An Informal Discussion with Members of Class of 2009
Nuclear Science and Engineering Department, MIT,
November 29, 2005

A Glimpse of MIT, Nuclear Engineering, and Multiscale Materials Modeling and Simulation

Sidney Yip
Department of Nuclear Science and Engineering
Department of Materials Science and Engineering

MIT

Nuclear Engineering at MIT

A few words, with meaning …

The MIT Mission

Develop the ability and passion to work wisely, creatively and effectively for the benefit of humankind.

Generate, disseminate and preserve knowledge, working with others to bring this knowledge on the world's great challenges.

Combine rigorous study with the excitement of discovery.

http://mit.edu/

Where To Put the X ?

(how MIT sees its future through the Capital Campaign – *Calculated Risks and Creative Revolutions*)

IT'S SAID THAT IN THE EARLY YEARS OF THIS CENTURY CHARLES PROTEUS STEINMETZ, THE GREAT ELECTRICAL ENGINEER, WAS BROUGHT TO GENERAL ELECTRIC'S FACILITIES IN SCHENECTADY, NEW YORK.

GE had encountered a performance problem with one of its huge electrical generators and had been absolutely unable to correct it. Steinmetz, a genius in his understanding of electromagnetic phenomena, was bought in as a Consultant – not a very common occurrence in those days, as it would be now.

Steinmetz also found the problem difficult to diagnose, but for some days he closeted himself with the generator, its engineering drawings, paper, and pencil. At the end of this period he emerged, confident that he knew how to correct the problem.

After he departed, GE's engineers found a large "X" marked with chalk on the side of the generator casing. There was also a note instructing them to cut the casing open at that location and remove so many turns of wire from the stator. The generator would then function properly.

And indeed it did.

Steinmetz was asked what his fee would be. Having no idea in the world what was appropriate, he replied with the absolutely unheard-of answer that his fee was $1,000.

Stunned, the GE bureaucracy then required him to submit a formally invoice.

They soon received it. It included two items:

1. Marking chalk X on side of generator: $1.
2. Knowing where to mark chalk X: $999."

President Charles M. Vest, Commencement address, June 1999

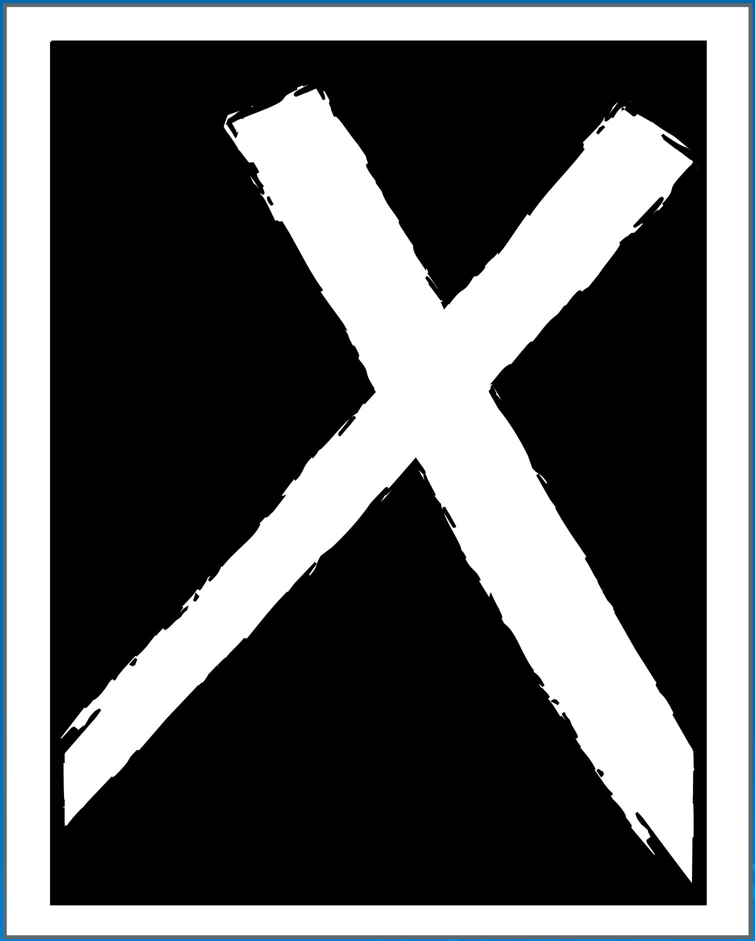


Figure by MIT OCW.

(how the School of Engineering sees its Mission)

Leadership Through Technical Excellence and Innovation

MIT (5 Schools)
School of Engineering (8 Departments)

Department of Nuclear Science and Engineering

17 Faculty, 110 Grad, 60 UG

Fission Technology

Plasma Science and Fusion

Nuclear Science and Technology

Energy/Technology Management and Policy

http://mit.edu/ned/

Nuclear Engineering Department

Fundamental Studies leading to diverse applications

Core Currriculum → Fission, Fusion, NST

Sow-Hsin Chen

Professor of Nuclear Engineering

Neutron and X-ray diffraction and spectroscopy applications of laser light scattering to complex fluids and biological problems.

Jeffrey A. Coderre

Associate Professor of Nuclear Engineering

Radiation biology; boron neutron capture therapy.

David G. Cory

Professor of Nuclear Engineering

Magnetic resonance and its applications (particularly to spatial characterization); advanced instrumentation; new methodologies; imaging; scattering; medical imaging; non-destructive analysis; quantum information processing; quantum computing; quantum complexity.

Richard Lanza

Senior Research Scientist

Radiation imaging; radiation detectors; nondestructive testing; radiological and industrial applications of radiation; development of new radiation sources.

Jacquelyn C. Yanch

Professor of Nuclear Engineering, and Whitaker College of Health Science and Technology

Computational methods in medical physics; nuclear medicine imaging; radiation therapy; accelerator neutron production.

Sidney Yip

Professor of Nuclear Engineering, and Material Science and Engineering

Theory and atomistic simulations in transport and collisional phenomena; multiscale materials modeling.

Down to the level of an individual professor whose research interests and activities are in

Modeling and Simulation

Computational Materials Research (Computational Materials)
is a unique complement to traditional theory and experiment

