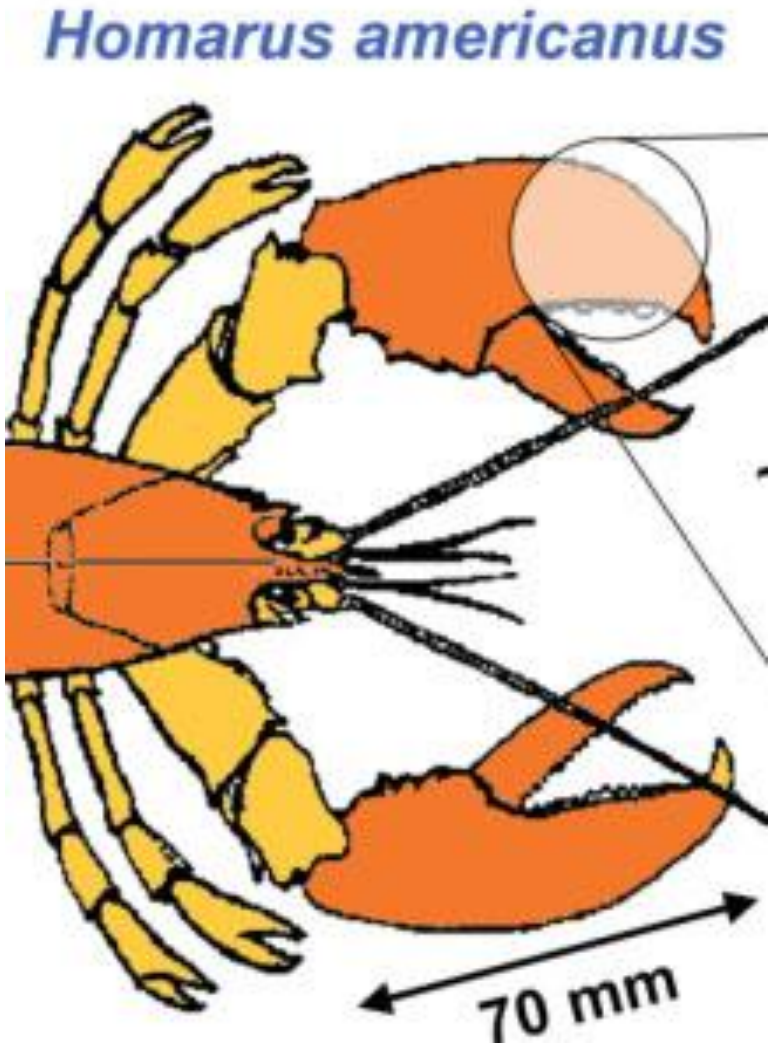
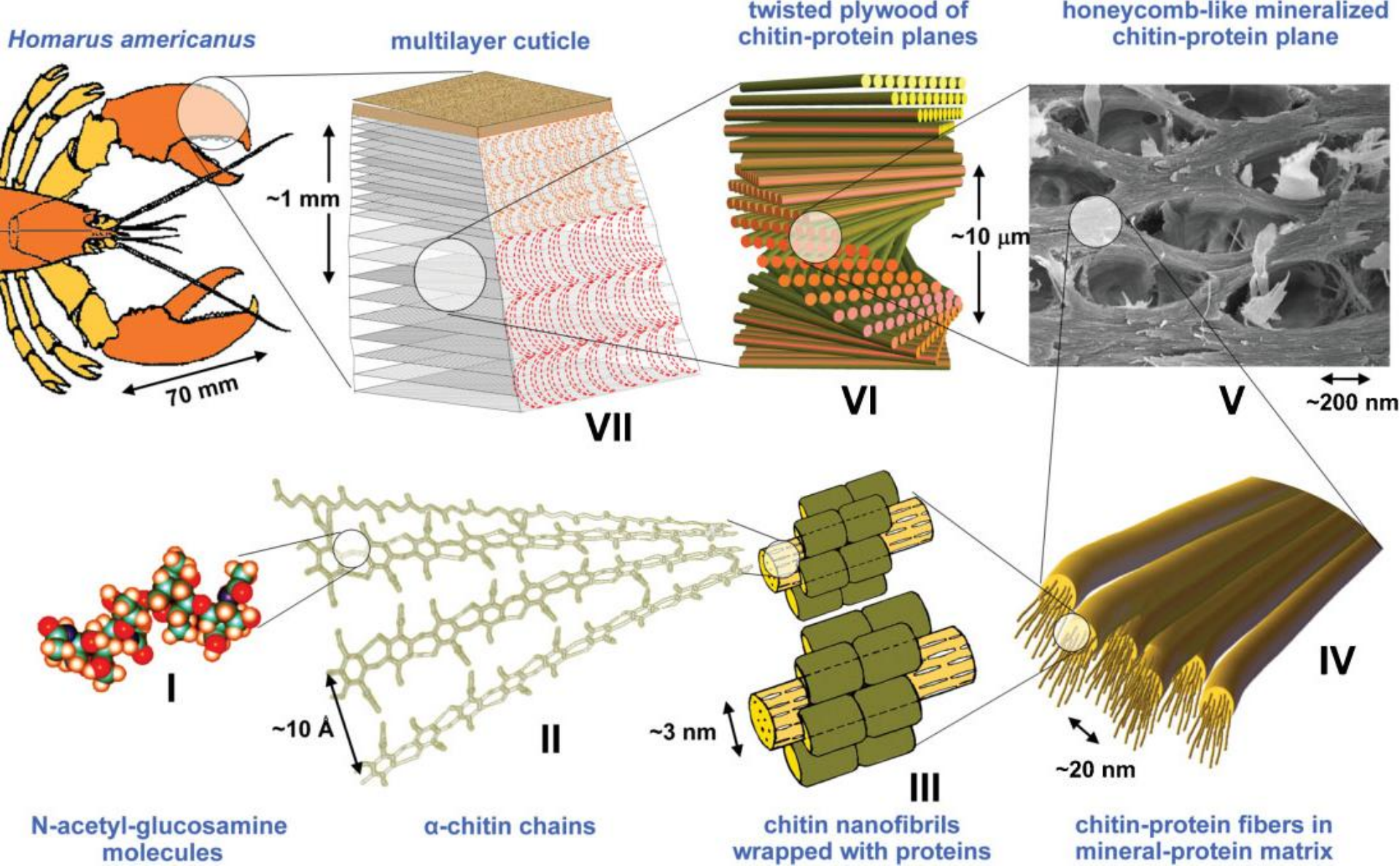
Homarus Americanus

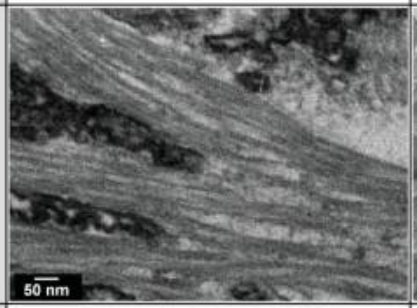
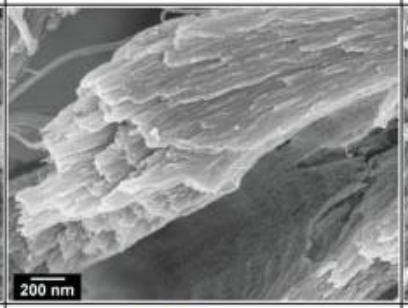
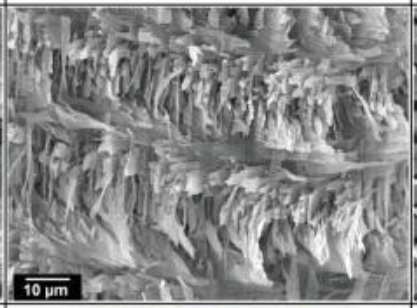
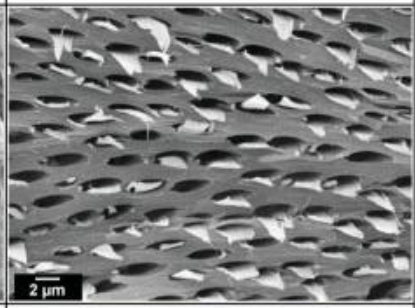
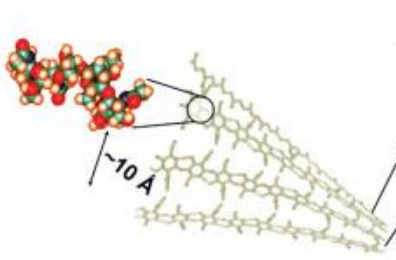
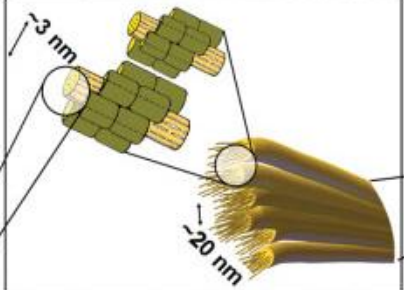
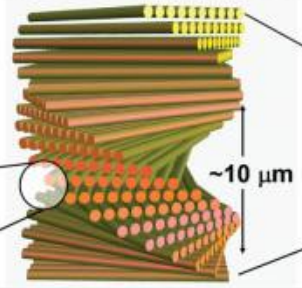
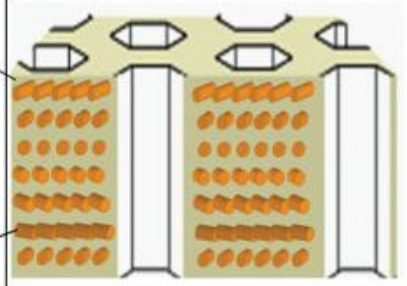
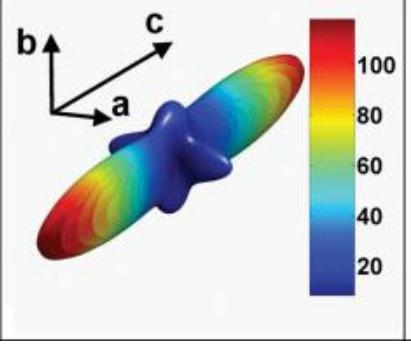
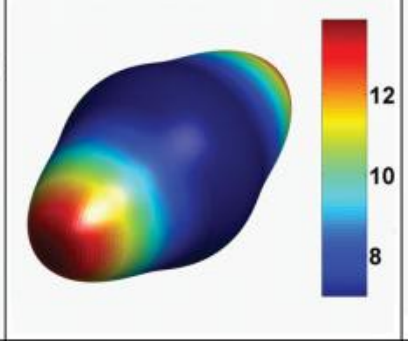
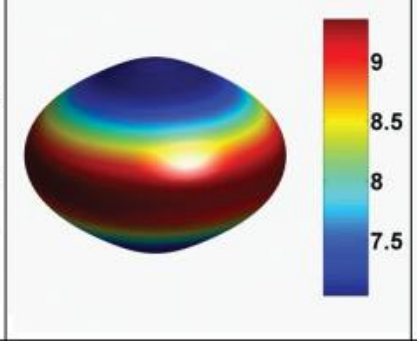
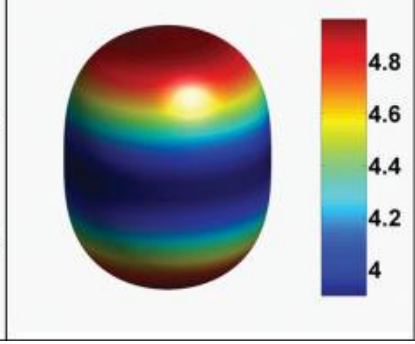


