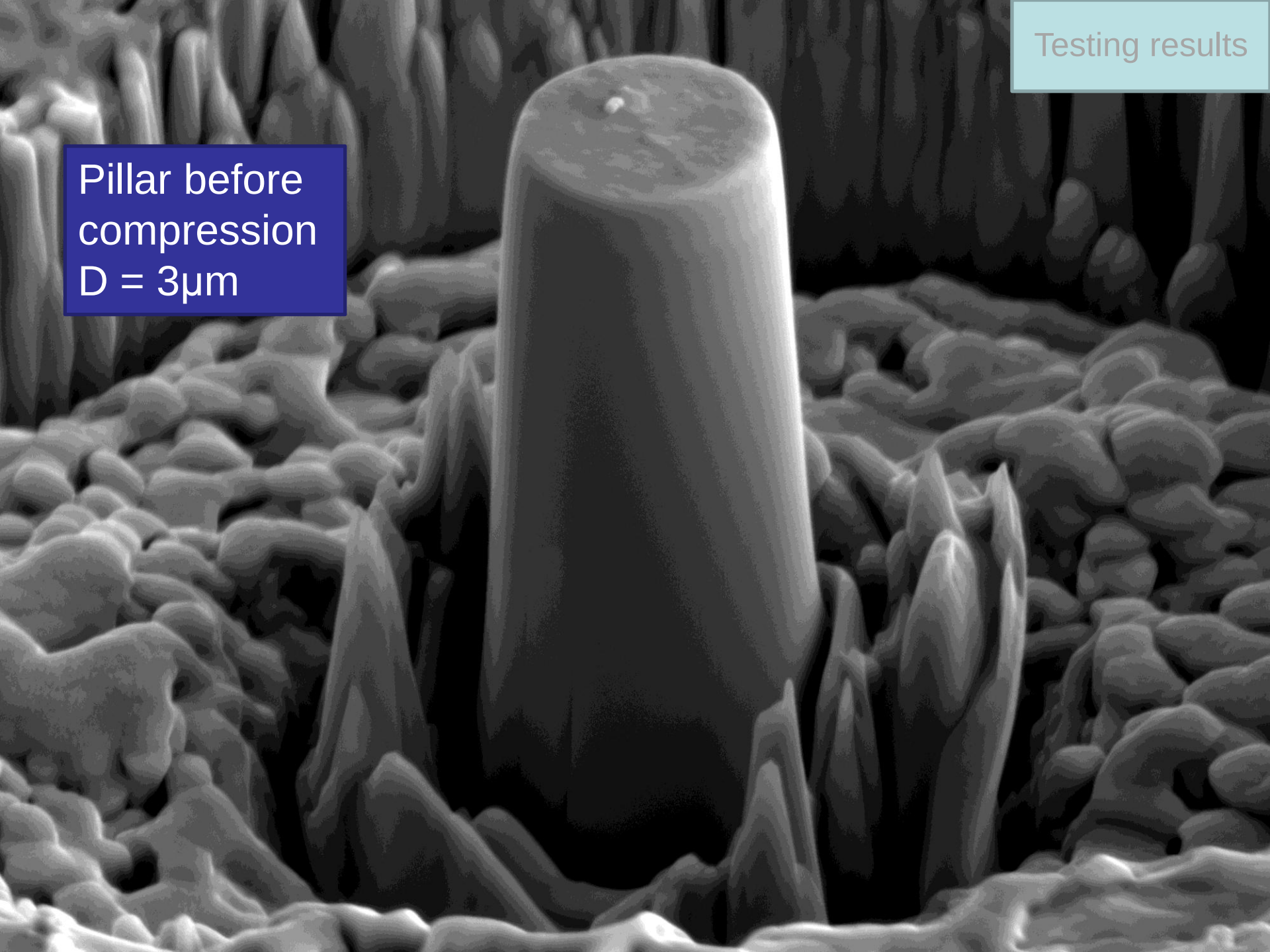
Compression

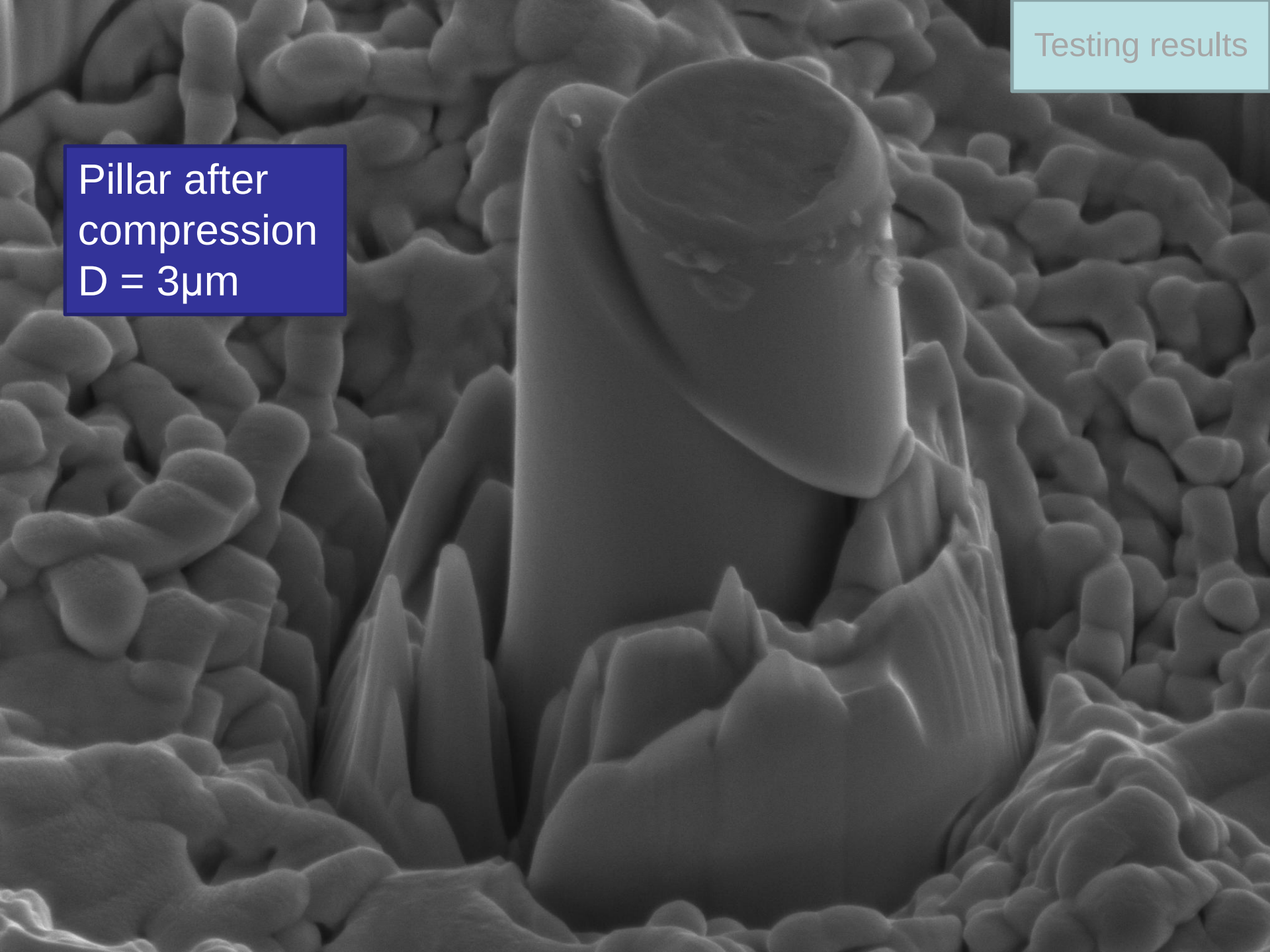


→**Yield stress (σ_y)**

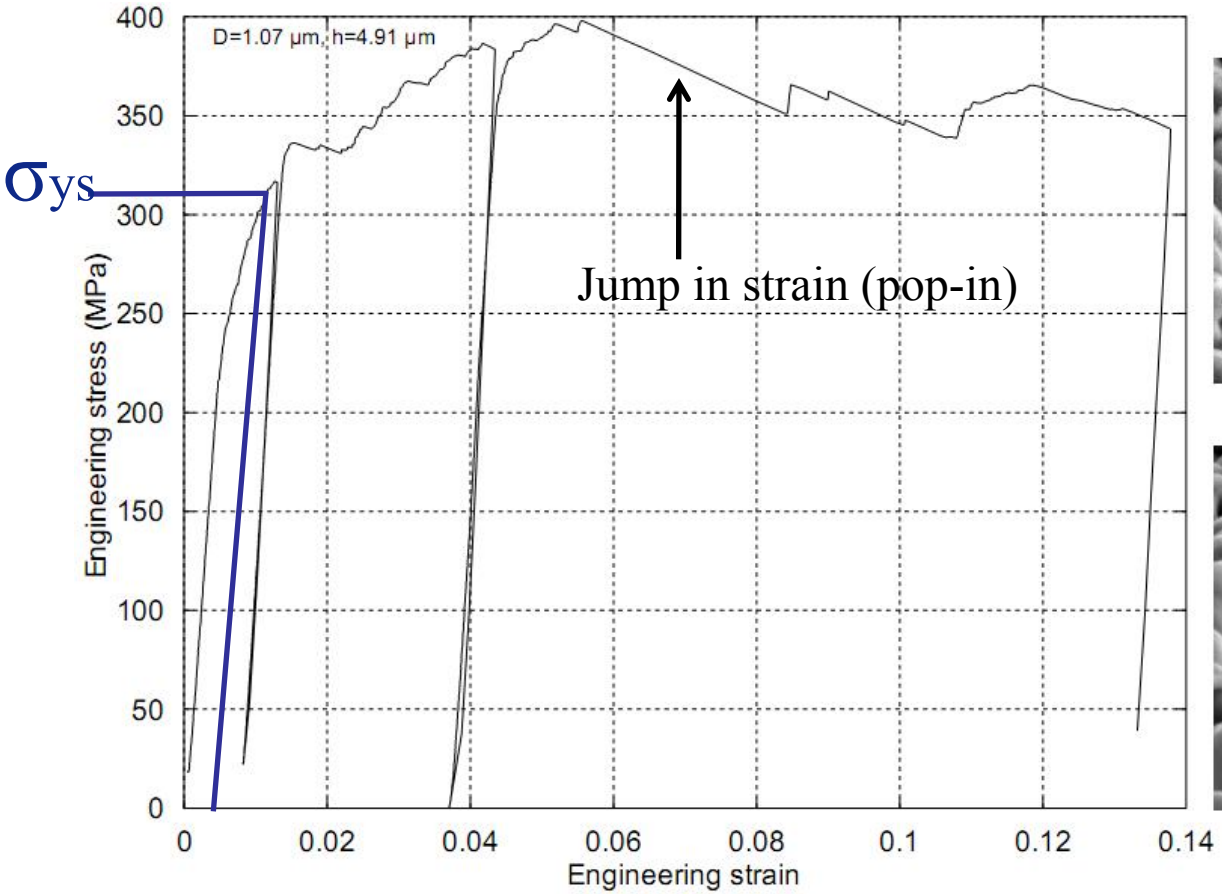
Testing results