High Performance Computing

Advances in theory and simulation

Scientific Visualization

Fundamental Understanding, Prediction, Design/Discovery

Modeling Challenges in Materials Processing

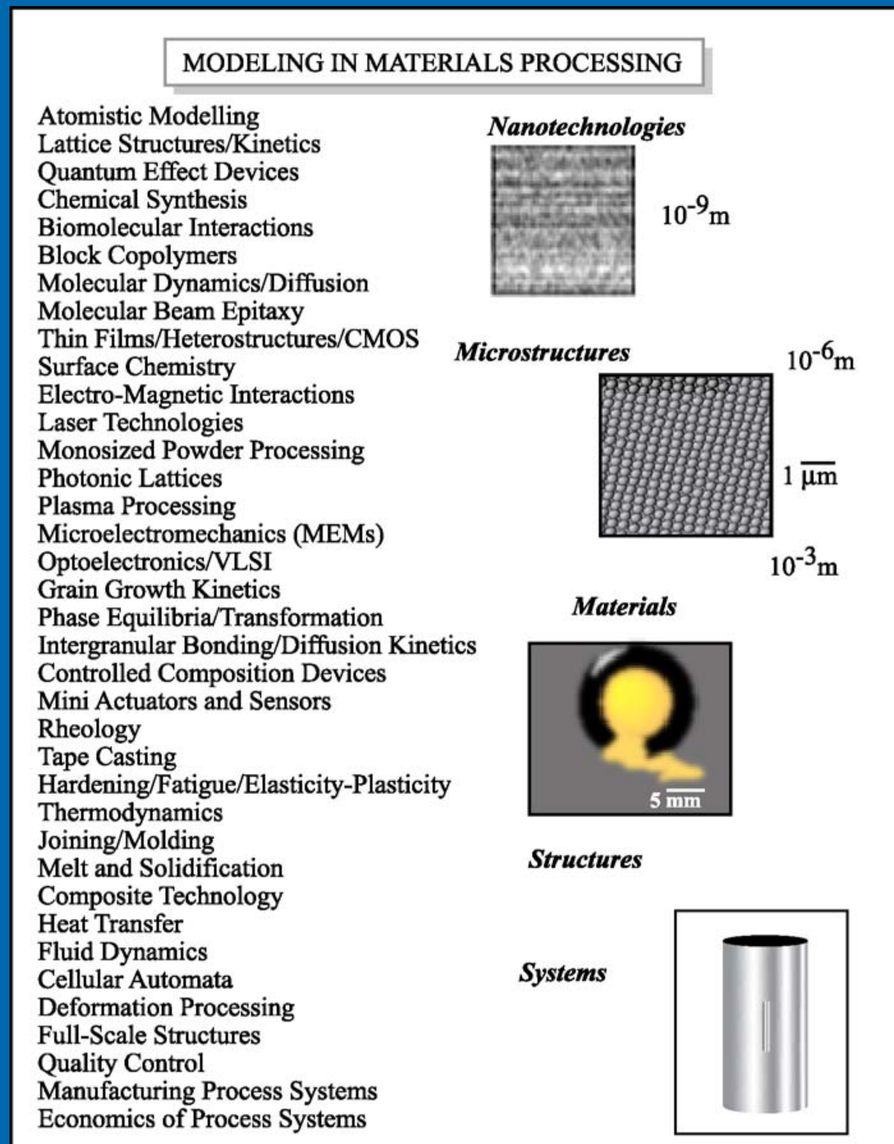


Fig. 1-1

Figure by MIT OCW.

Multiscale Modeling – theory, simulation and visualization of physical phenomena from electrons to atoms, macromolecules and beyond

Modeling is the physicalization of a concept, Simulation its computational realization

"If, in some cataclysm, all of scientific knowledge were to be destroyed, and only sentence passed on to the next generations of creatures, what statement would contain the most information in the fewest words? I believe it is the *atomic hypothesis* (or the atomic *fact*, whatever you wish to call it) that *all things are made of atoms – little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon squeezed into one another*. In that one sentence, you will see, there is enormous amount of information about the world, if just a little imagination and thinking are applied."

Richard P. Feynman, *Six Easy Pieces*, (Addison-Wesley, Reading,1963), p.4, *Matter is made of atoms*

For understanding and prediction --

atoms	$\{\underline{r}^N(t)\}$	Newton
electrons	ψ_i	Schrödinger

→ statistical Thermodynamics
solid and fluid mechanics
condensed matter physics, etc. → Science and Technology of Materials