0.55 Gyr age

The cuticle is one of the oldest natural materials for structural and armor applications, already present in the fossil records of crab, lobster or shrimp about 550Myr ago, and thus, among the most successful animals living on the earth

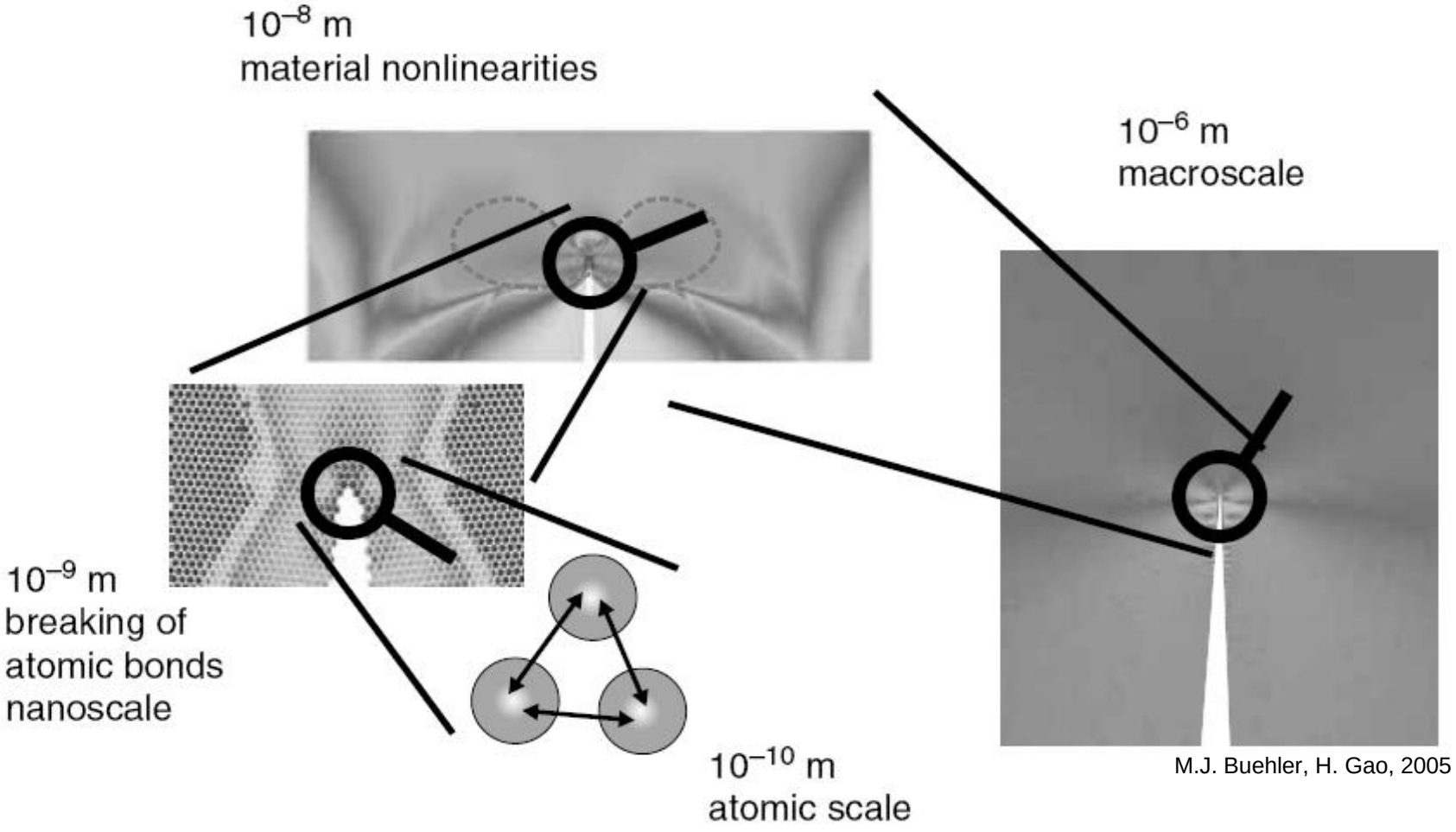


Nikolov, S, Petrov, M, Lymperakis, L, Friak, M, Sachs, C, Fabritius, H-O, Raabe, D and Neugebauer, J.: "Revealing the Design Principles of High-Performance Biological Composites using Ab initio and Multiscale Simulations: The Example of Lobster Cuticle" Advanced Materials,21 (2009), 1-8

Scale	0.1 nm – 10 nm	10 nm – 100 nm	100 nm – 10 μm	10 μm – 1 mm
Hierarchical structure unit	α-chitin (H-bonded anti-parallel N-acetyl-glucosamine molecular chains)	Mineralized chitin-protein nanofibrils in a planar array	Twisted plywood stack of mineralized chitin-protein planes without pore canals	Twisted plywood stack of mineralized chitin-protein planes with pore canals
Experimental method	Transmission electron microscope	Field emission scanning electron microscope	Field emission scanning electron microscope	Field emission scanning electron microscope
Microstructure				
Schematic				
Simulation method	Ab initio; density functional theory	Mori-Tanaka scheme (chitin-protein fiber); Torquato 3-point scheme (mineral-protein matrix)	Dilute approximation, tensor rotation	Torquato 3-point homogenization
Elastic behavior, 3D maps of Young's modulus [GPa] a,b-axes: basal directions of the chitin unit cell c-axis: longitudinal (chain) axis of the chitin molecule				

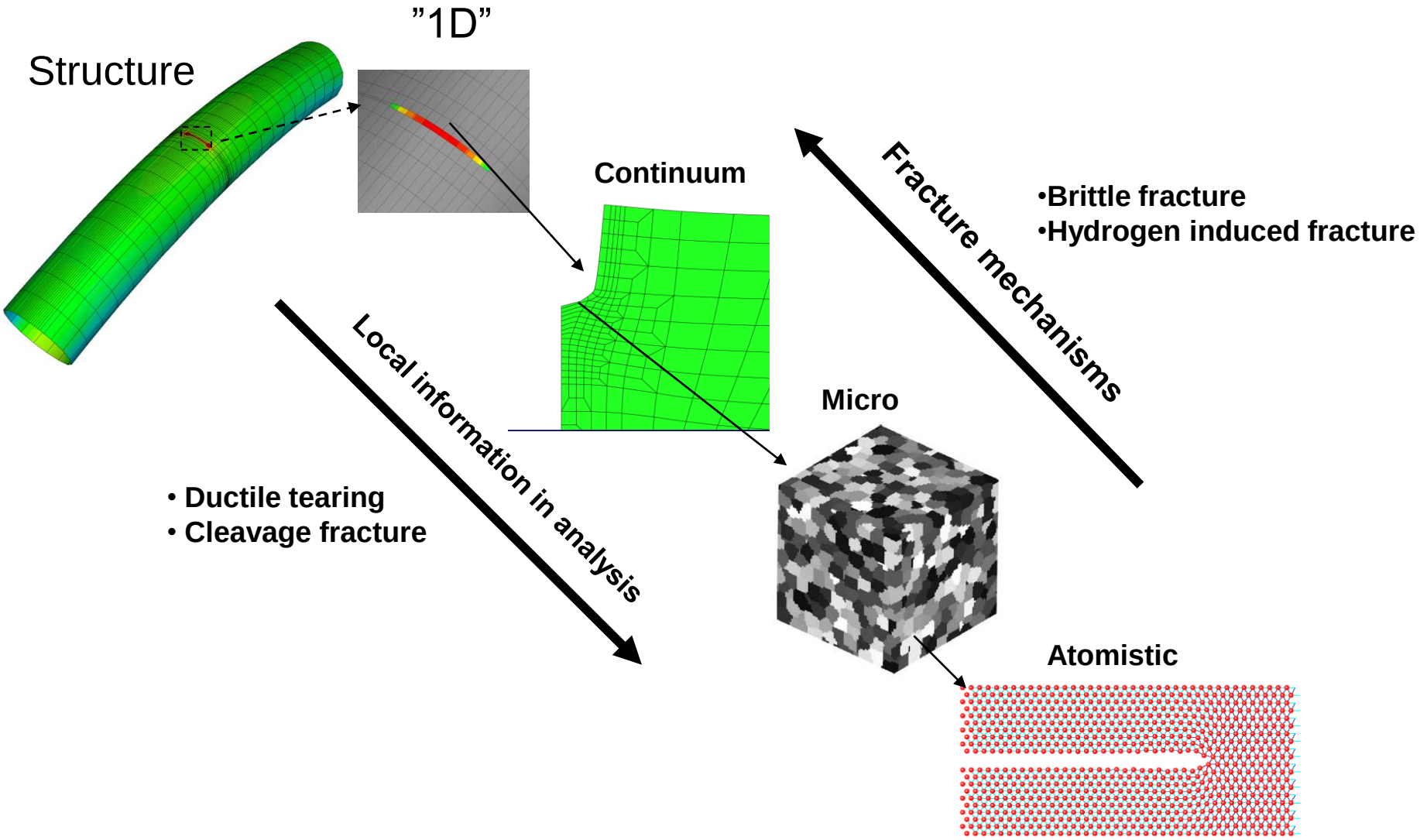
Links between scales – Multiscale Material Modeling

Fracture mechanics problem is a complex multiscale phenomenon

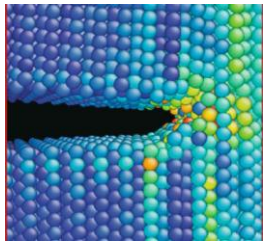
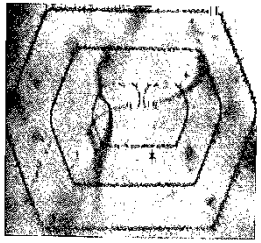
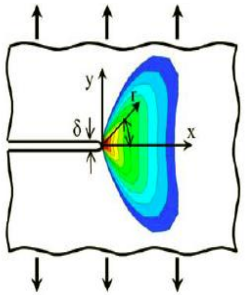