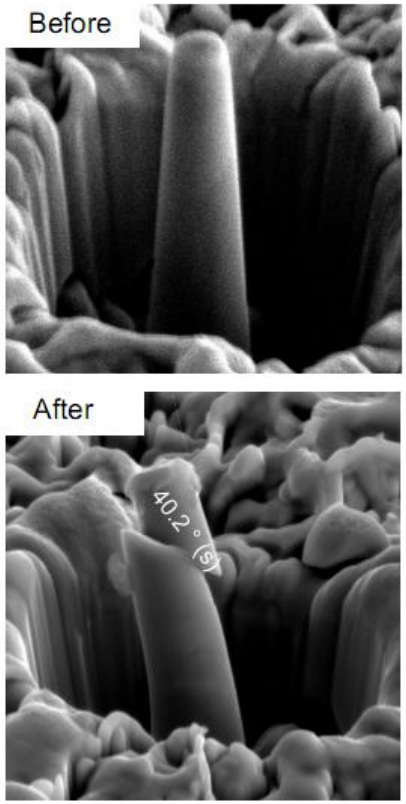



Pillar before
compression
D = 3μm


Pillar after
compression
D = 3μm

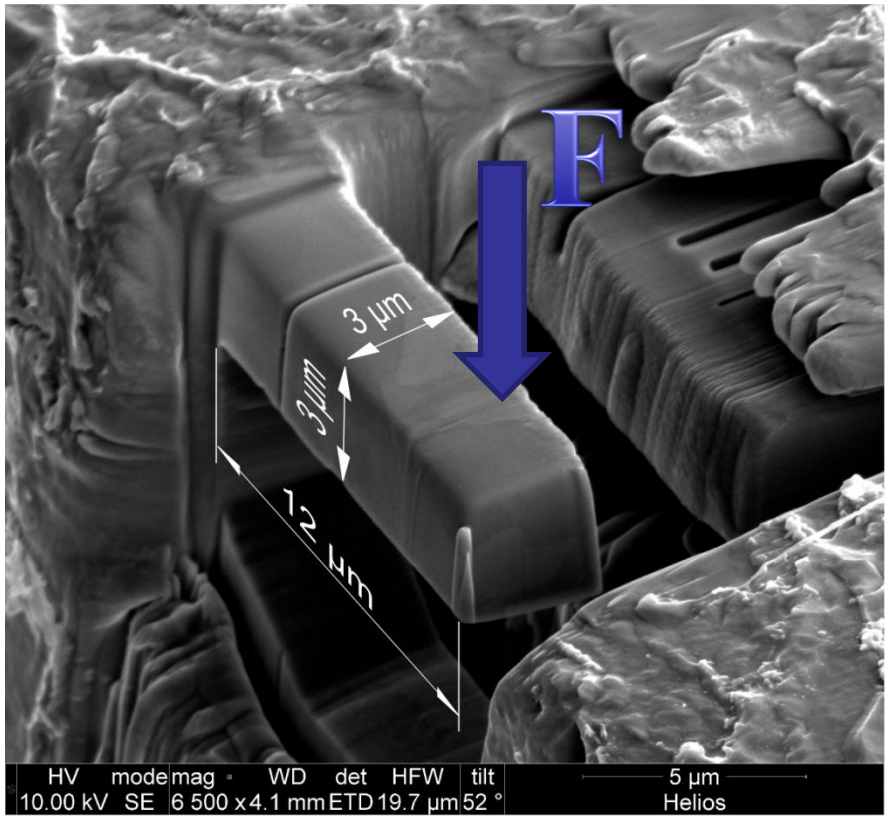
Stress-strain test result from compression testing of pillars