funding agencies, universities, national labs, corporate research

workshops, symposia, publications

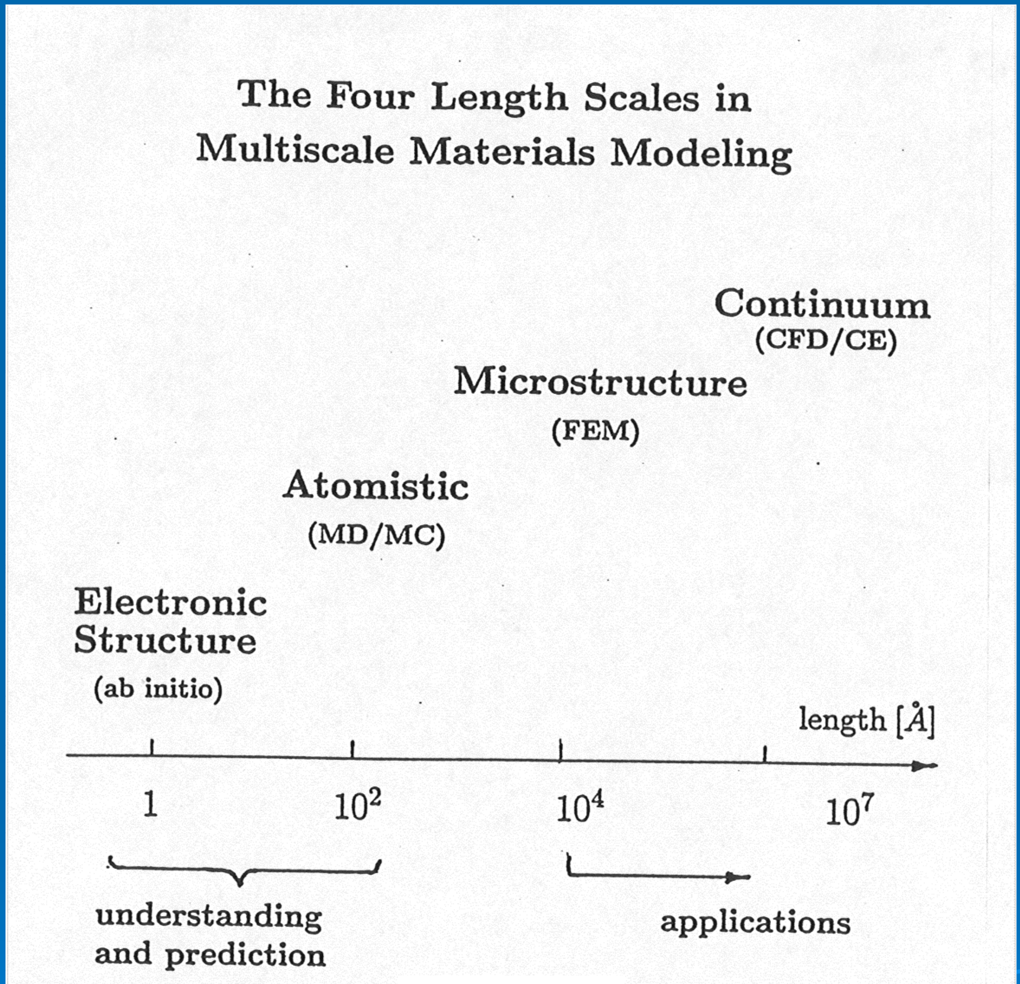


Fig. 1-2

There exist corresponding time scales

Scales of Microstructure

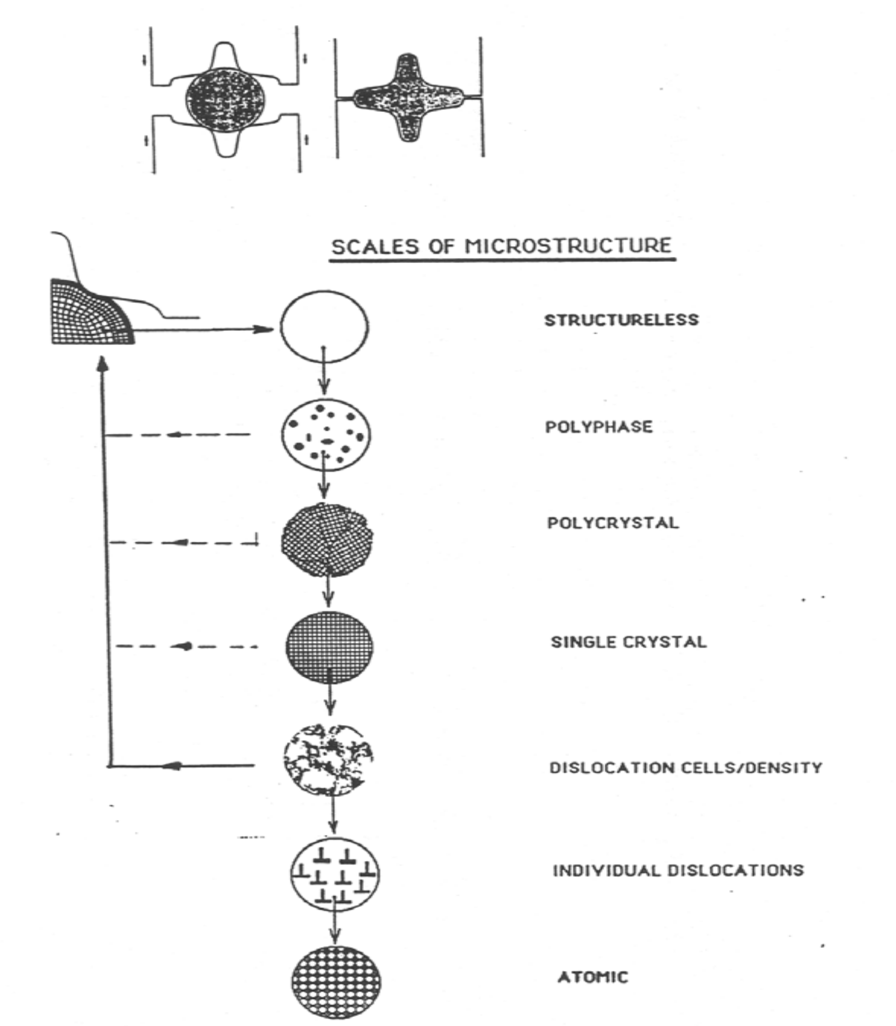


Fig. 1-3

Courtesy of Prof. Lalit Anand. Used with permission.

A large multiscale modeling project (the dynamics of metals) at the Lawrence Livermore National Laboratory

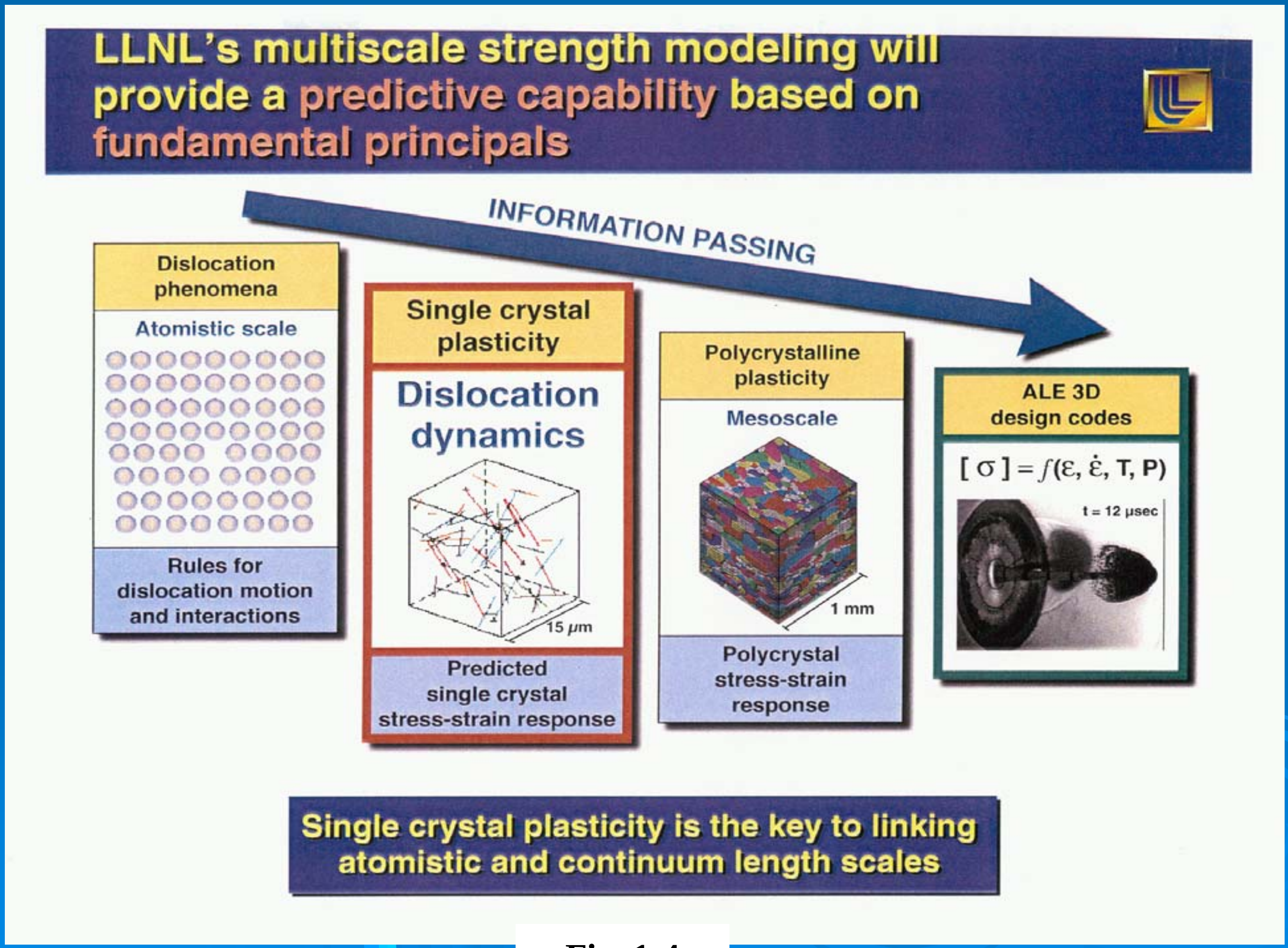


Fig. 1-4

The most challenging problem in thermodynamics is the calculation of free energy

MD determination of Argon melting curve

Image removed due to copyright restrictions

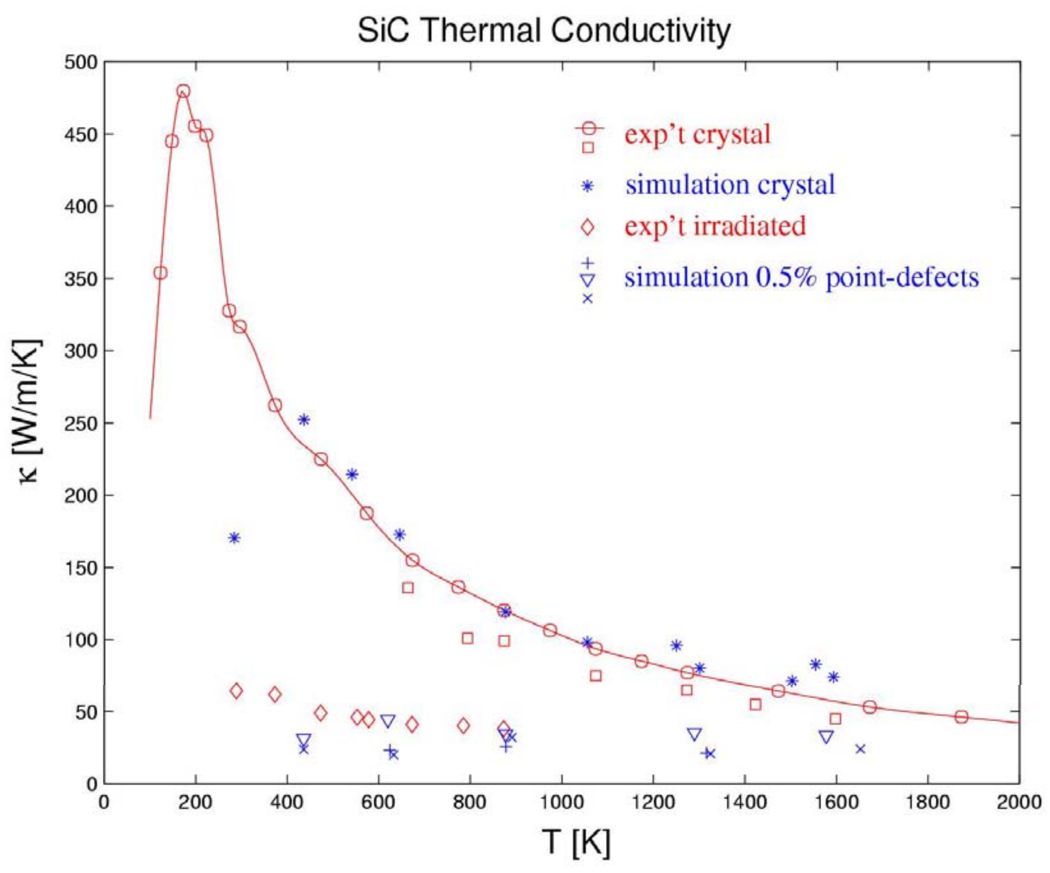
Solca, J. *et al.* “Melting curve for argon calculated from pure theory.” *Chemical Physics* 224 (December1997): 253-261. *Figure 3.*