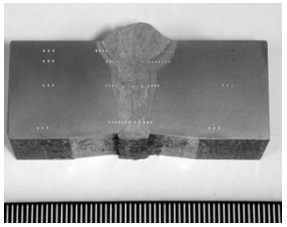
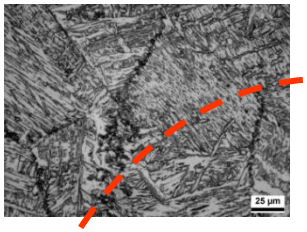
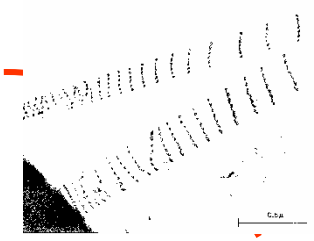
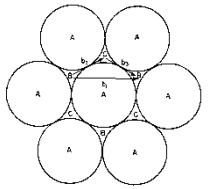
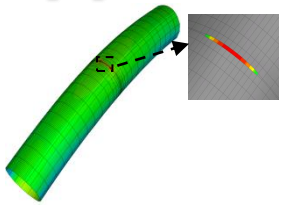
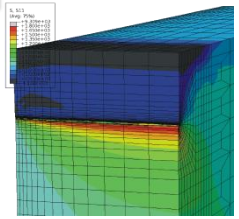
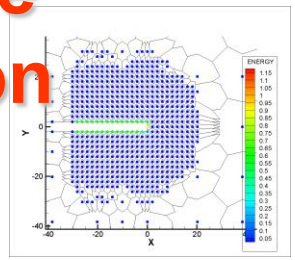
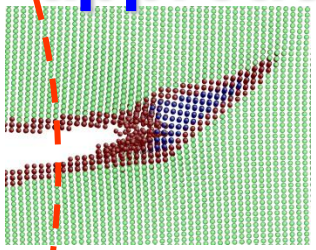
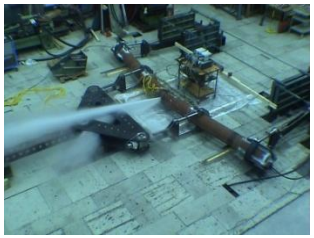
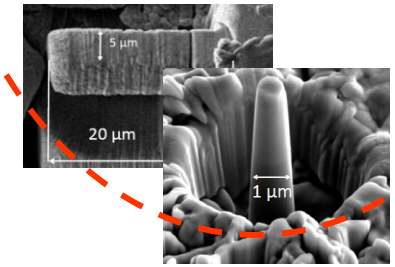
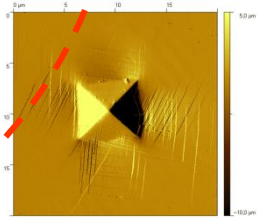
M.J. Buehler, H. Gao, 2005

Multiscale approach to fracture in steels



Multiscale Materials Modeling

Atoms Precipitates	Dislocations Plastic flow	Grains Primary particles	Continuum laws	Load Geometry
				
1nm	1µm	100µm	10mm	10m
New interatomic potentials for steel	Stacking fault energy	Crystal plasticity	Mechanics modeling	Constraint

Scale	$1\text{-}10^5$ m	0.01-1 m	$10^{-6}\text{-}10^{-3}$ m	$10^{-8}\text{-}10^{-7}$ m	$10^{-10}\text{-}10^{-9}$ m
Structure/ material					
Modelling techniques	 Continuum mechanics		 Crystal plasticity	 Quasi-continuum	 Molecular dynamics
Experimental techniques	 Large-scale testing	 Small-scale testing	 Micor-pillars/ Focused ion beam	 Nano indentation	

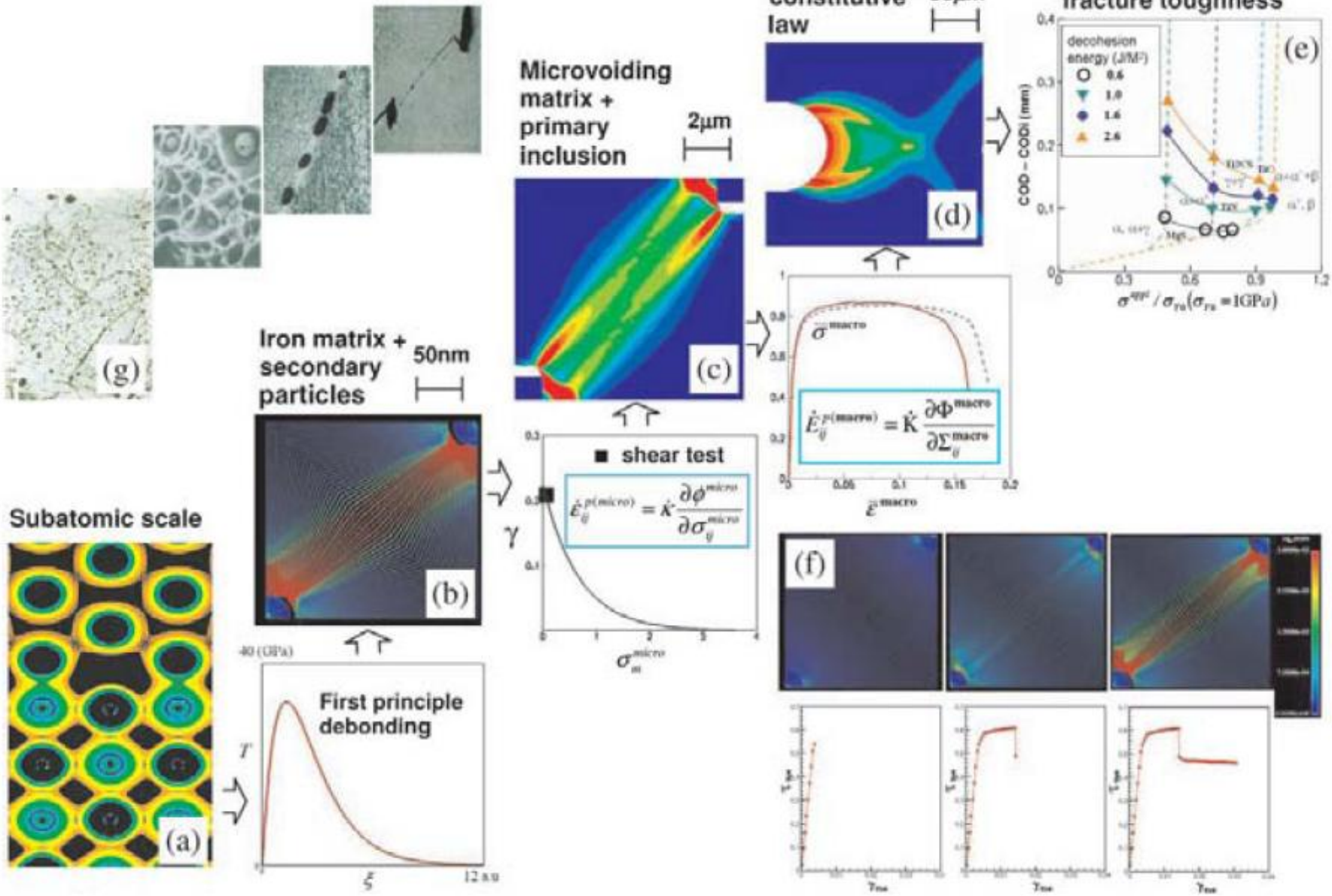
Top-down approach

"Hand-shake" region

Bottom-up approach

E Østby and C Thaulow

Cybersteel 2020
Multiscale modeling of ductile fracture



Hao S, B. Moran, W. K. Liu and G.B. Olson 2004

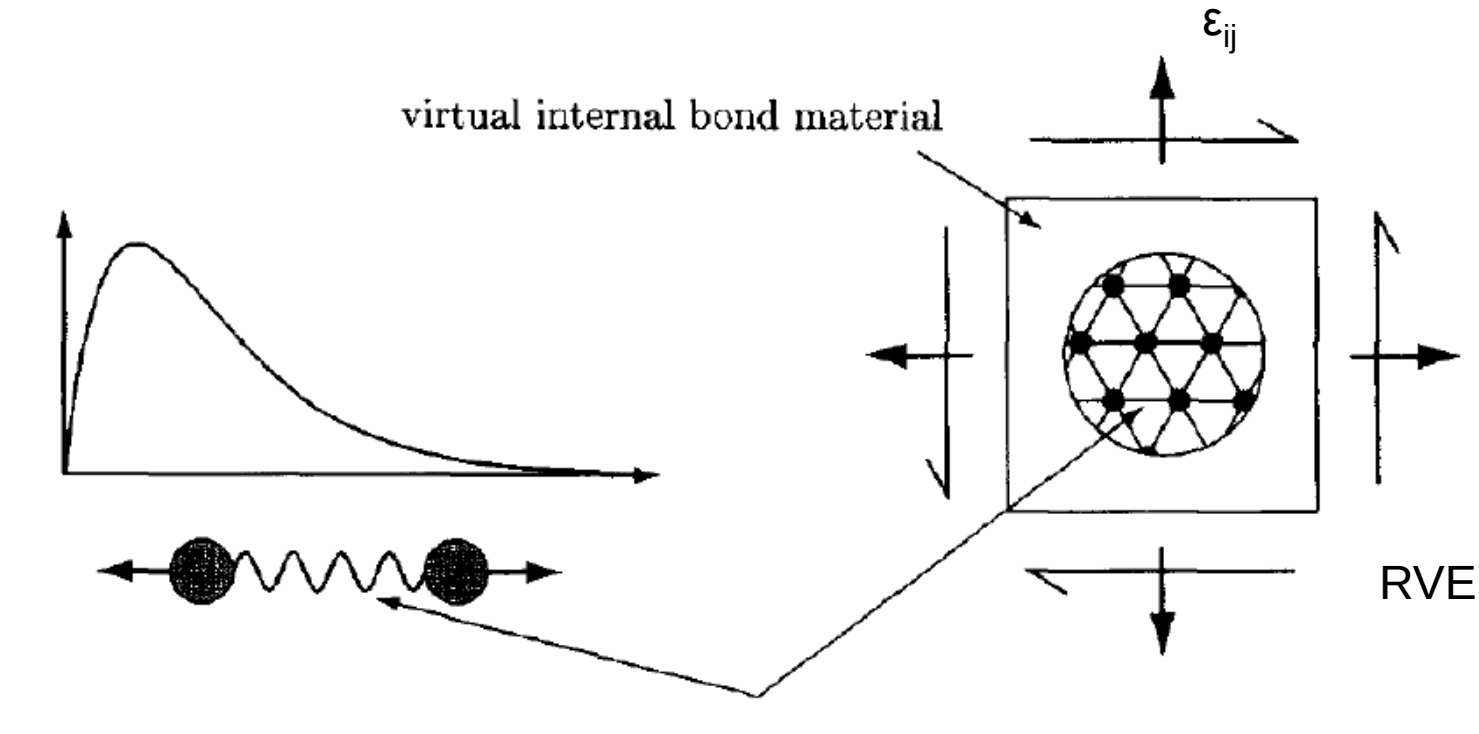
- **Virtual internal bond (VIB) method**
  Suitable for fracture applications, "*hierarchical coupling*"

- **Quasicontinuum method (QC)**
  Suitable for fracture and plasticity applications, "*concurrent coupling*"