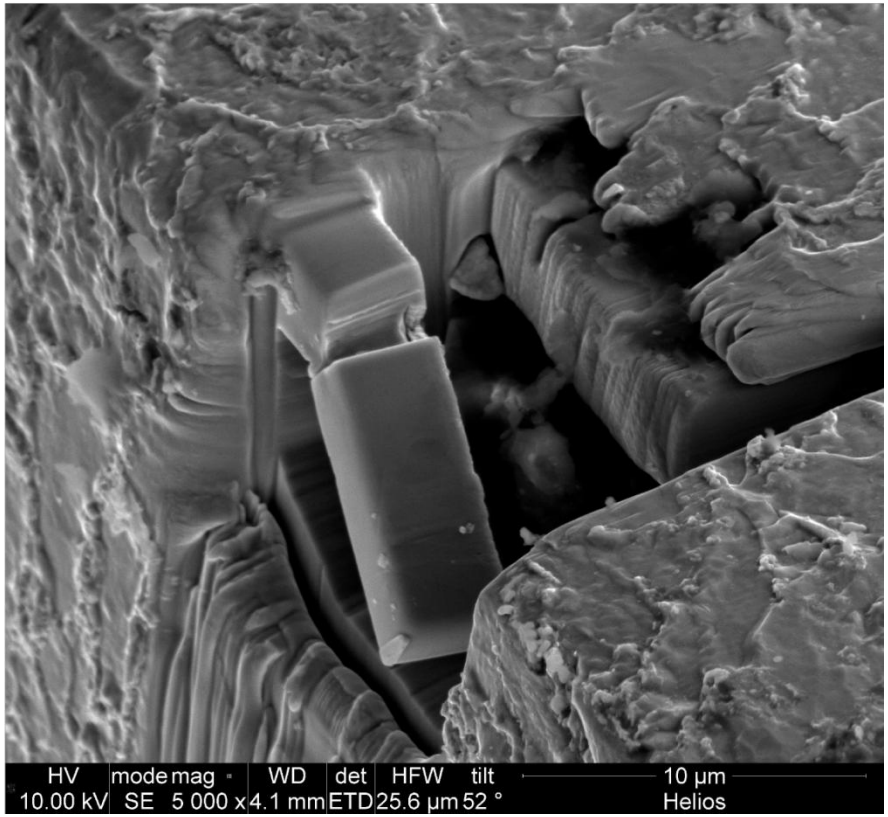


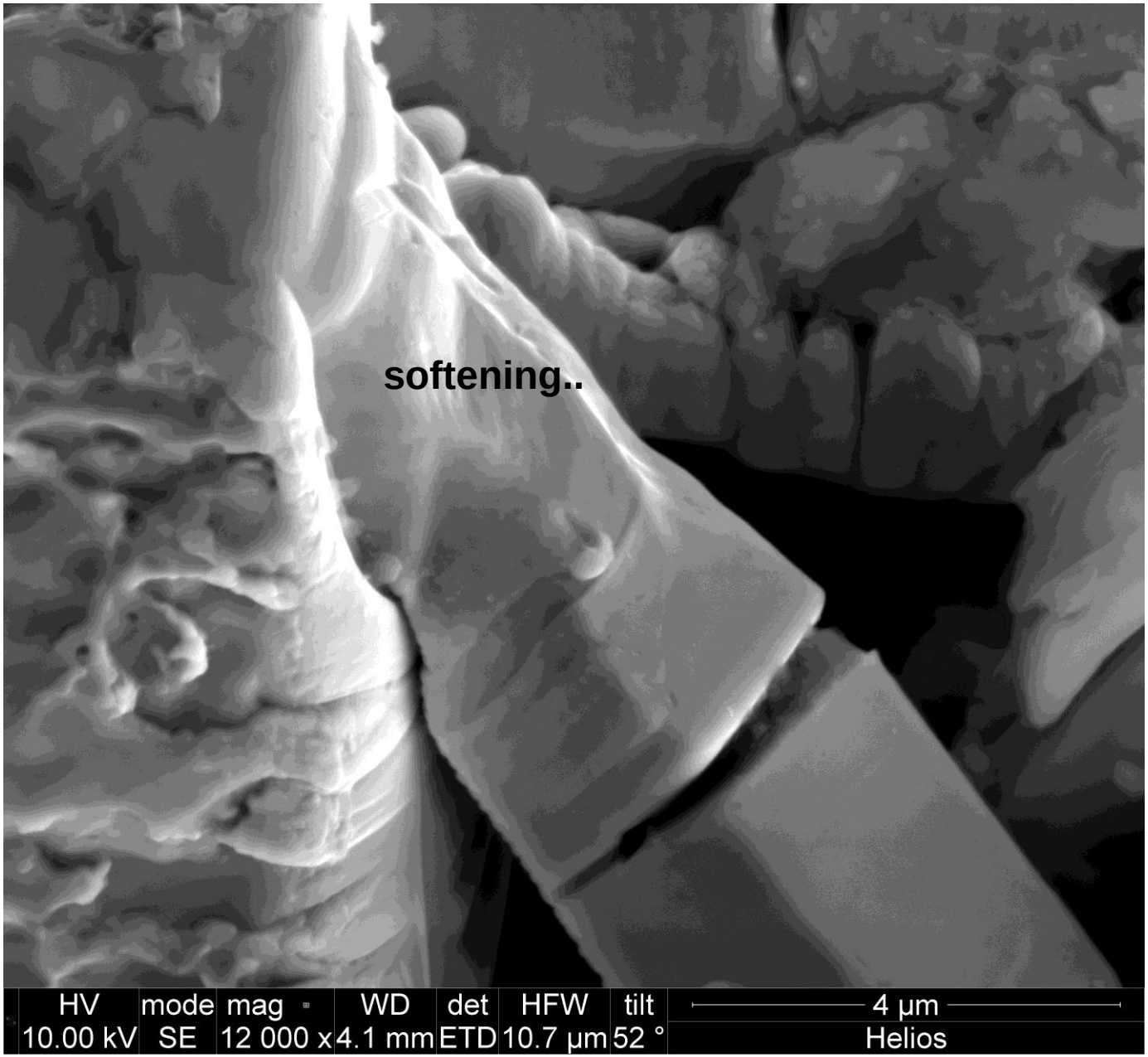
Fracture mechanics test: cantilever beam with notch