Melting curves from defect-nucleation MD and from direct free-energy calculations

Image removed due to copyright restrictions

de Koning, Maurice, Alex Antonelli, and Sidney Yip. “Single-simulation determination of phase boundaries: A dynamic Clausius-Clapeyron integration method. *Journal of Chemical Physics* 115, no. 24 (December 2001): 11025-11035. *Figure 9.*

Understanding the mechanical and thermal behavior of irradiated SiC is a basic nuclear materials issue for fission and fusion technologies



J. Li, L.J. Porter, S. Yip, J. Nuclear Materials 255, 139 (1998).
L.J. Porter, J. Li, S. Yip, J. Nuclear Materials 246, 53 (1997).

The Jiggling and Wiggling of Atoms

"Certainly no subject is making more progress on so many fronts than biology, and if we were to name the most powerful assumption of all, which leads one on and on in an attempt to understand life, it is that *all things are made of atoms*, and that everything that living things do can be understood in terms of the jiggling and wiggling of atoms."

-- Richard Feynman, Lectures on Physics, vol. 1, p.3-6 (1963)

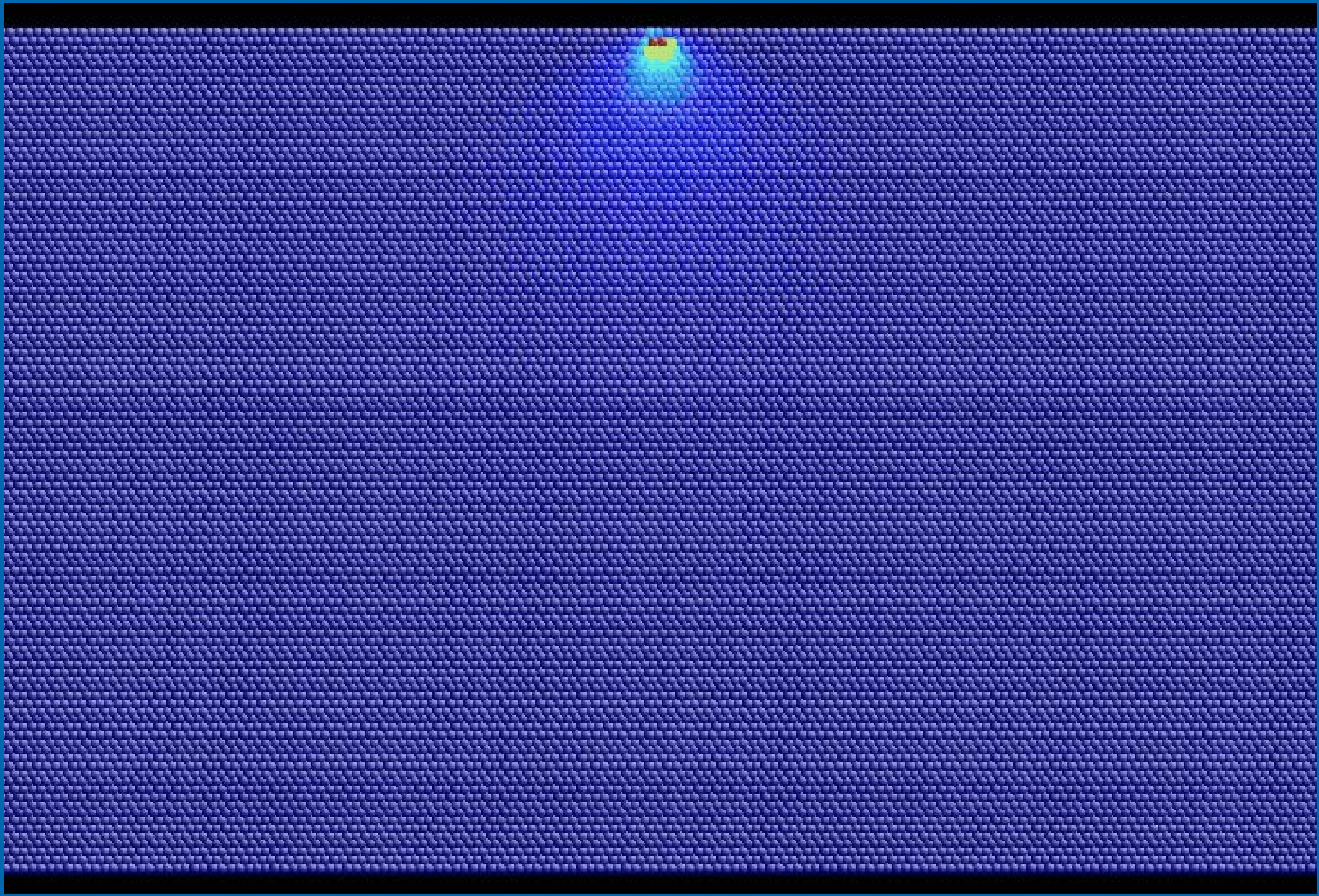
Experimental Observations of yield onset