- **Hierarchical coupling**: sequentially feed parameters (e.g. QM (DFT) to MD to FEM etc.), only one level of discretization during simulation

- **Concurrent coupling**: concurrently carrying out simulations of different discretization in one domain; parameter feeding "on-the-fly"

VIB approach



P. Klein and H. Gao, 1998 (and following years)

Fundamentals of VIB

calculate

Once free energy density is known, calculate constitutive relations

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl} \qquad c_{ijkl} = \frac{\partial^2 \psi}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}}$$

Concept of VIB: use Cauchy-Born rule (C-B) to develop expression of free energy density; use to obtain constitutive relation for finite element model

Cauchy-Born rule

- **Concept:** Express potential energy U for a atomistic representative volume element (RVE) as a function of applied strain

$$\psi(\varepsilon_{ij}) = \frac{1}{\Omega_0}\int_{\Omega_0} U(\varepsilon_{ij}) d\Omega$$

T=0, no entropy

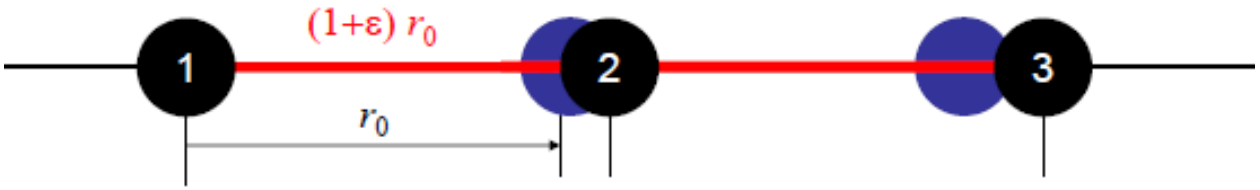
$U(\varepsilon_{ij})$: potential energy of RVE as function of ε_{ij}

Ω_0 : volume of RVE

- Impose macroscopic deformation gradient on atomistic volume element, then calculate atomic stress – this corresponds to the macroscopic stress
- Strictly valid only far away from defects in periodic lattice (homogeneous deformation, perfect lattice, amorphous solid-average)
- Allows direct link of potential to macroscopic continuum elasticity

1D example: Cauchy-Born rule

- Impose homogeneous strain field on 1D string of atoms
- Then obtain $\sigma_{ij} = c_{ijkl}\varepsilon_{kl}$ from that



$$r = (1+\varepsilon)\cdot r_0$$

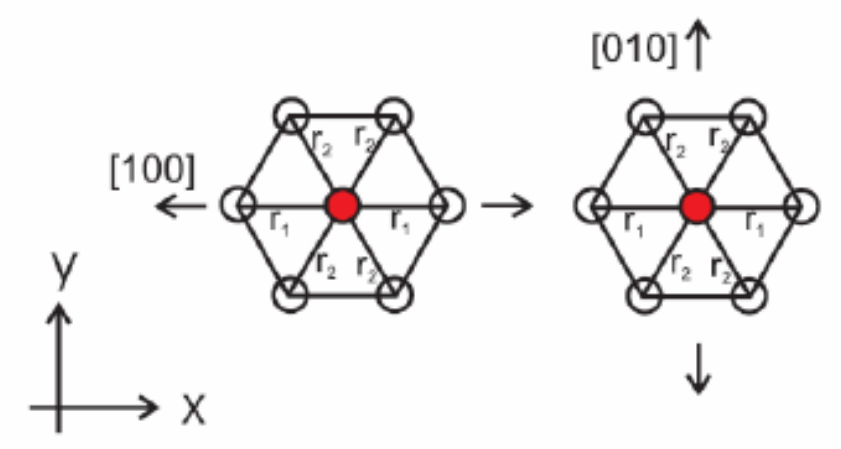
$$\psi(\varepsilon) = \frac{1}{r_0 \cdot D}\phi(r) = \frac{1}{r_0 \cdot D}\phi((1+\varepsilon)\cdot r_0)$$

Strain energy density function

interatomic potential

out-of-plane area ⟶ $r_0 \cdot D$ *atomic volume*

2D hexagonal lattice

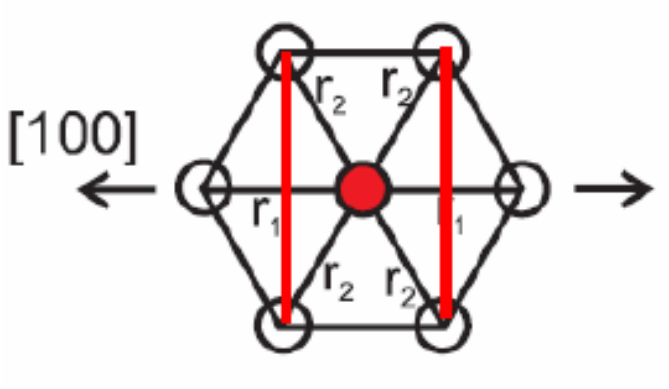


$$\psi = \frac{\sqrt{3}}{8}\phi''\left(3\varepsilon_{xx}^2 + 2\varepsilon_{xx}\varepsilon_{yy} + 3\varepsilon_{yy}^2 + (\varepsilon_{yx} + \varepsilon_{xy})^2\right) \longleftarrow \psi(\varepsilon_{ij}) = \frac{1}{\Omega_0}\int_{\Omega_0} U(\varepsilon_{ij})d\Omega$$

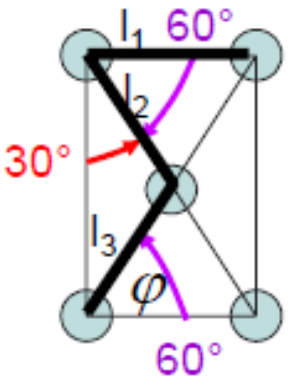
$$\sigma_{ij} = \frac{\partial \psi(\varepsilon_{ij})}{\partial \varepsilon_{ij}} \qquad c_{ijkl} = \frac{\partial^2 \psi(\varepsilon_{ij})}{\partial \varepsilon_{ij}\partial \varepsilon_{kl}}$$

How is this expression obtained?

Geometry triangular lattice



one atom with six neighbors



Need bond length as function of strain

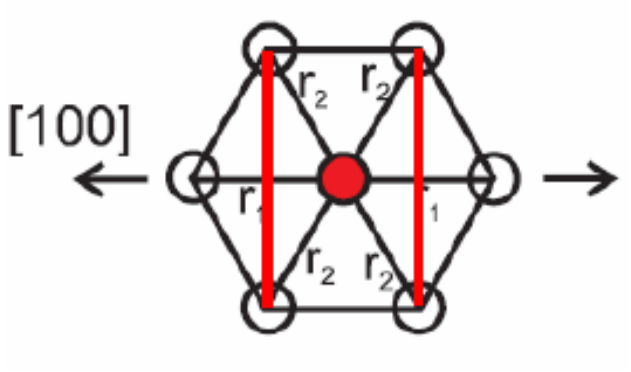
$$\varepsilon_{\alpha\alpha} = \vec{e}_\alpha \cdot \underline{\underline{\varepsilon}} \cdot \vec{e}_\alpha \rightarrow \boxed{l_\alpha = 1 + \vec{\xi}^{(I)} \cdot \underline{\underline{\varepsilon}} \cdot \vec{\xi}^{(I)}}$$

$$l_\alpha = \frac{L_{0,\alpha} + \Delta L_\alpha}{L_{0,\alpha}}$$

General vector to describe bonds:

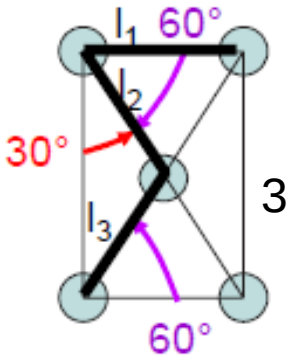
$$\vec{\xi}^{(I)} = [\cos(\varphi), \sin(\varphi)]$$

Geometry triangular lattice



$$l_\alpha = \left(1 + \xi_i^{(I)} \varepsilon_{ij} \xi_j^{(I)}\right) \cdot r_0$$

$$\vec{\xi}^{(I)} = [\cos(\varphi), \sin(\varphi)]$$



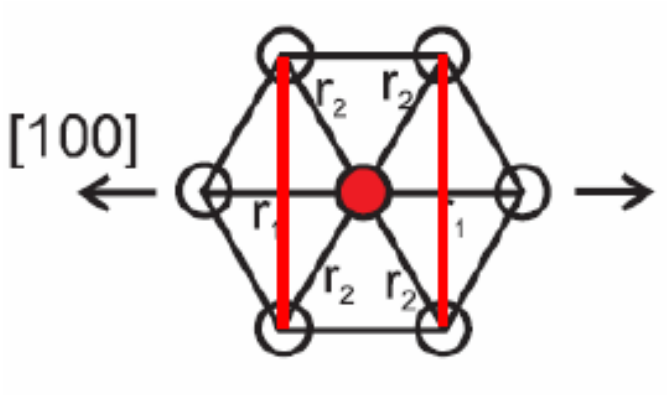
3 bonds

$$\vec{\xi}^{(1)} = [1,0] \qquad \varphi = 0°$$

$$\vec{\xi}^{(2)} = [\tfrac{1}{2}, -\tfrac{\sqrt{3}}{2}] \qquad \varphi = -60°$$

$$\vec{\xi}^{(3)} = [\tfrac{1}{2}, \tfrac{\sqrt{3}}{2}] \qquad \varphi = 60°$$

Geometry triangular lattice



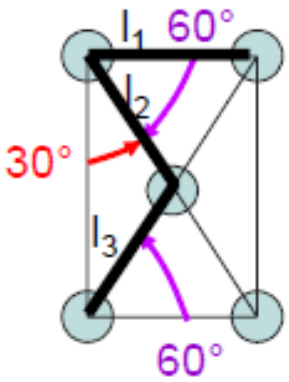
$$l_I = \left(1 + \xi_i^{(I)} \varepsilon_{ij} \xi_j^{(I)}\right) \cdot r_0$$

$$\vec{\xi}^{(I)} = [\cos(\varphi), \sin(\varphi)]$$

$$\vec{\xi}^{(1)} = [1,0] \quad \varphi = 0°$$

$$\vec{\xi}^{(2)} = [\tfrac{1}{2}, -\tfrac{\sqrt{3}}{2}] \quad \varphi = -60°$$

$$\vec{\xi}^{(3)} = [\tfrac{1}{2}, \tfrac{\sqrt{3}}{2}] \quad \varphi = 60°$$



$$l_1 = (1 + \varepsilon_{11}) \cdot r_0$$

$$l_2 = \left(1 + \tfrac{1}{4}\varepsilon_{11} + \tfrac{3}{4}\varepsilon_{22} - \tfrac{\sqrt{3}}{4}(\varepsilon_{12} + \varepsilon_{21})\right) \cdot r_0$$

$$l_3 = \left(1 + \tfrac{1}{4}\varepsilon_{11} + \tfrac{3}{4}\varepsilon_{22} + \tfrac{\sqrt{3}}{4}(\varepsilon_{12} + \varepsilon_{21})\right) \cdot r_0$$