Before loading



After loading

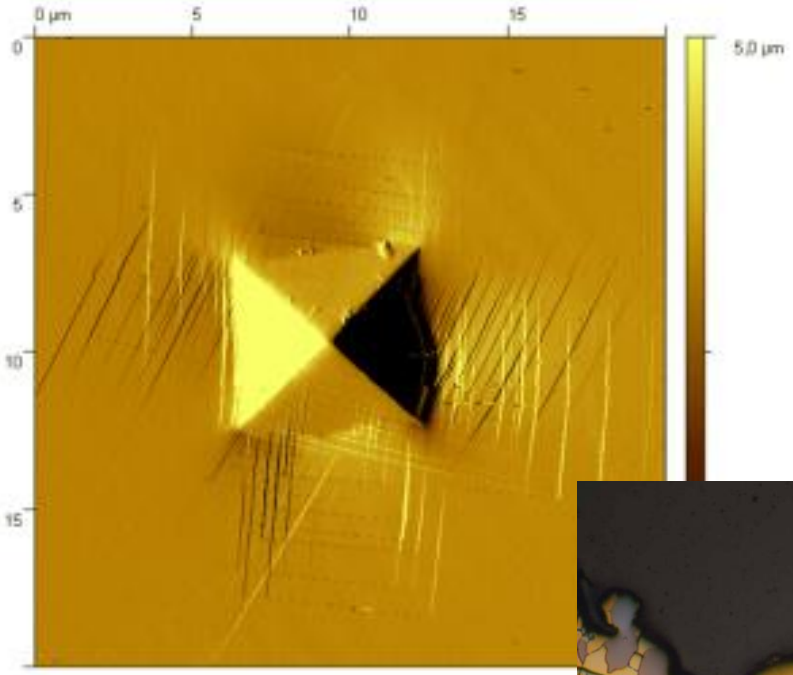


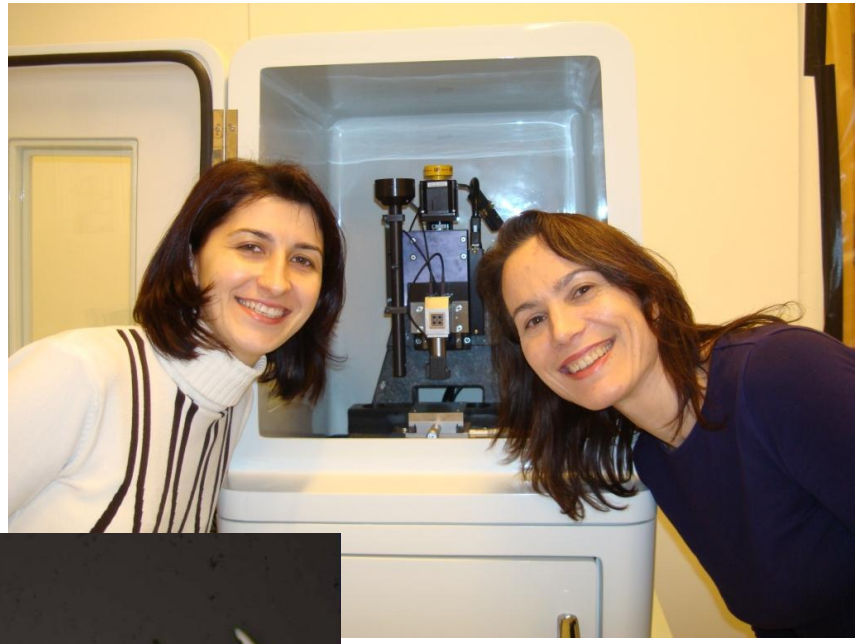

softening..
HV
10.00 kV
mode
SE
mag
12 000 x
WD
4.1 mm
det
ETD
HFW
10.7 µm
tilt
52 °
4 µm
Helios

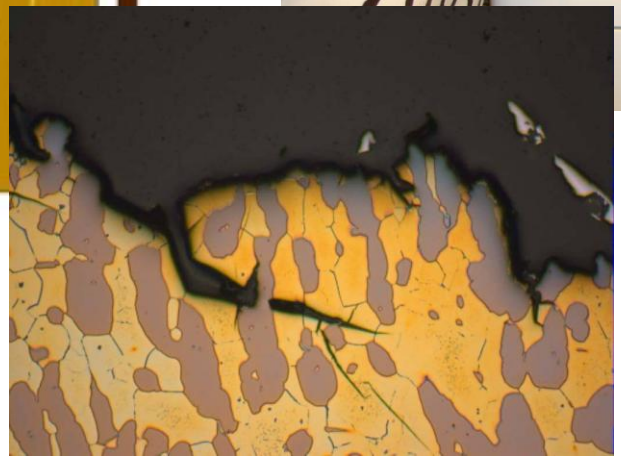

My first pillar
HV
10.00 kV
mode
SE
mag
6 500 x
WD
4.1 mm
det
ETD
HFW
19.7 µm
tilt
52 °
5 µm
Helios