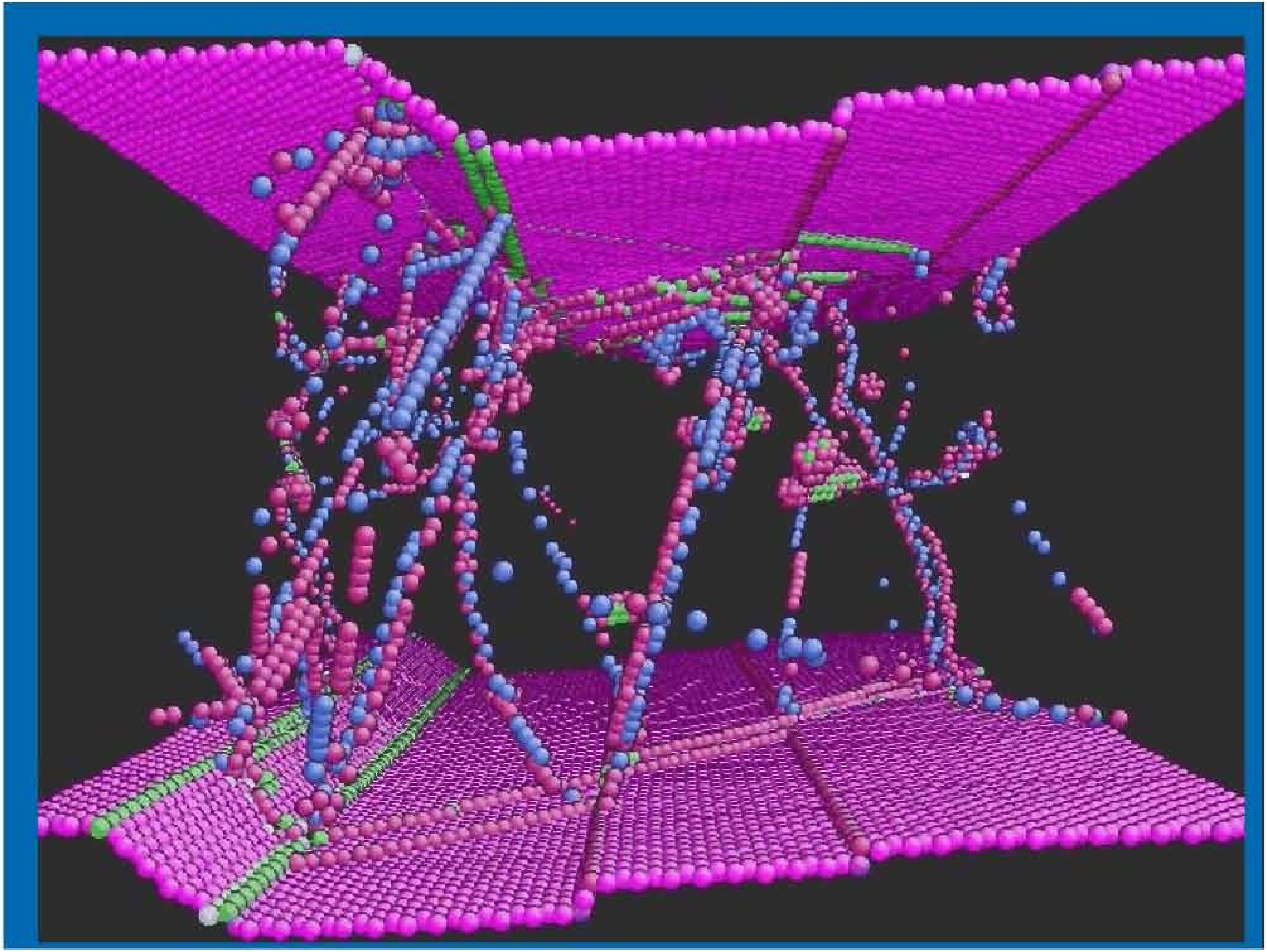
- formation of slip step

Image removed due to copyright restrictions.

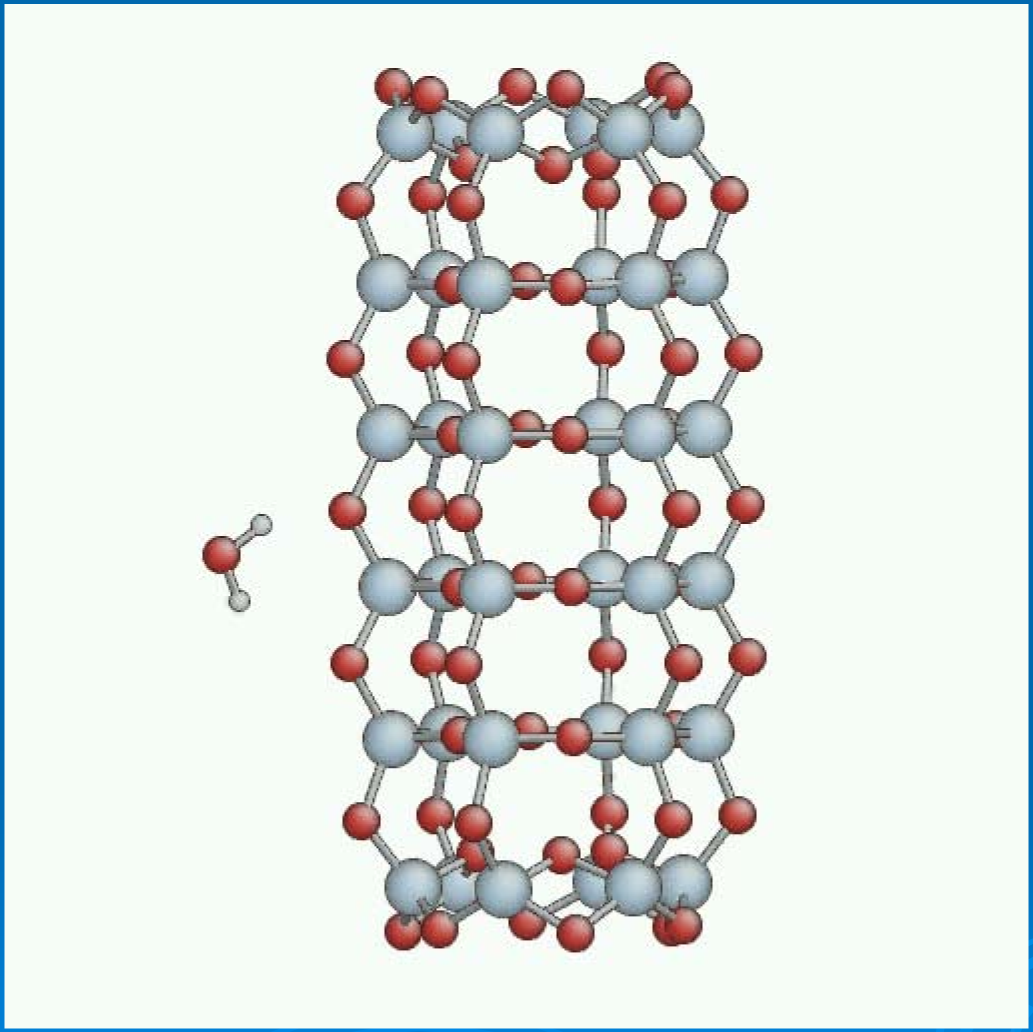
Gouldstone, A., K. Van Vliet, and S. Suresh. "Simulation of defect nucleation in a crystal." *Nature* 411 (2001): 656. *Figure 1.*

Nanoindentation in 2D (MD)
coordination number encoding

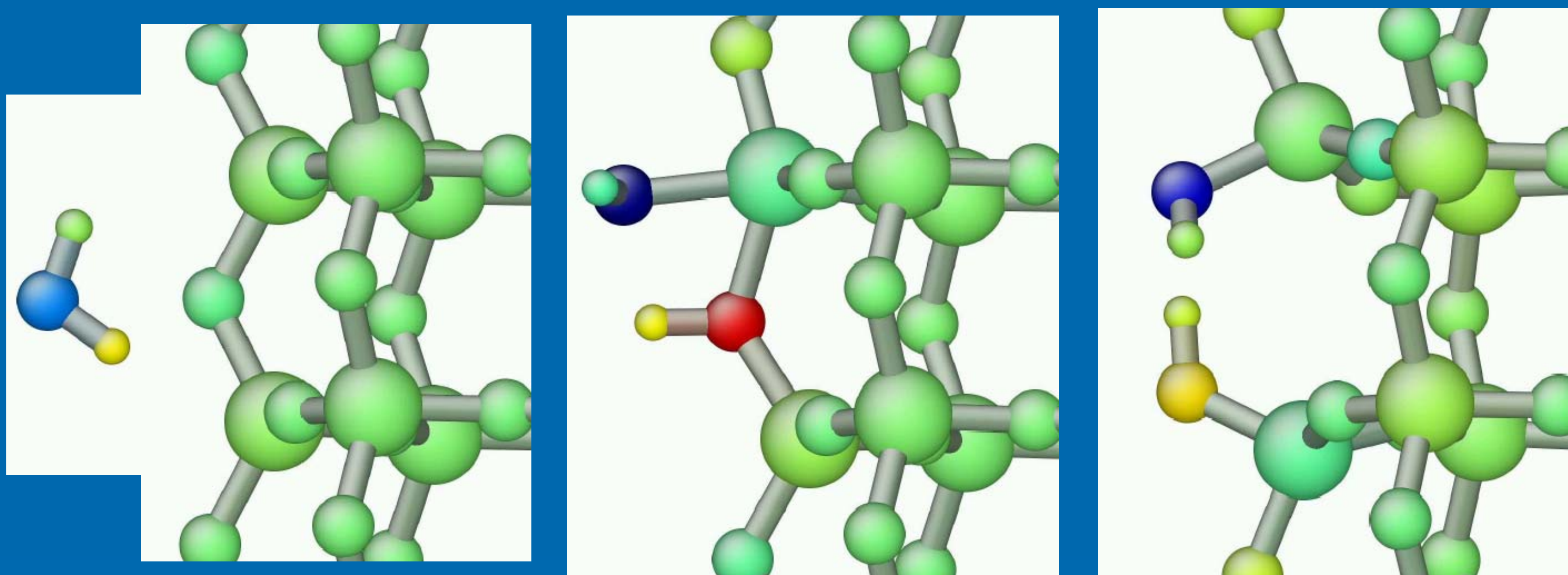




Attack of water molecule on quartz (SiO_2)