Expression of free energy density

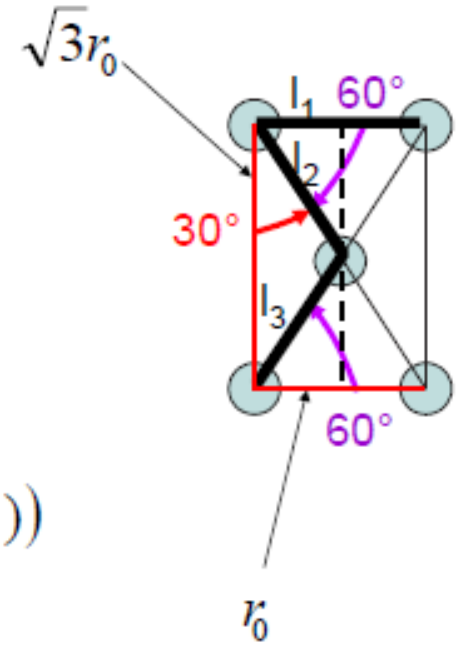
$$\psi(\varepsilon_{ij}) = \frac{1}{\Omega}\sum_i \phi_i(r_i)$$

$$\Omega = \sqrt{3}r_0^2$$

Account for all bonds

6 neighbors

$$\psi(\varepsilon_{ij}) = \frac{2}{\sqrt{3}}\frac{1}{r_0^2}\left(\phi(l_1)+\phi(l_2)+\phi(l_3)\right)$$



Taylor expansion of interatomic potential

$$\psi(\varepsilon_{ij}) = \frac{2}{\sqrt{3}} \frac{1}{r_0^2} \left(\phi(l_1) + \phi(l_2) + \phi(l_3)\right)$$

only the two first terms

$$l \equiv r$$

$$\phi(r) = a_0 + a_1(r - r_0) + a_2 / 2(r - r_0)^2 + \ldots$$

$$a_0 = const.$$

$$a_1 = \phi'(r_0) = 0$$

Valid for any pair potential

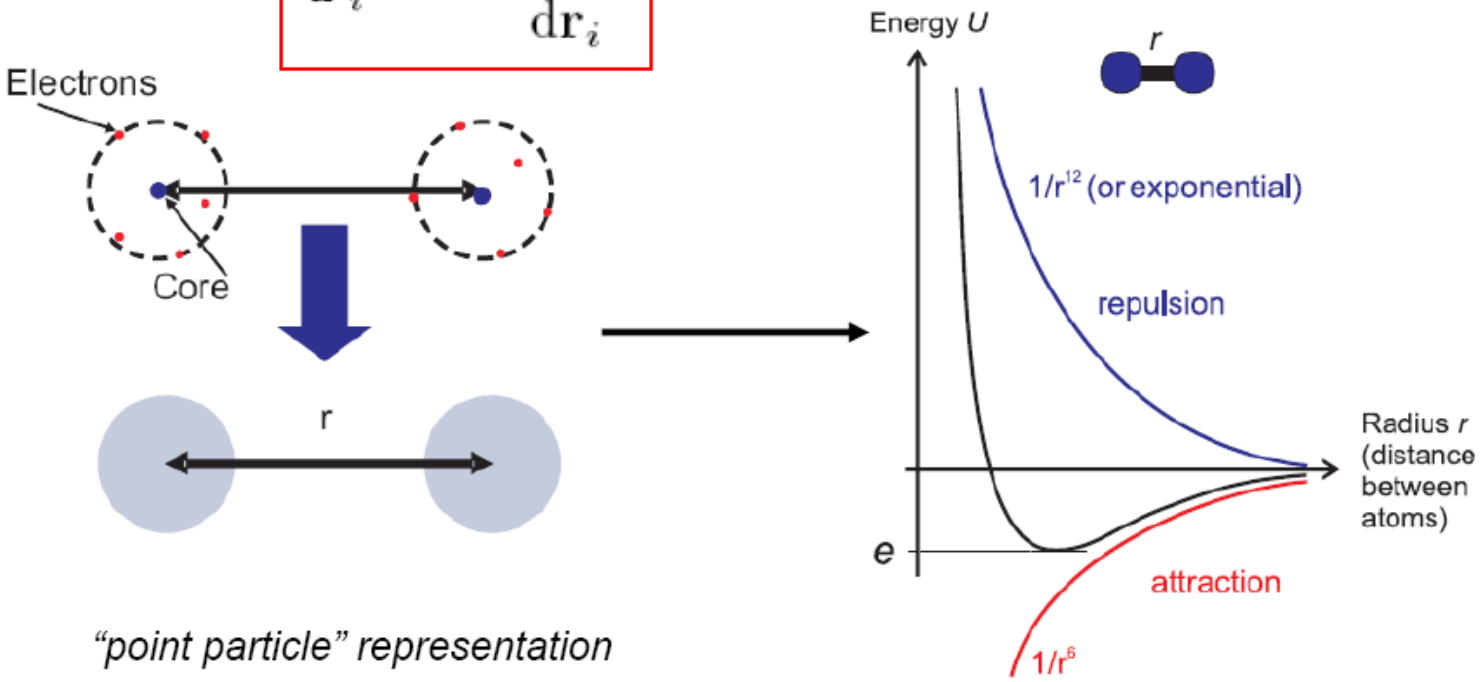
$$a_2 = \phi''(r_0) = k$$

$$\boxed{\phi(r) \approx \frac{k}{2}(r - r_0)^2}$$

Harmonic approximation

Concept: Interatomic potential

$$\mathbf{F}_i = -\frac{\mathrm{d}U(\mathbf{r}_i)}{\mathrm{d}\mathbf{r}_i}$$



"point particle" representation

Attraction: Formation of chemical bond by sharing of electrons
Repulsion: Pauli exclusion (too many electrons in small volume)

- **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)

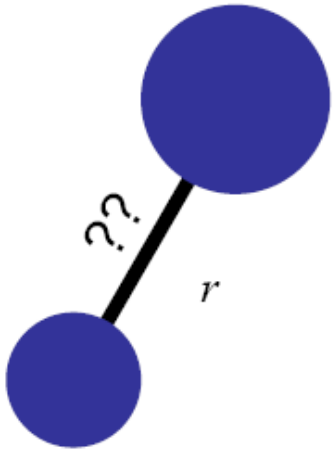
$$\phi_i = \sum_{j=1..N_{neigh}} \frac{1}{2} \phi(r_{ij}) + F(\rho_i(r_{ij}))$$

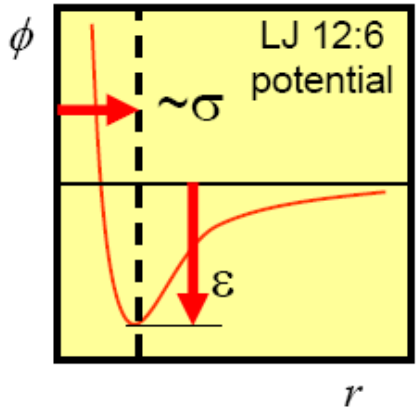
depends on all neighbors of i (multi-body)

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

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

Lennard-Jones potential: schematic





ε: well depth (energy per bond)

σ: force vanishes (EQ distance between atoms)

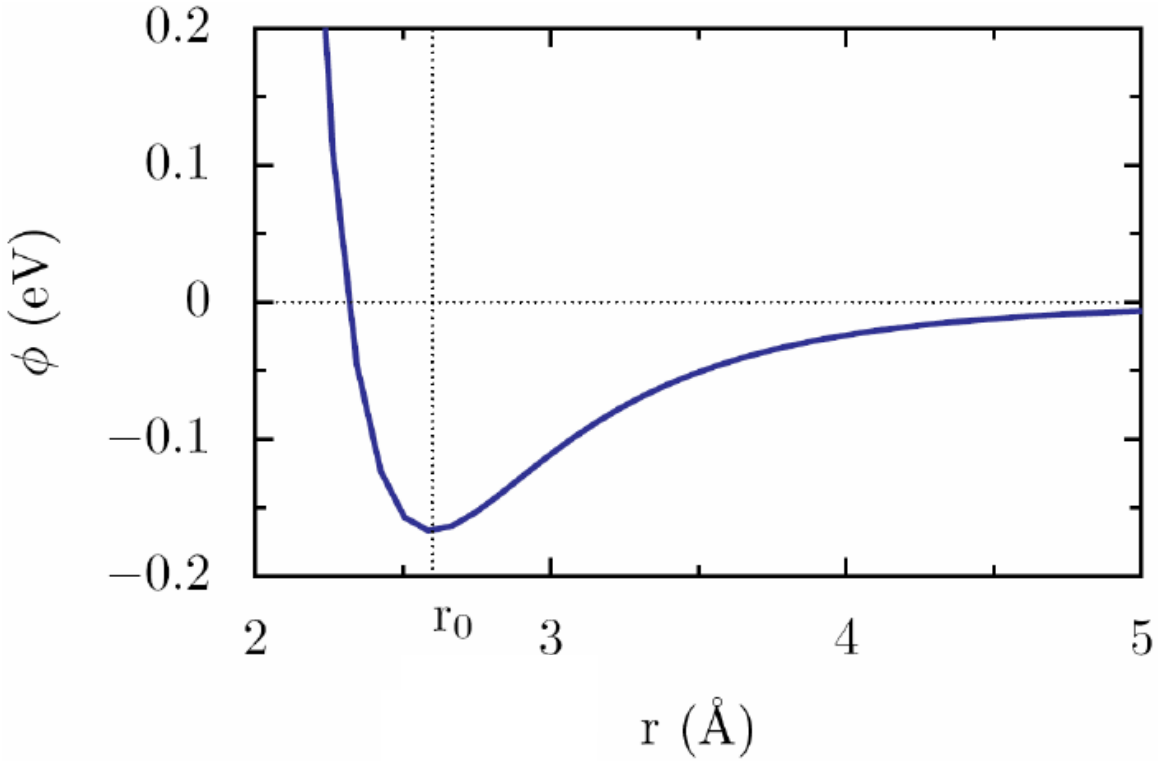
Sir J. E. Lennard-Jones (Cambridge UK)

Parameters

$$\phi(r) = 4\varepsilon\left(\left[\frac{\sigma}{r}\right]^{12} - \left[\frac{\sigma}{r}\right]^{6}\right)$$