Adina Basa, PhD HISC project

Nanoindentation of stainless steels with in situ hydrogen charging

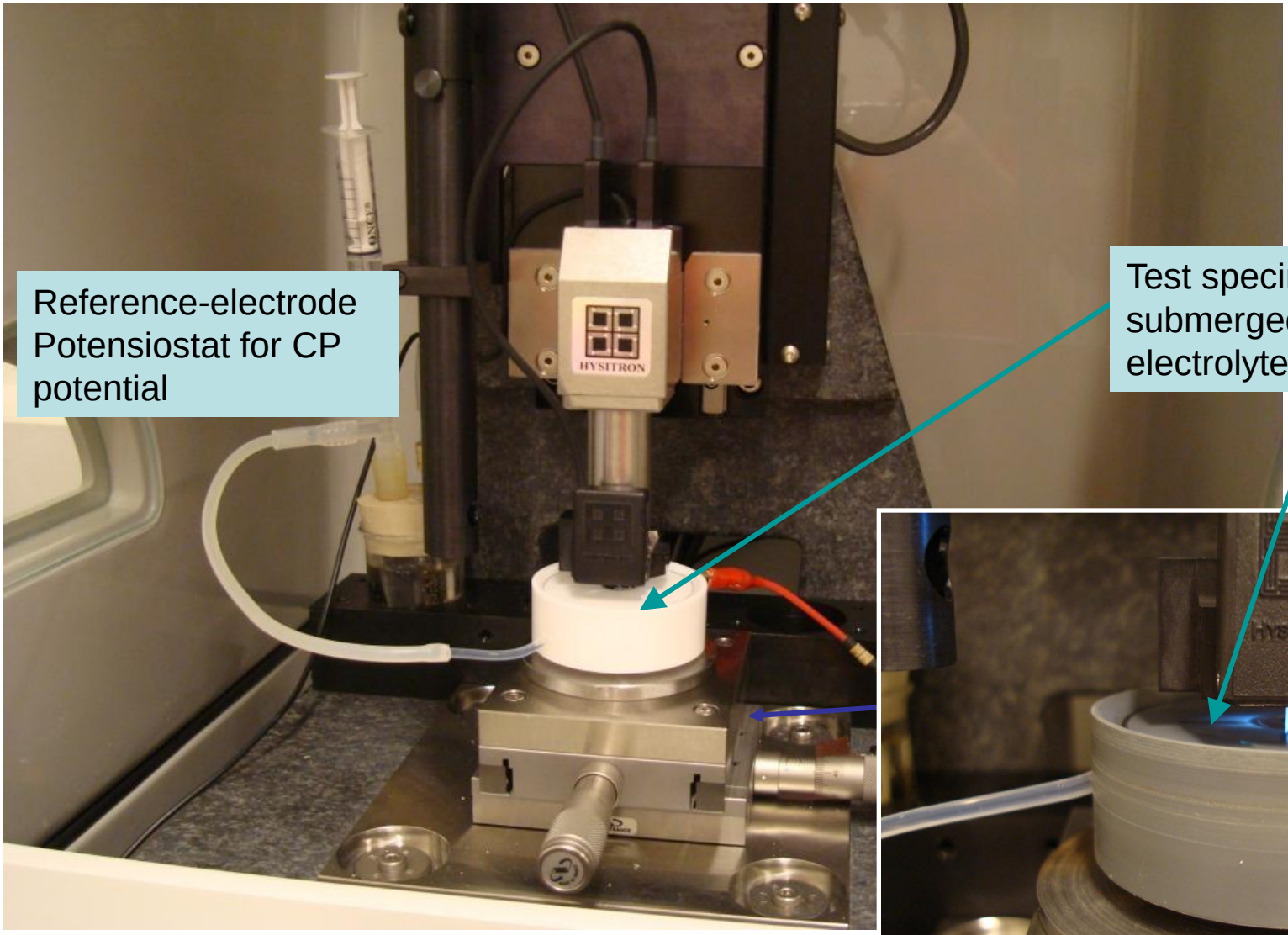


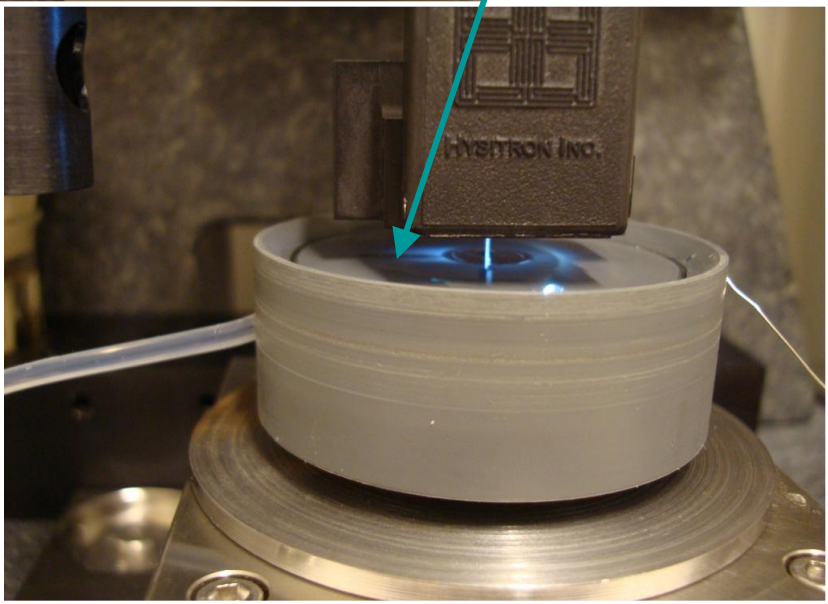




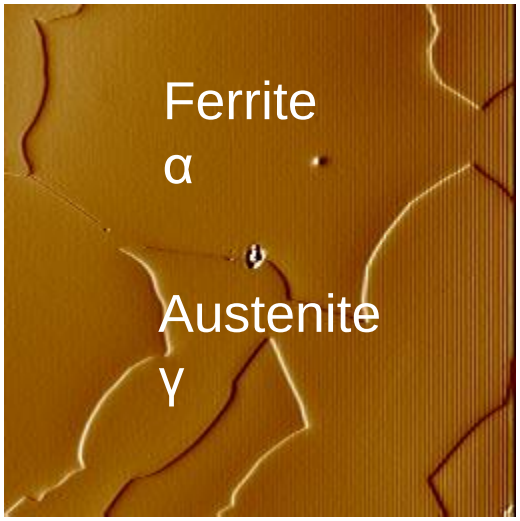
Superduplex stainless steel
26%Cr-7%Ni-4%Mo
austenite - ferrite

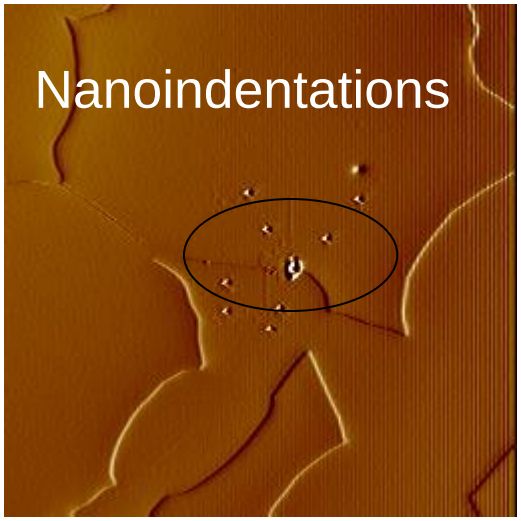
Nanoindentation with in situ hydrogen charging of stainless steel

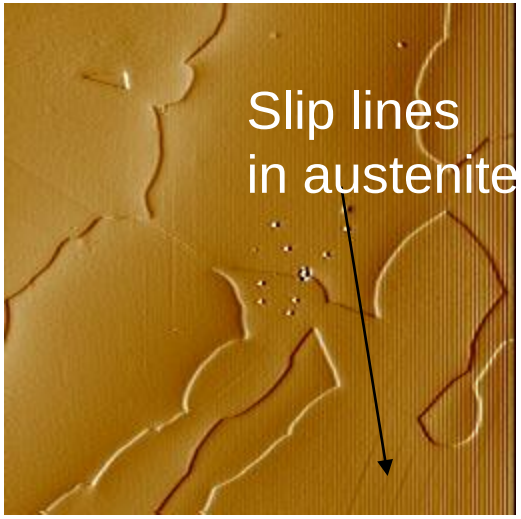




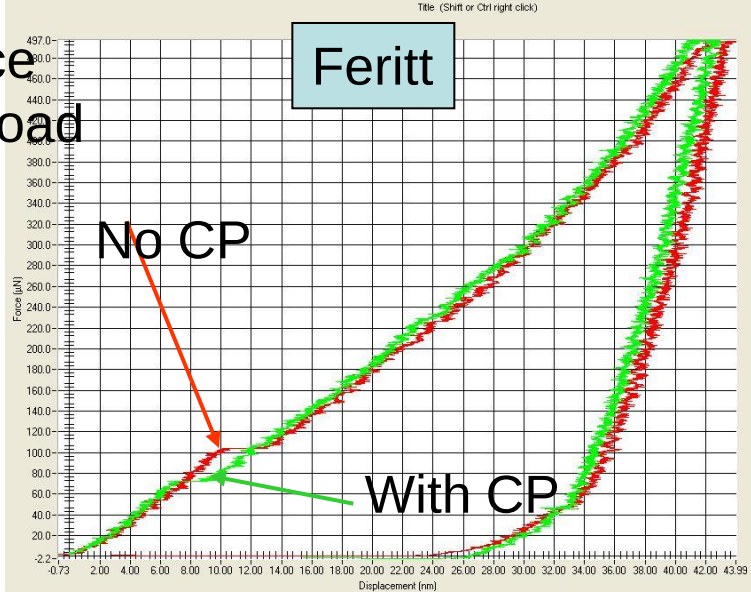
CP for 1 hour at -1050mV$_{sce}$







CP reduce
”pop in”-load



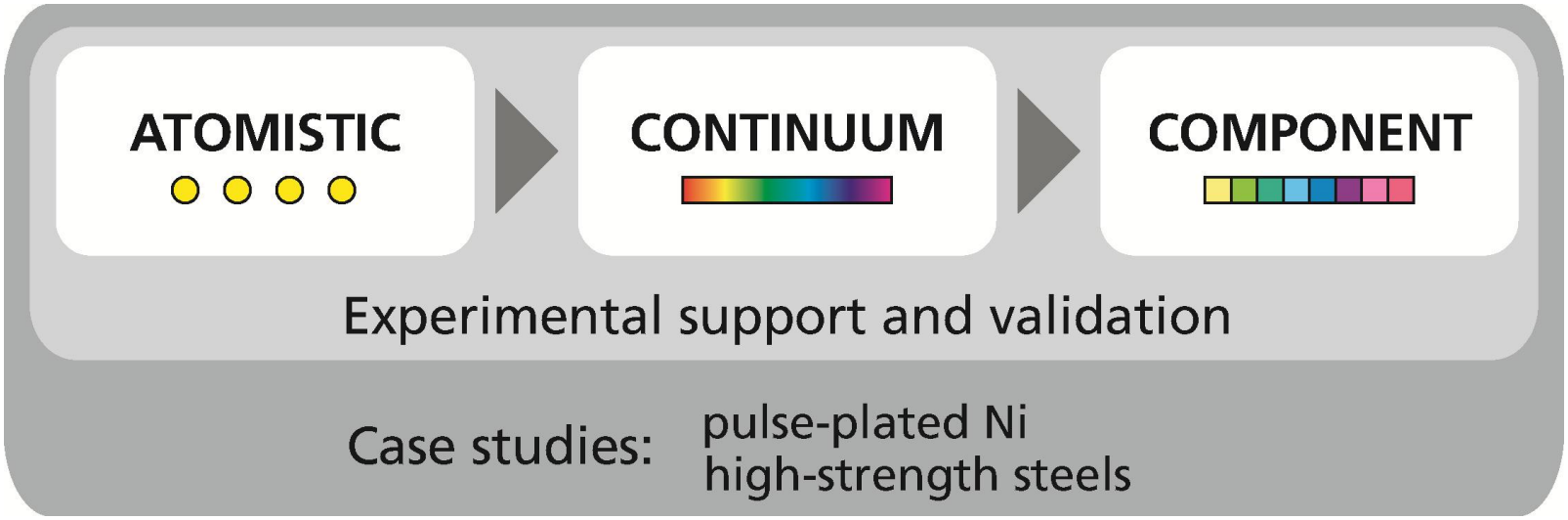
Multiscale modelling of hydrogen embrittlement in crystalline materials