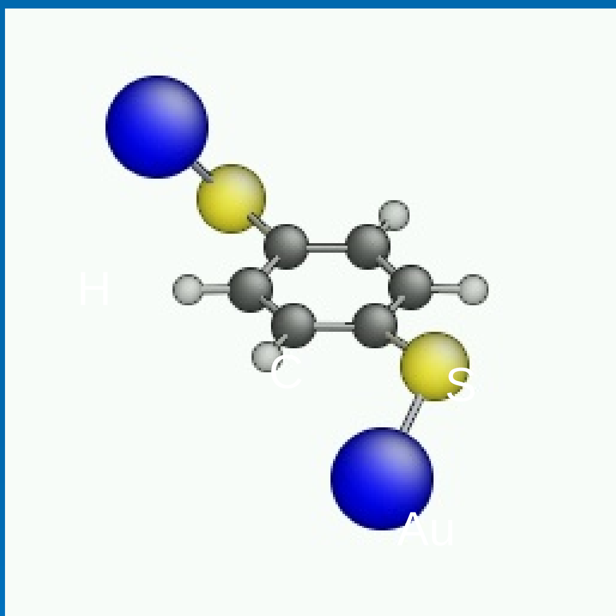
H_2O + Si-O-Si → 2SiOH

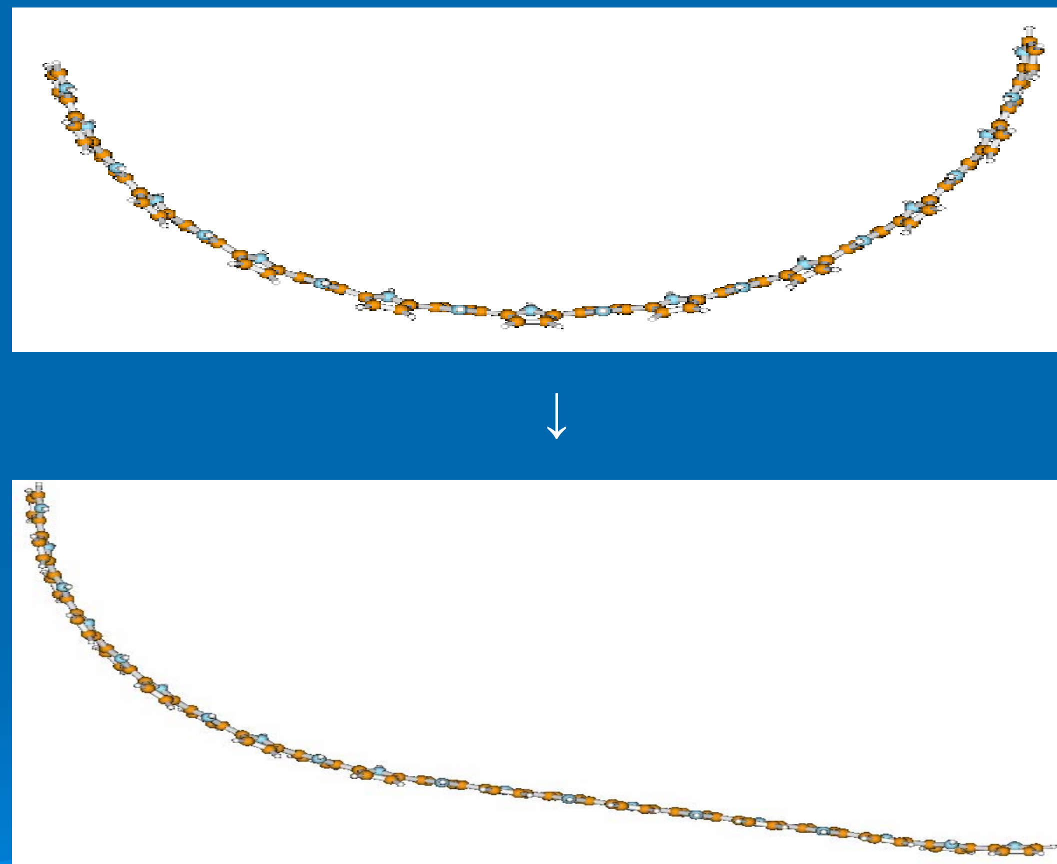


charge transfer during hydrolysis of Si-O-Si bridge

charging a single polypyrrole chain causing
a conformation change is an intrinsic mechanism

electron conductance across
a molecular junction





charge transport and localization in functional nanostructures
– molecular electronics, molecular actuators

Conjugated Polymer Actuators

Examples of big companies using conjugated polymer actuator technology include:

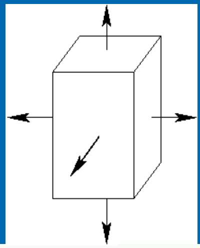
• Honda Asimo Technology

•EAMEX

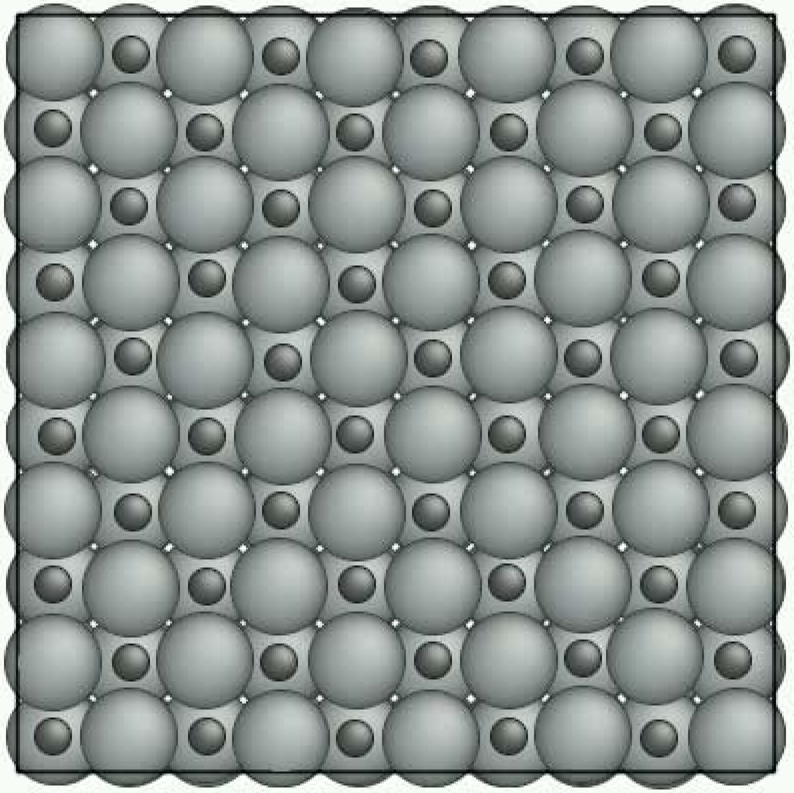
http://www.eamex.co.jp/index_e.html

Effects of temperature on deformation and bond breaking

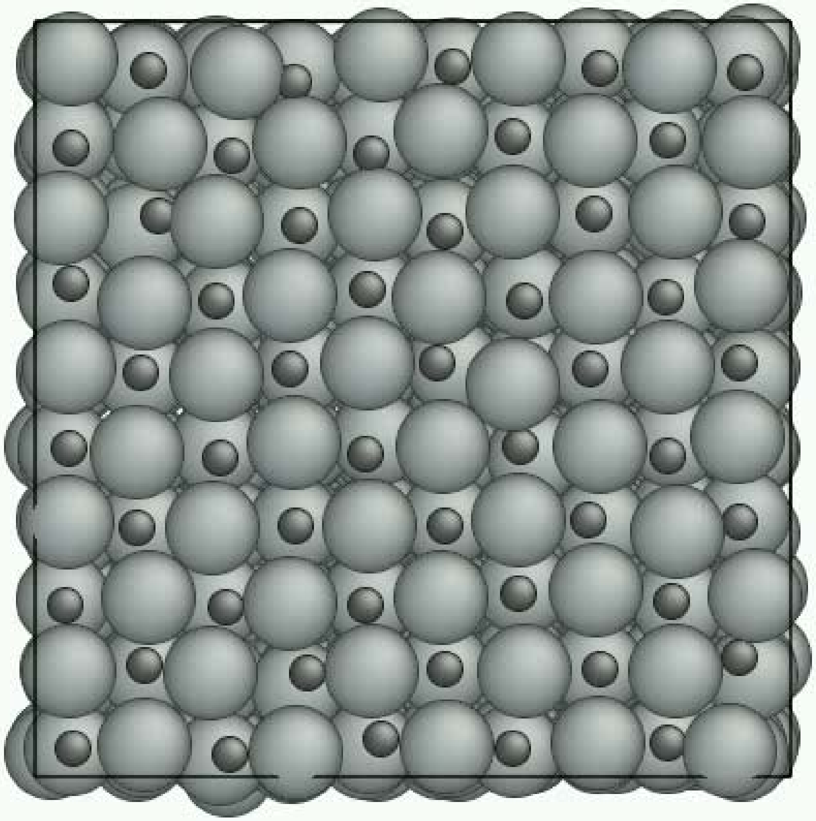
Failure of ZrC under Hydrostatic Tension – Temperature Effects



Low T (300^{o}K) Cleavage

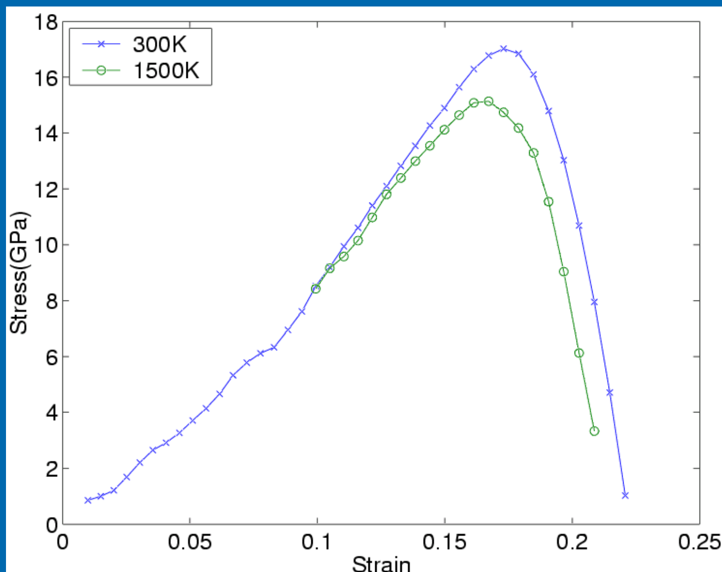


High T (3500^{o}K) Cavitation



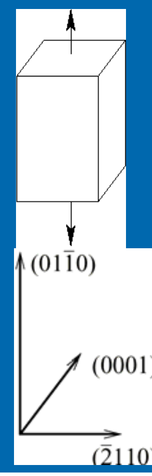
[2]

Extension of Elliptical Crack in Quartz



T_m=1700K

300K



Fracture Toughness of Quartz (300°K)

Griffith: $K_{IC} = \sqrt{2E\gamma/(1-\nu^2)}$

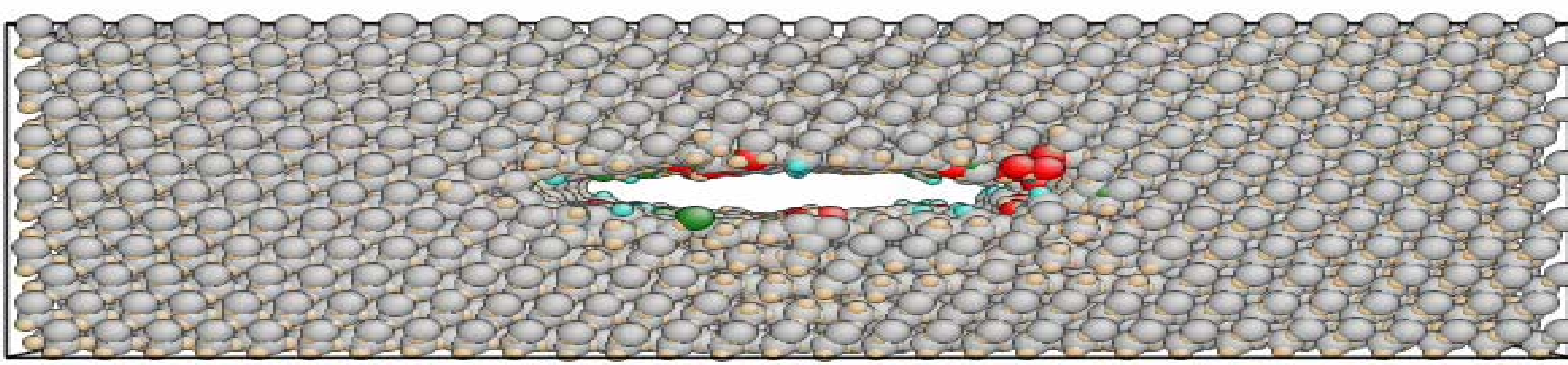
K_{IC}=0.91 [MPa m1/2] (from E,γ,ν)

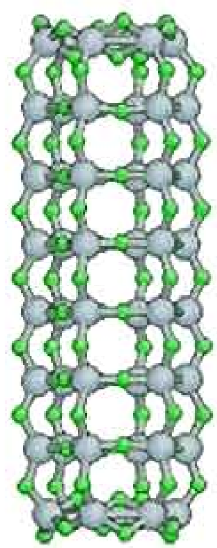
=0.97 (expt – Iwasa & Ueno '81)

Direct Simulation: $K_{IC} = \sigma_c\sqrt{\pi c}$

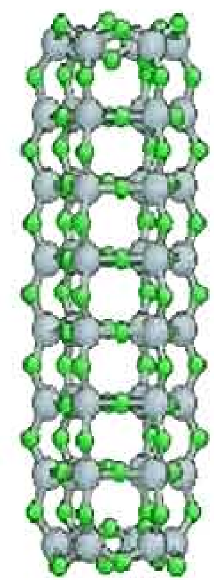
K_{IC}=1.55 (simulation)

K_{IC}=1.63 (unrelaxed γ')





nanorod_1K.avi



nanorod_100K.avi

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Real-time imaging gold nanojunctions

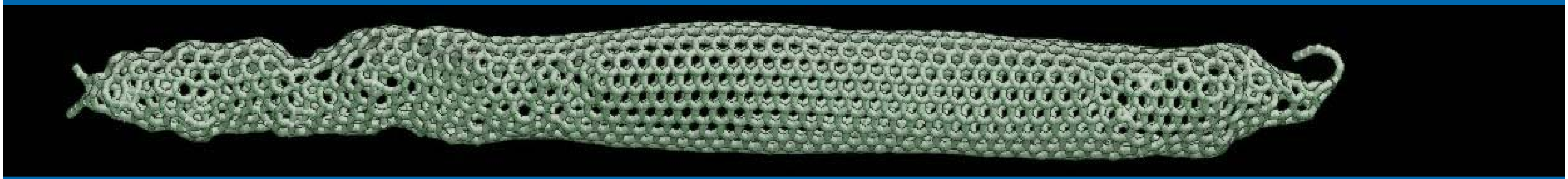
Rodrigues and Ugarte. “Real-time imaging of atomistic process in one-atom-thick metal junctions *Physical Review B* 63 no. 073405 (2001). *Figure 1*.