Lennard-Jones 12:6

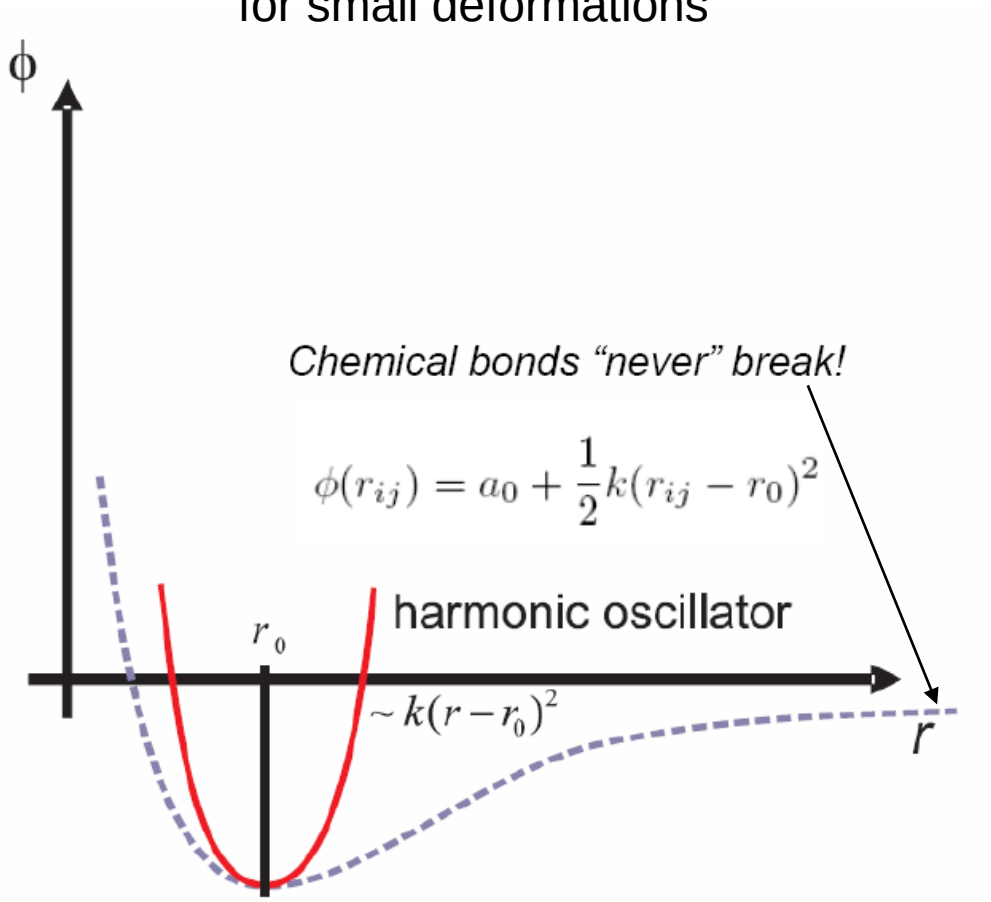
Lennard-Jones potential – example for copper



LJ potential – parameters for copper (Cleri *et al.*, 1997)

Harmonic approximation

for small deformations



Free energy density

harmonic pot

$$\psi(\varepsilon_{ij}) = \frac{2}{\sqrt{3}r_0^2}\left(\phi(l_1) + \phi(l_2) + \phi(l_3)\right) \qquad \phi(r) \approx \frac{k}{2}(r - r_0)^2$$

$$l_k = f(\varepsilon_{ij})$$

$$l_1 = (1 + \varepsilon_{11}) \cdot r_0$$

$$l_2 = \left(1 + \tfrac{1}{4}\varepsilon_{11} + \tfrac{3}{4}\varepsilon_{22} - \tfrac{\sqrt{3}}{4}(\varepsilon_{12} + \varepsilon_{21})\right) \cdot r_0$$

$$l_3 = \left(1 + \tfrac{1}{4}\varepsilon_{11} + \tfrac{3}{4}\varepsilon_{22} + \tfrac{\sqrt{3}}{4}(\varepsilon_{12} + \varepsilon_{21})\right) \cdot r_0$$

After lengthy algebra…

$$\psi(\varepsilon_{ij}) = \frac{\sqrt{3}}{8}\phi''\left(3\varepsilon_{11}^2 + 2\varepsilon_{11}\varepsilon_{22} + 3\varepsilon_{22}^2 + (\varepsilon_{21} + \varepsilon_{12})^2\right)$$

$\phi'' = k$ spring constant

Can now be used to determine constitutive relations

$$\sigma_{ij} = \frac{\partial \psi(\varepsilon_{ij})}{\partial \varepsilon_{ij}} \qquad c_{ijkl} = \frac{\partial^2 \psi(\varepsilon_{ij})}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}}$$

$$\sigma_{11} = \frac{\partial \psi(\varepsilon_{ij})}{\partial \varepsilon_{11}} = k\frac{\sqrt{3}}{4}(3\varepsilon_{11} + \varepsilon_{22}) \qquad \sigma_{22} = \frac{\partial \psi(\varepsilon_{ij})}{\partial \varepsilon_{22}} = k\frac{\sqrt{3}}{4}(3\varepsilon_{22} + \varepsilon_{11})$$

$$\sigma_{12} = \frac{\partial \psi(\varepsilon_{ij})}{\partial \varepsilon_{12}} = k\frac{\sqrt{3}}{4}(\varepsilon_{12} + \varepsilon_{21})$$

$$\varepsilon_{12} = \varepsilon_{21} \qquad \sigma_{12} = \frac{\partial \psi(\varepsilon_{ij})}{\partial \varepsilon_{12}} = k\frac{\sqrt{3}}{2}\varepsilon_{12}$$

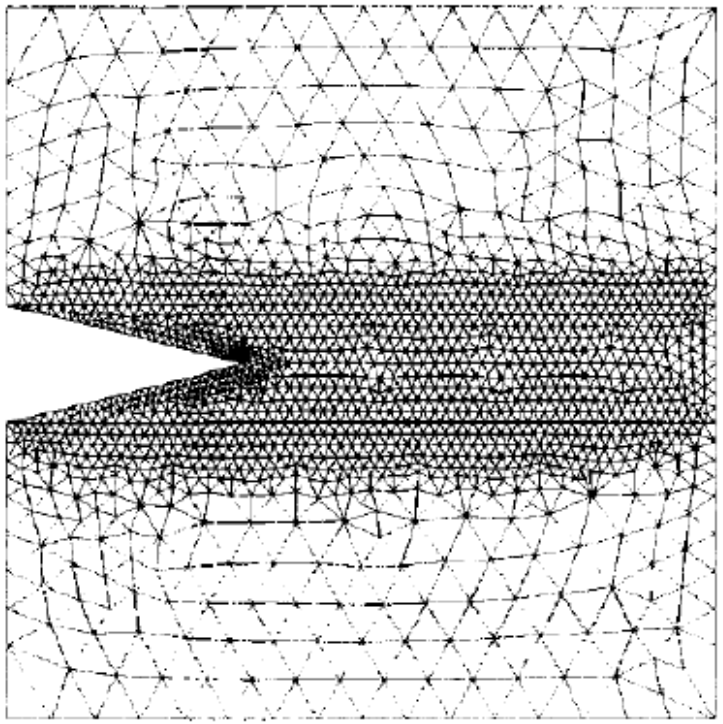
Summary

- Have model that **makes direct link between atomistic potential and structure** (e.g. random bonds as in amorphous materials) and **constitutive model**

- Have model that **describes failure of material** at point of loss of stiffness (instability)

- Can apply to **describe fracture of materials**!

Example: brittle fracture

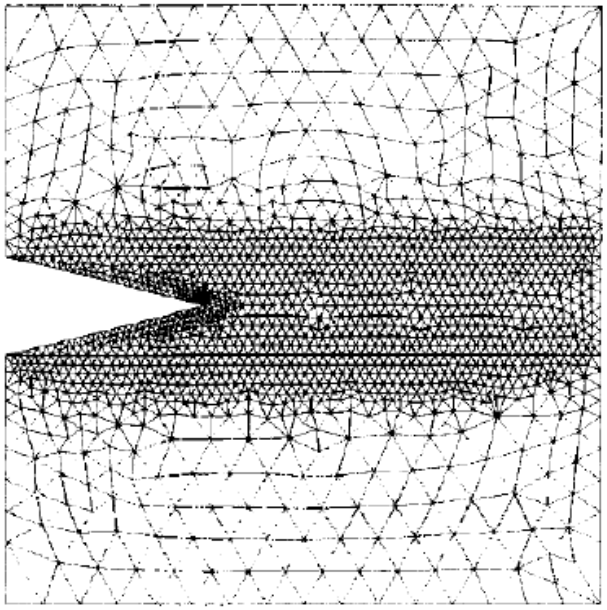


Mode I loaded crystal with crack

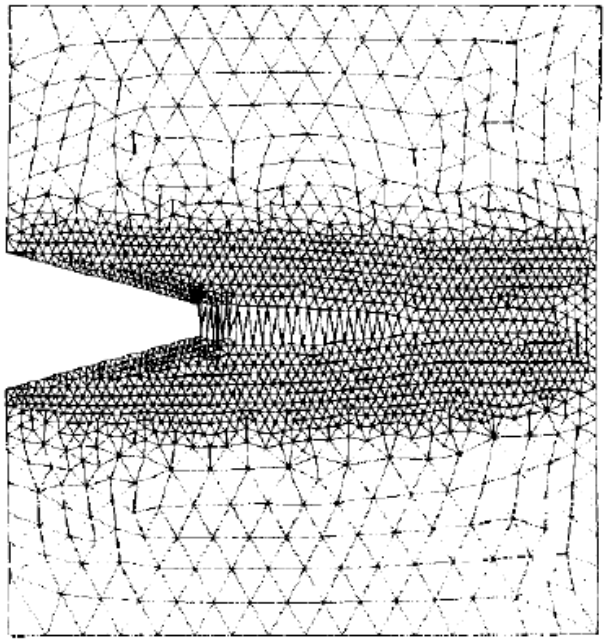
FE mesh denser around crack tip

Calculate constitutive relation directly from interatomic potential; depends on deformation state