MultiHy

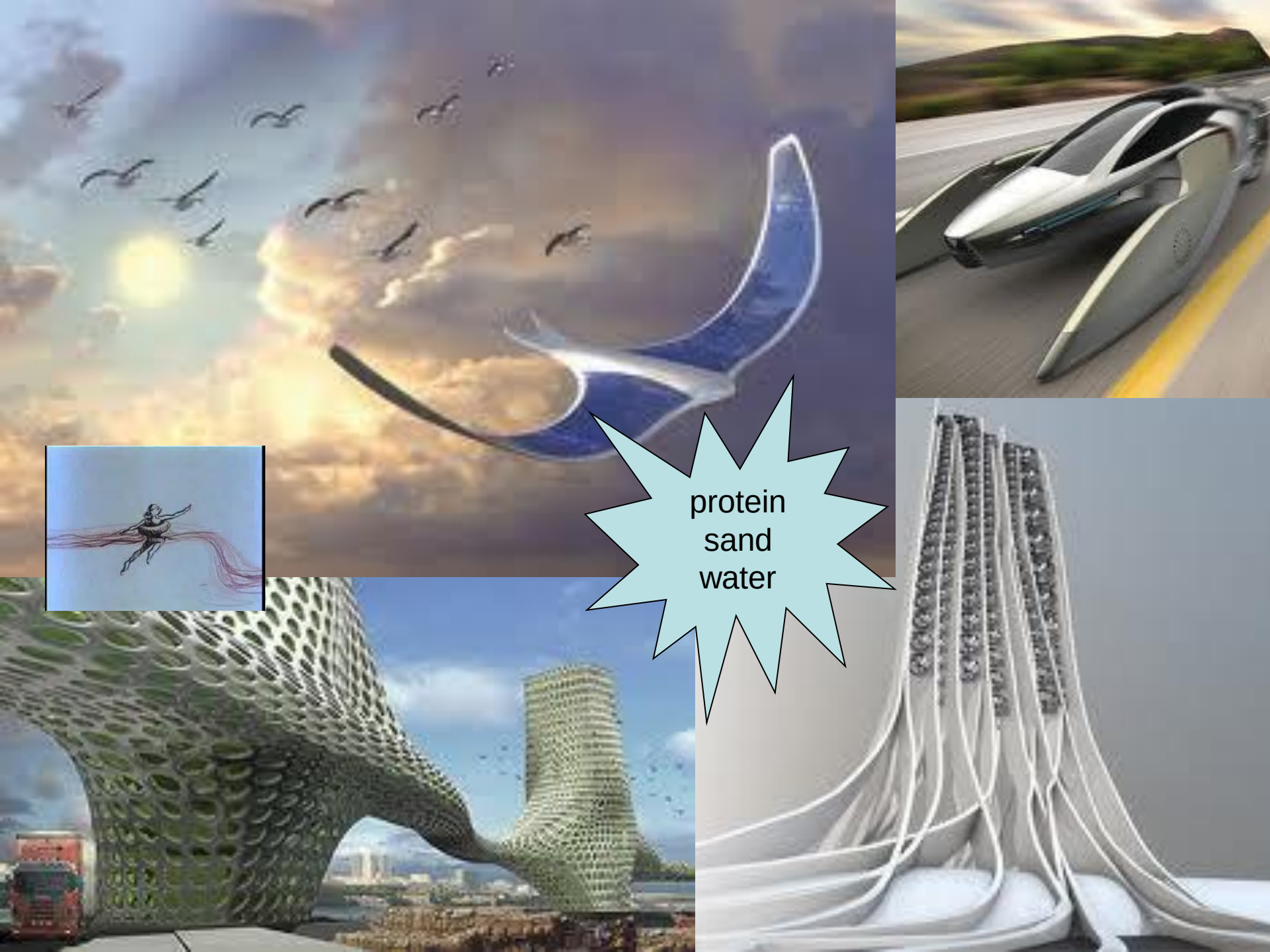
Collaborative Project
(Small or medium-scale focused research project)

SEVENTH FRAMEWORK PROGRAMME

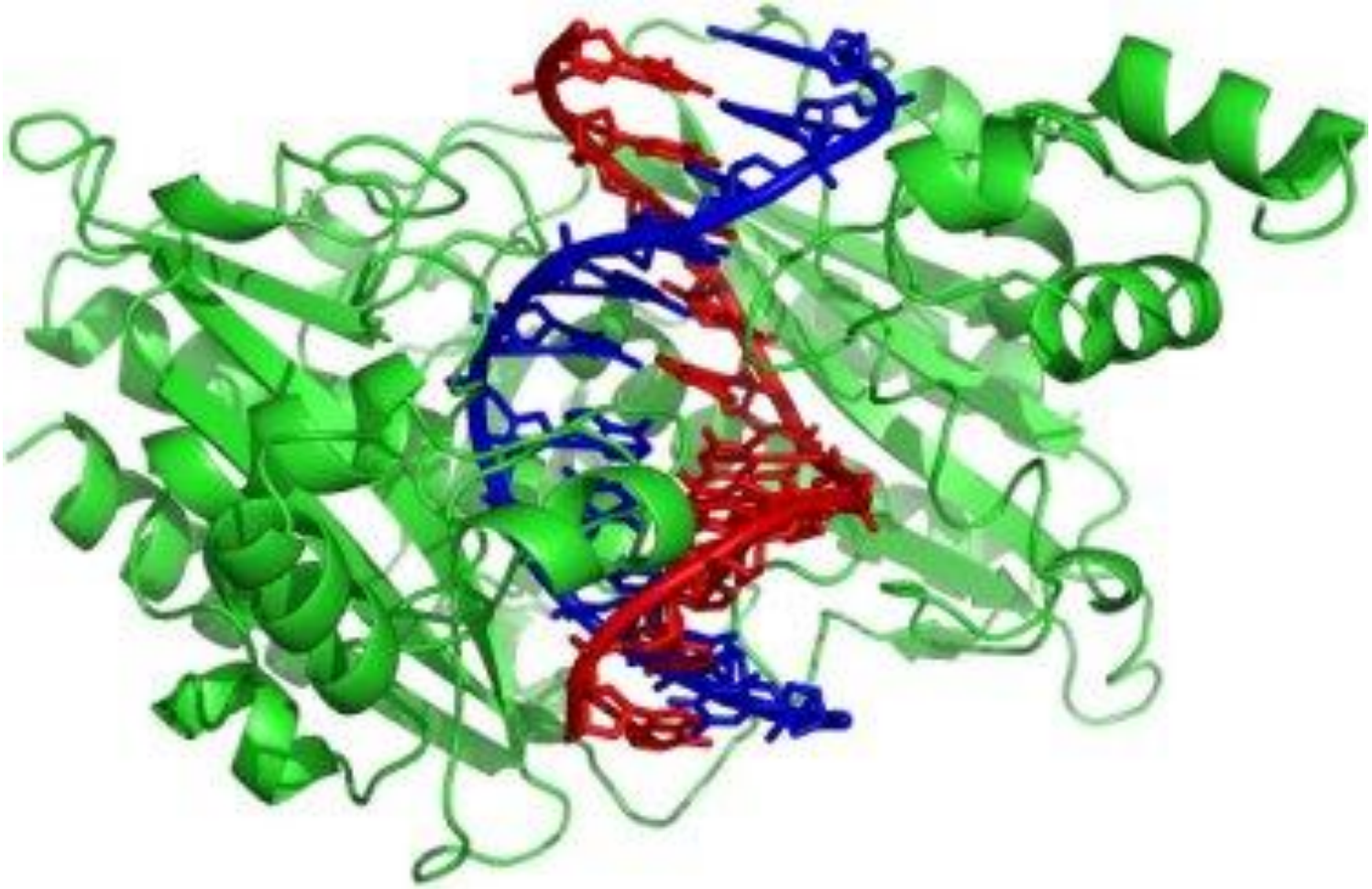
NMP Theme
Call Identifier: FP7-NMP-2010-SMALL-4