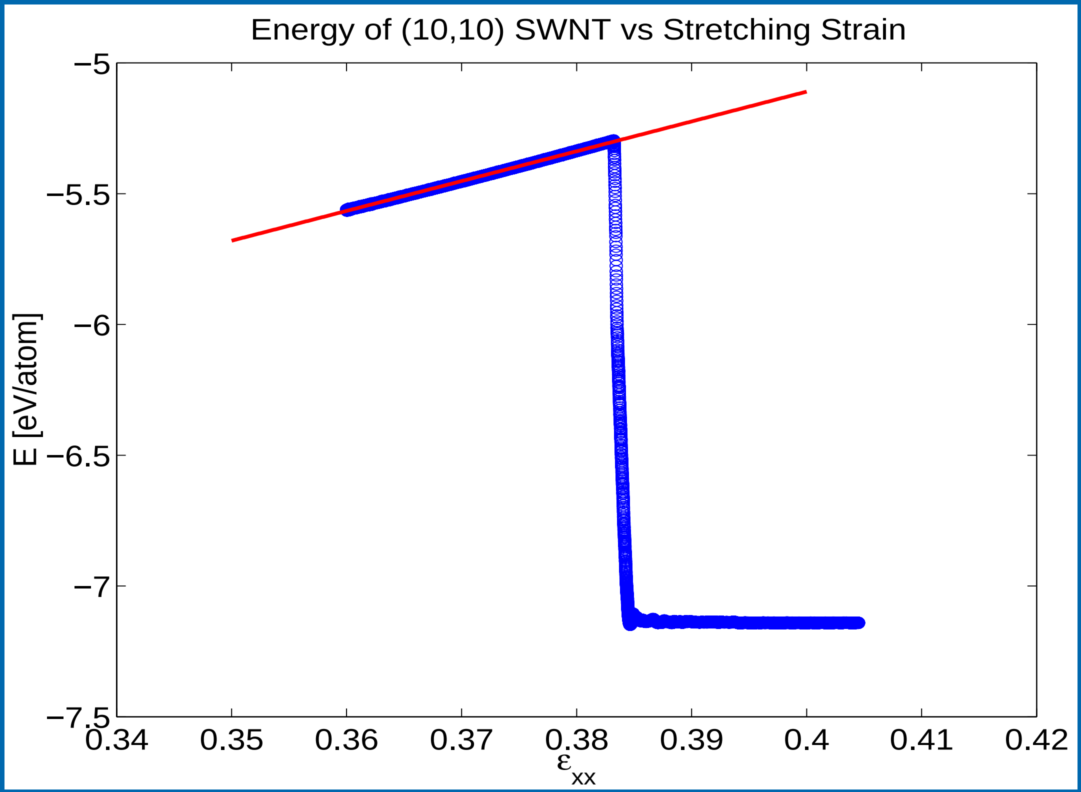
Image removed due to copyright restrictions.

TB-MD simulations

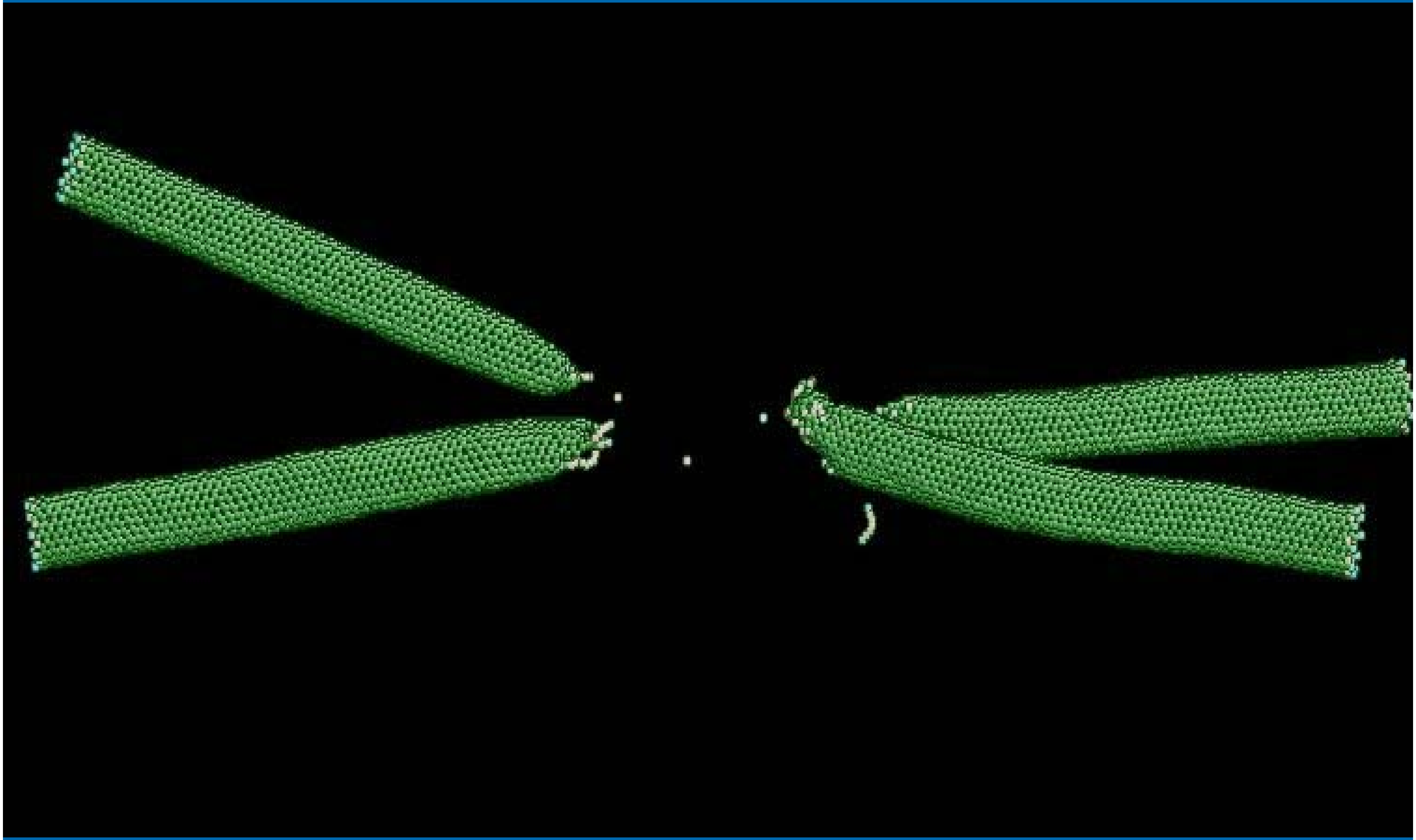
da Silva, E.Z., Antonio da Silva, and A. Fazzio. “How Do Gold Nanowires Break?” *Physical Review Letters* 87, no. 25 (2001). *Figure 1*.

Tensile Strength of Carbon Nanotube
(molecular dynamics simulation)





(10,10) SWNT Junction Strength



back to the MIT experience …

It’s Not What We Know. It’s What We Don’t Know.

“In our lifetime, technology and science will change and converge in abundant and bewildering ways. We may find ourselves in a place where we won’t know what to do, and we’ll have to figure it out. But if you’ve been to MIT, you’ve been there before.”

-- *Calculated Risks, Creative Revolutions*: The Campaign for MIT (1999)

The MIT Style --

Intelligent, Irreverent, and To the Point

Four qualities that will serve you well at MIT

Excellence
Perseverance
Boldness
Optimism