Example: brittle fracture



fracture initiation

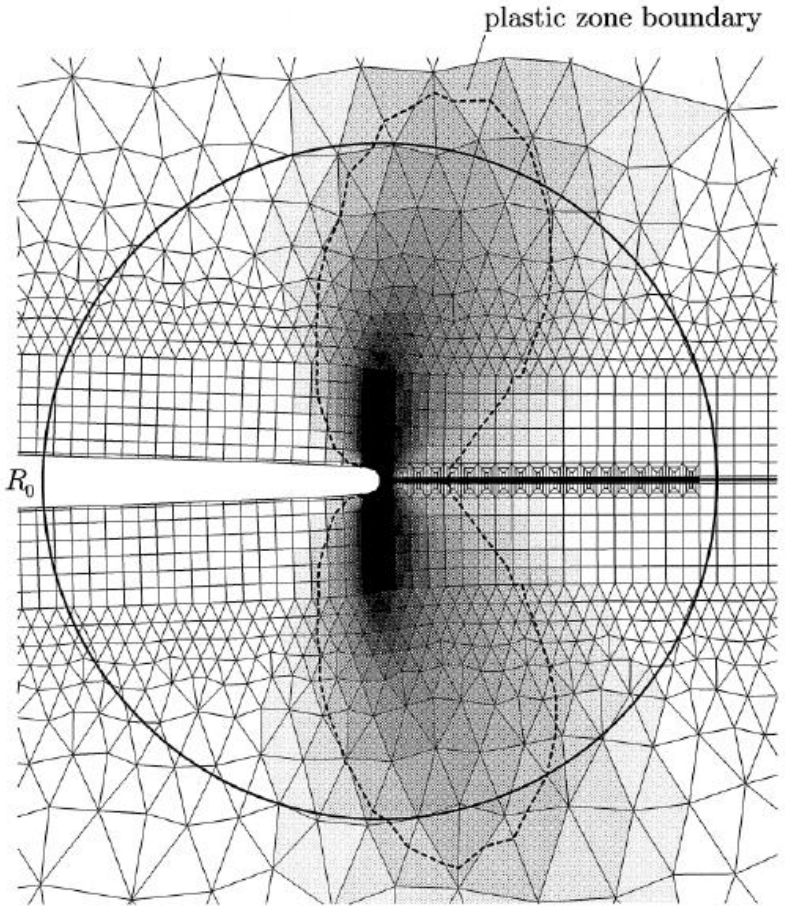


$$\min(c_i) = 0$$

Element failed when one wave speed equal to zero

Atomistic FE

Fracture simulations with VIB



Further developments…

VIB can not treat finite temperature effects

$$c_{ijkl} = \frac{\partial^2 \psi}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}}$$

zero temperature

$$\psi = U - TS$$

Finite temperature atomistic-continuum methods

Need an additional term to account for temperature:

the entropy due to the vibrations

A Finite-Temperature Continuum Theory Based on Interatomic Potentials

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Y. Huang

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University of Illinois, Urbana, IL 61801

K. C. Hwang
Department of Engineering Mechanics, Tsinghua University, Beijing, China 100084

There are significant efforts to develop continuum theories based on atomistic models. These atomistic-based continuum theories are limited to zero temperature (T=0 K). We have developed a finite-temperature continuum theory based on interatomic potentials. The effect of finite temperature is accounted for via the local harmonic approximation, which relates the entropy to the vibration frequencies of the system, and the latter are determined from the interatomic potential. The focus of this theory is to establish the continuum constitutive model in terms of the interatomic potential and temperature. We have studied the temperature dependence of specific heat and coefficient of thermal expansion of graphene and diamond, and have found good agreements with the experimental data without any parameter fitting. We have also studied the temperature dependence of Young's modulus and bifurcation strain of single-wall carbon nanotubes. [DOI: 10.1115/1.2019865]

Keywords: Finite Temperature, Local Harmonic Approximation, Interatomic Potential, Constitutive Model

Planck's constant

vibration frequencies of the system

$$S = -k_B \sum_{n=1}^{3N} \ln\left[2\sinh\left(\frac{h\omega_n}{4\pi k_B T}\right)\right]$$

Boltzmann constant

$$\psi = U - TS$$

Concept: account for entropic effects

Achieved by considering atomic vibrations

Atomistically informed finite temperature finite element method

$$S = -k_B \sum_{n=1}^{3N} \ln\left[2\sinh\left(\frac{h\omega_n}{4\pi k_B T}\right)\right] \qquad \psi = U - TS$$

$$\left| \omega_n^2 \boldsymbol{I}_{3N\times 3N} - \frac{1}{m}\frac{\partial^2 U_{\text{tot}}}{\partial \boldsymbol{x}\,\partial \boldsymbol{x}} \right| = 0$$

vibration frequencies of the system (eigenvalue problem)

Determine atomic vibrations, determined for specific crystal structure and interatomic potential

Jiang, Huang *et al.*, JEMT, 2005

Atomistically informed finite temperature finite element method

Free energy: $\psi = U - TS (=: A)$

Vibration frequencies For all atoms and all directions in RVE

$$\psi(r,T) = U_{\text{tot}}(r) + k_B T \sum_{i=1}^{N} \sum_{\kappa=1}^{3} \ln\left[2 \sinh\left(\frac{h\omega_{i\kappa}}{4\pi k_B T}\right)\right]$$

"regular" potential energy term (sum over all contributions in RVE)

entropic contribution (new)

Key concept: use free energy in Cauchy-Born rule instead of potential energy

$$\psi^* r,T) = U_{\text{tot}}(r) + k_B T \sum_{i=1}^{N} \sum_{\kappa=1}^{3} \ln\left[2 \sinh\left(\frac{h\omega_{i\kappa}}{4\pi k_B T} \right) \right]$$

volume of unit cell

$$\psi = \frac{\psi^*}{\Omega_0}$$

$$c_{ijkl} = \frac{\partial^2 \psi}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}}$$

Similar method (developed by W.K. Liu's group)

Comput Mech (2008) 42:531–541
DOI 10.1007/s00466-007-0239-x

ORIGINAL PAPER

A finite temperature continuum theory based on interatomic potential in crystalline solids

Albert C. To · Wing Kam Liu · Adrian Kopacz

Received: 14 June 2007 / Revised: 11 September 2007 / Accepted: 14 December 2007 / Published online: 8 January 2008

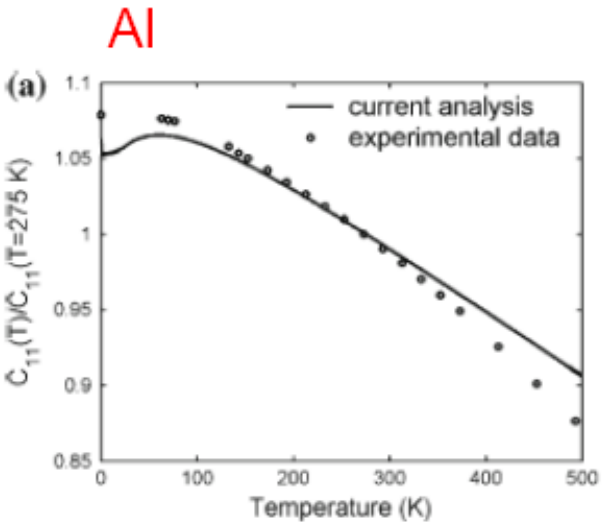
Abstract A finite temperature continuum theory of crystalline solid based on an approximate Helmholtz free energy expression is proposed. The free energy expression is specifically derived for simple implementation in atomistic-based continuum methods (i.e. quasicontinuum method) via the Cauchy–Born rule at finite temperature. It is obtained by the method of statistical moments via the quasi-harmonic approximation together with Taylor series expansion of a given interatomic potential. The phonons are assumed to follow the Bose–Einstein distribution so that the quantum effects at low temperature are accounted for. The resulting free energy is in terms of a given interatomic potential and a simple function of displacement that accounts for thermal expansion. It is employed to formulate two finite temperature continuum methods via Cauchy–Born rule and via the virtual atomic cluster (VAC). It is validated through comparison with experimental results of various thermodynamic quantities. In the case of fcc metals, the proposed free energy expression is shown to be valid for a wide range of temperatures above 50 K.

Keywords Quasicontinuum · Finite temperature continuum · Cauchy–Born rule · Interatomic potential · Crystalline solids

scale. Traditional single-scale modeling methods encounter great difficulties analyzing nanoscale structures due to its long length and time scales that make computation very inefficient [1–3]. Mesoscale systems consist of billions of atoms, which is simply too many for direct atomistic simulations such as molecular dynamics (MD). Neither scale can be modeled by traditional continuum methods because the correct physics at the nano- and meso-scale cannot be captured by these methods. Recently, many multiscale modeling methods and continuum theories based on interatomic potentials have been developed to address the issues of length and time scales while keeping some essential atomistic features [4–18]. At the continuum level in many of these multiscale methods and in the atomistic-based continuum theories, the equations of motion are derived from the interatomic potential via either the Cauchy–Born rule [6,19], or the recently developed virtual atomic cluster (VAC) [1,2,20]. In addition, the heterogeneous multiscale method (HMM) framework developed by E and co-workers obtains multiscale constitutive behavior by conserving energy and momentum at different scales [7,21].

There has been a recent surge of interest to account for finite temperature effects in these multiscale methods and atomistic-based continuum theories, namely the change in