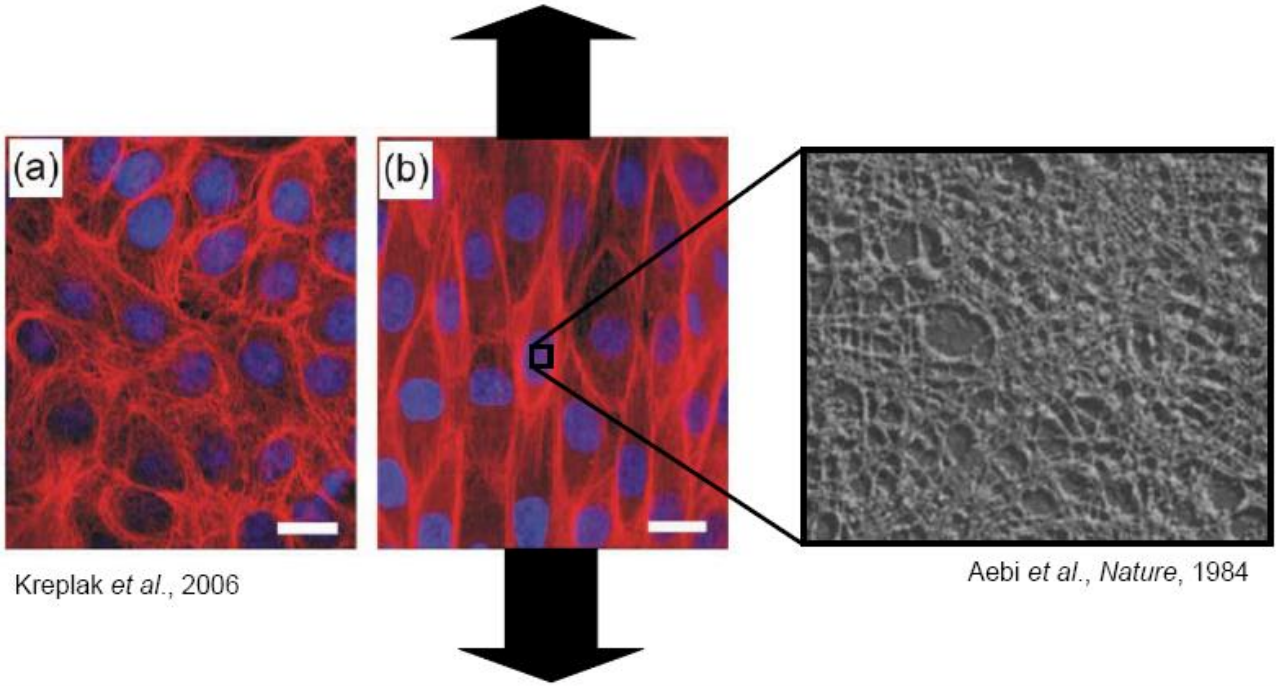
Nanomechanical properties and fracture toughness from local microstructural constituents charged with hydrogen


protein
sand
water

Proteins



Cell deformation



Kreplak *et al.*, 2006

Aebi *et al.*, *Nature*, 1984

How does behavior of protein network at larger scale depend on the structure?

OPEN ACCESS Freely available online PLoS one

Alpha-Helical Protein Networks Are Self-Protective and Flaw-Tolerant

Theodor Ackbarow[1], Dipanjan Sen[1,2], Christian Thaulow[1], Markus J. Buehler[1,3]*

1 Laboratory for Atomistic and Molecular Mechanics, Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States of America, **2** Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States of America, **3** Center for Computational Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States of America

Abstract

Alpha-helix based protein networks as they appear in intermediate filaments in the cell's cytoskeleton and the nuclear membrane robustly withstand large deformation of up to several hundred percent strain, despite the presence of structural imperfections or flaws. This performance is not achieved by most synthetic materials, which typically fail at much smaller deformation and show a great sensitivity to the existence of structural flaws. Here we report a series of molecular dynamics simulations with a simple coarse-grained multi-scale model of alpha-helical protein domains, explaining the structural and mechanistic basis for this observed behavior. We find that the characteristic properties of alpha-helix based protein networks are due to the particular nanomechanical properties of their protein constituents, enabling the formation of large dissipative yield regions around structural flaws, effectively protecting the protein network against catastrophic failure. We show that the key for these self protecting properties is a geometric transformation of the crack shape that significantly reduces the stress concentration at corners. Specifically, our analysis demonstrates that the failure strain of alpha-helix based protein networks is insensitive to the presence of structural flaws in the protein network, only marginally affecting their overall strength. Our findings may help to explain the ability of cells to undergo large deformation without catastrophic failure while providing significant mechanical resistance.

Citation: Ackbarow T, Sen D, Thaulow C, Buehler MJ (2009) Alpha-Helical Protein Networks Are Self-Protective and Flaw-Tolerant. PLoS ONE 4(6): e6015. doi:10.1371/journal.pone.0006015

Editor: Laurent Kreplak, Dalhousie University, Canada

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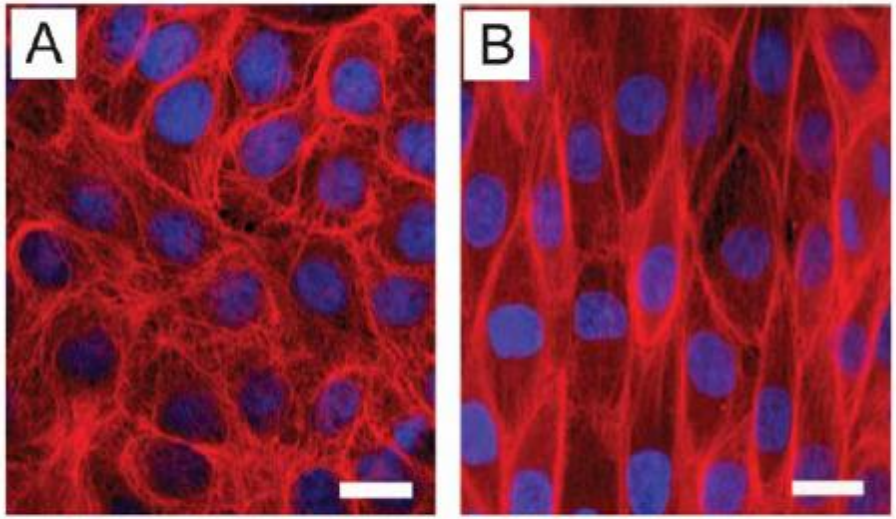
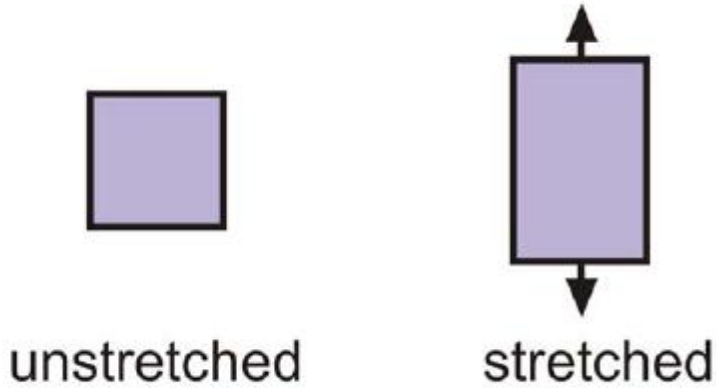
Competing Interests: The authors have declared that no competing interests exist.

* E-mail: mbuehler@mit.edu





Alpha-Helical Protein Networks

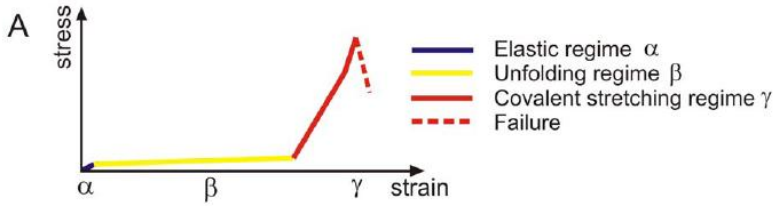
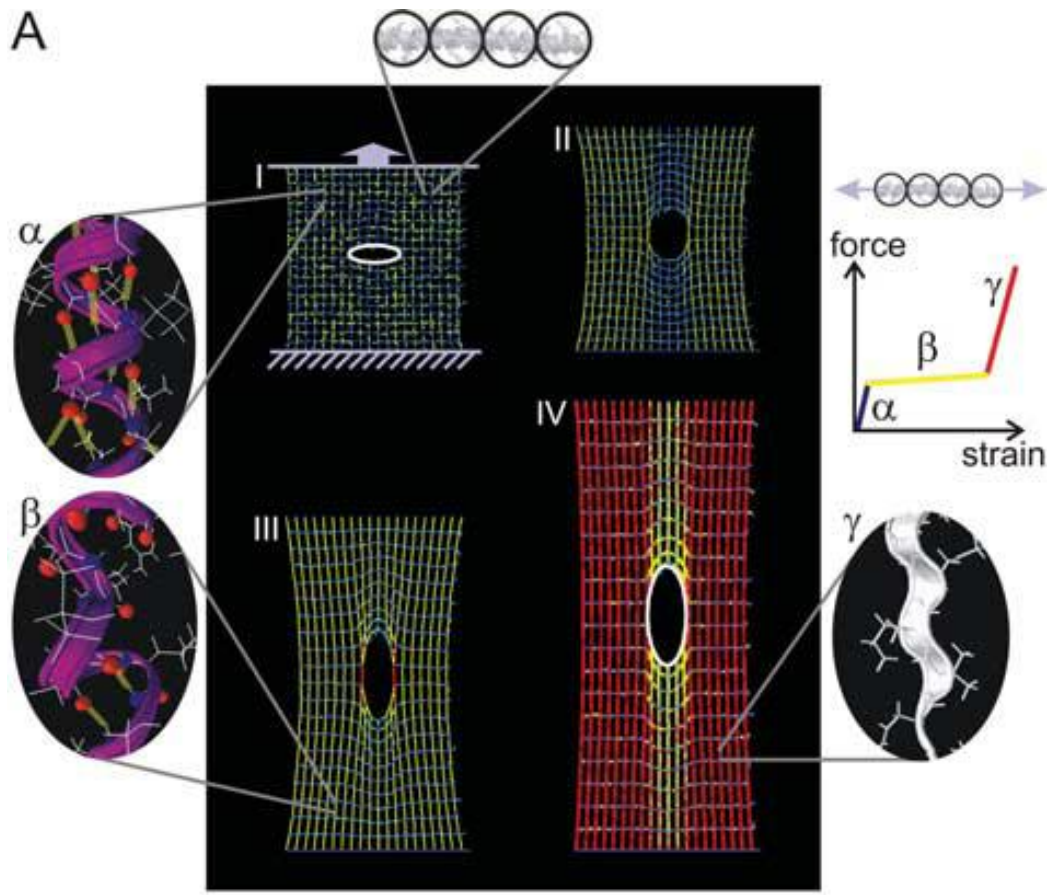
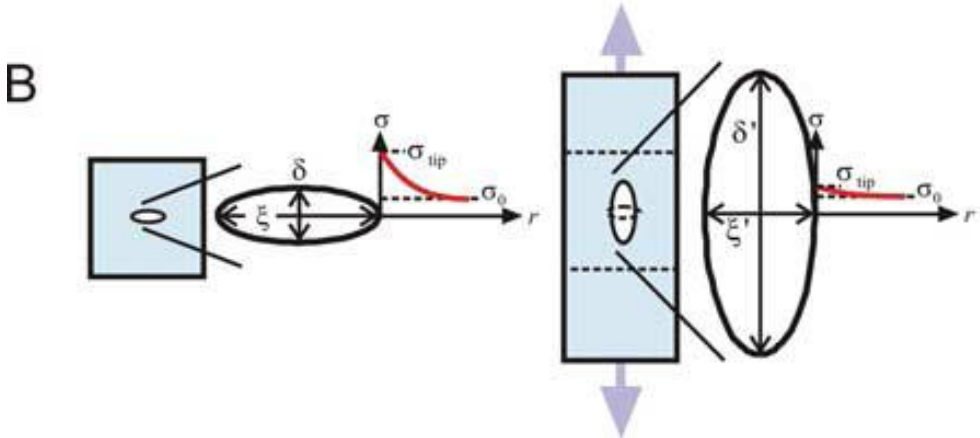


Figure 2. Effect of large uniaxial stretch on the intermediate filament network in MDCK cells, illustrating the ability of intermediate filament network to undergo very large deformation without catastrophic failure. The cells were grown on collagen-coated silastic membranes and stretched using a custom cell stretcher that was mounted on a confocal microscope. Cells were fixed and stained for immunofluorescence (red = keratin IFs, blue = DNA). Subplot A: Control cells were processed on a relaxed silastic membrane. Subplot B: Stretched cells were fixed, stained and imaged on membranes that were held in the stretched state. The approximate uniaxial strain in stretched cells is 75%. Scale bar is approximately 25 μm. Images reprinted with permission of John Wiley & Sons, Inc. from reference [46], *Biomechanical properties of intermediate filaments: from tissues to single filaments and back*, Vol. 29, No. 1, 2007, pp. 26–35, copyright © 2007 John Wiley & Sons, Inc.
doi:10.1371/journal.pone.0006015.g002

Self-protecting and flaw-tolerant protein material networks





Ackbarow, T, Sen, D, Thaulow, C, and Buehler, MJ. "Alphahelical protein networks are self protective and flaw tolerant." *PLoS ONE* **4**(6), (2009) e6015.