Elasticity as function of temperature



Quasicontinuum (QC) method

E Tadmor, R Miller, W Curtin et al

The code can be downloaded

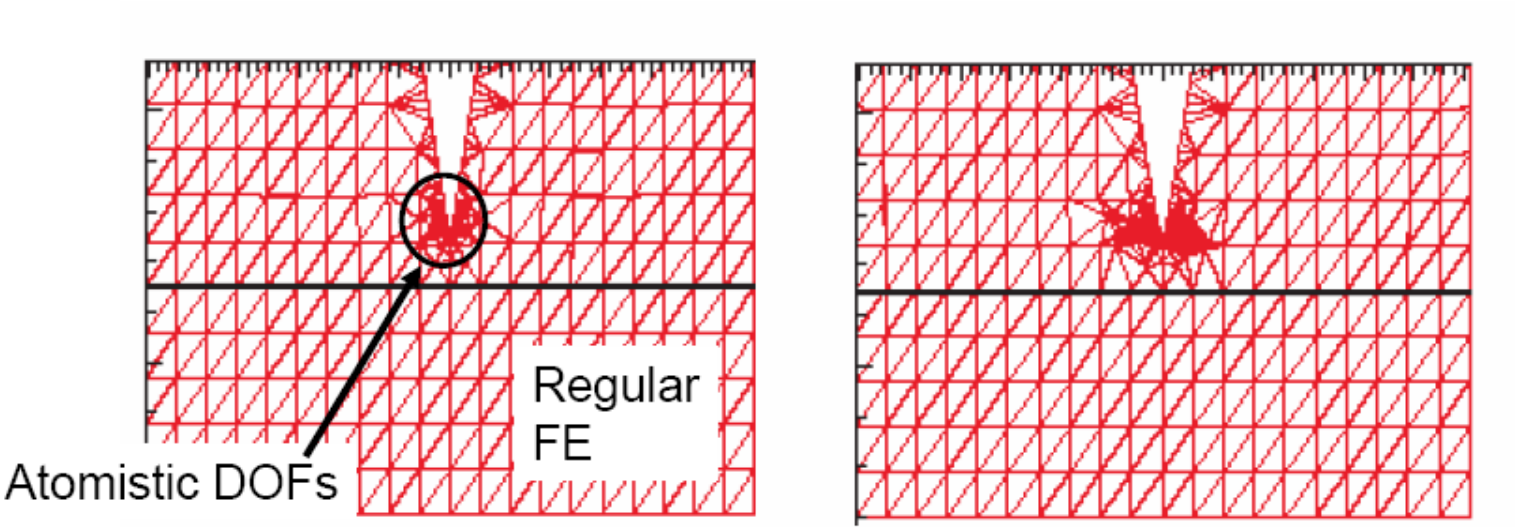
http://www.qcmethod.com/

Fundamentals of QC

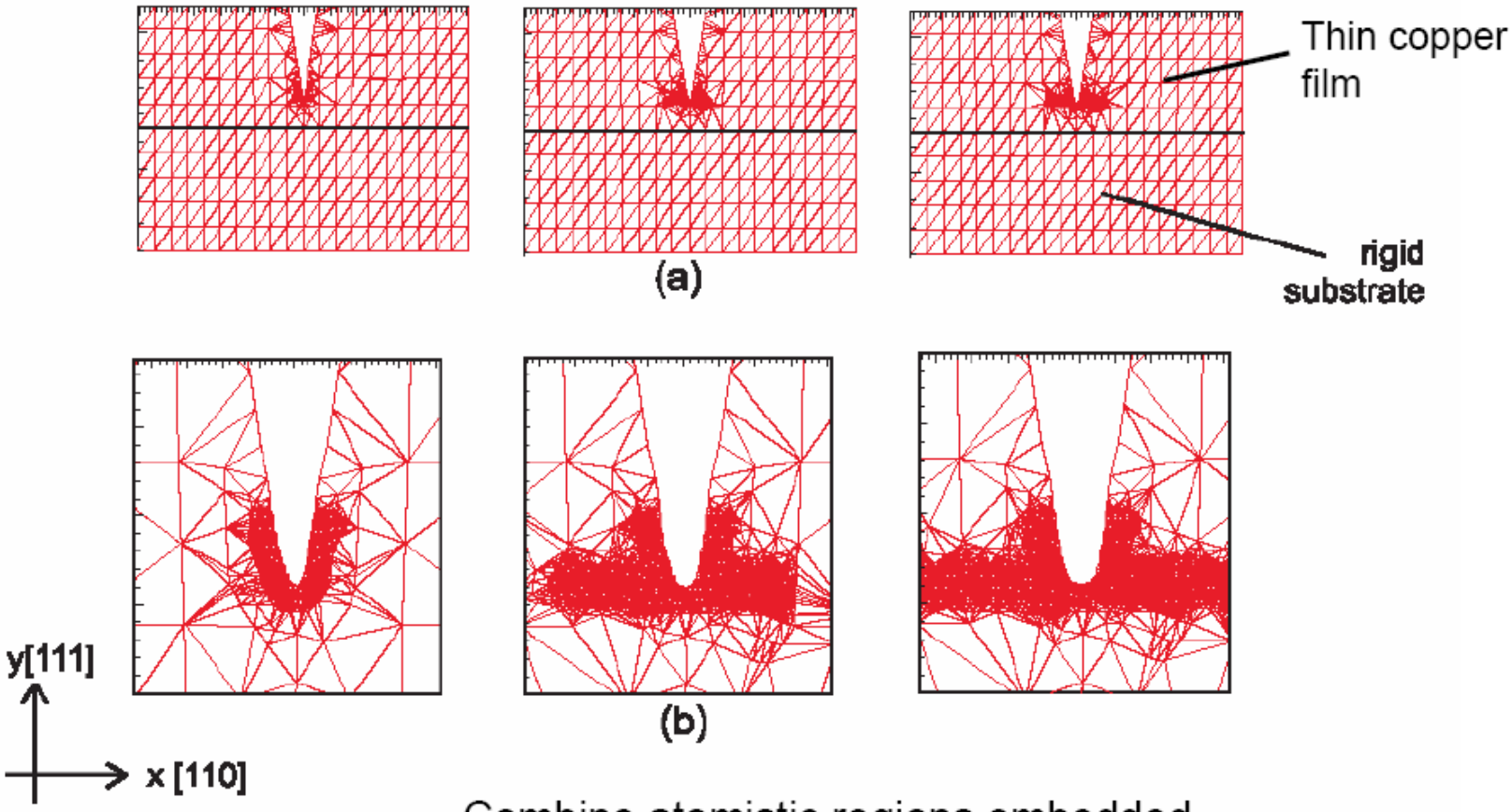
Use a **coupled atomistic-finite element domain**

Atomistic resolution of FE mesh possible (one FE node point = one atom)

In rest of domain, use C-B rule to obtain constitutive relation (similar to VIB, for small deformation only since FE model is linear elastic)



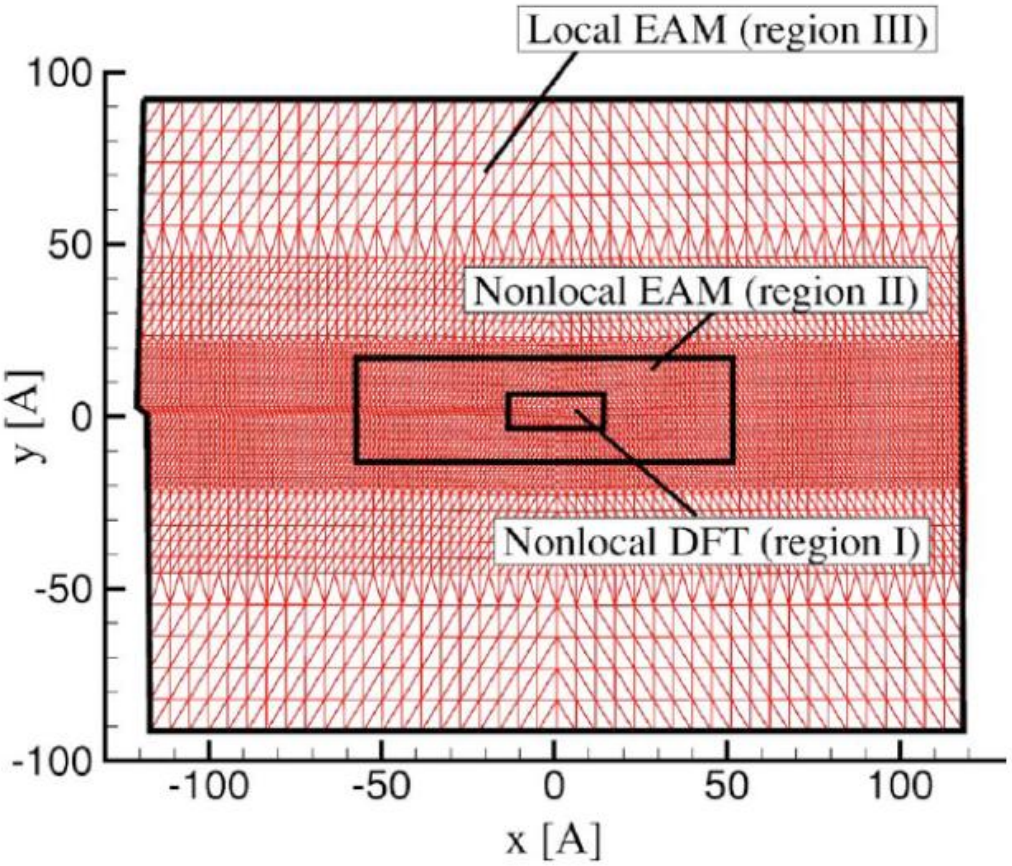
Crack in thin copper film



Combine atomistic regions embedded in continuum region

Buehler *et al.*, 2006

QC method to link DFT, EAM and FE



Lu, Tadmor, Kaxiras, PRB, 2005

Advantages & features

- Significantly reduced # of DOFs: atomistic description only where needed, in parts of the domain where strain is large (atomic bonds about to break, shear, rotate etc.)

- Compared with VIB can not only model brittle fracture, but also microscopic processes such as dislocation plasticity, grain boundary processes, etc.

Limited to 0 degree

A Unified Framework and Performance Benchmark of Fourteen Multiscale Atomistic/Continuum Coupling Methods*

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May 8, 2009

Abstract

A partitioned-domain multiscale method is a computational framework in which certain key regions are modeled atomistically while most of the domain is treated with an approximate continuum model (such as finite elements). The goal of such methods is to be able to reproduce the results of a fully-atomistic simulation at a reduced computational cost. In recent years, a large number of partitioned-domain methods have been proposed. Theoretically, these methods appear very different to each other making comparison difficult. Surprisingly, it turns out that at the implementation level these methods are in fact very similar. In this paper, we present a unified framework in which fourteen leading multiscale methods can be represented as special cases.

We use this common framework as a platform to test the accuracy and efficiency of the fourteen methods on a test problem; the structure and motion of a Lomer dislocation dipole in face-centered cubic aluminum. This problem was carefully selected to be sufficiently simple to be quick to simulate and straightforward to analyze, but not so simple to unwittingly hide differences between methods. The analysis enables us to identify generic features in multiscale methods that correlate with either high or low accuracy and either fast or slow performance.

All tests were performed using a single unified computer code in which all fourteen methods are implemented. This code is being made available to the public along with this paper.

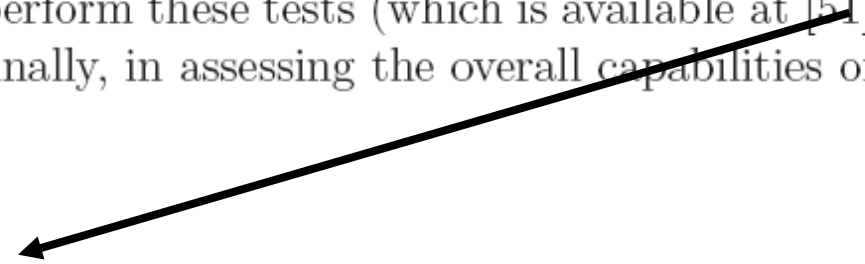
*To appear in *Modeling and Simulation in Materials Science and Engineering*, 2009. This article will also appear in a modified form as a chapter in the upcoming book: E. B. Tadmor and R. E. Miller, *Modeling Materials: Continuum, Atomistic and Multiscale Techniques*, Cambridge University Press.

Method	Acronym	Key References	Continuum Model	Handshake	Coupling Boundary Condition	Governing Formulation
Quasicontinuum	QC	[53, 45] section 4.1	Cauchy-Born	None	Strong Compatibility	Energy-Based
Coupling of Length Scales	CLS	[44] section 4.2	Linear Elasticity	None	Strong Compatibility	Energy-Based
Bridging Domain	BD	[60] section 4.3	Cauchy-Born	Linear mixing of energy	Weak Compatibility (penalty)	Energy-Based
Bridging Scale Method	BSM	[59, 39] section 4.4	Cauchy-Born	None	Weak/Stong Mix (least-squares fit)	Energy-Based
Composite Grid Atomistic Continuum Method	CACM	[10] section 4.5	Linear Elasticity	None	Weak Compatibility (average atomic positions)	Iterative Energy-Based (two energy functionals)
Cluster-Energy Quasicontinuum	CQC(m)-E	[15] section 4.6	Averaging of atomic clusters	None	Strong Compatibility	Energy-Based
Ghost-force corrected Quasicontinuum	QC-GFC	[46] section 4.7.1	Cauchy-Born	None	Strong Compatibility	Energy-Based with dead load GFC
Ghost-force corrected Cluster-Energy QC	CQC(m)-GFC	[15] section 4.7.2	Averaging of atomic clusters	None	Strong Compatibility	Energy-Based with dead load GFC
Finite-Element/Atomistics Method	FEAt	[25] section 6.1	non-linear, nonlocal elasticity	None	Strong Compatibility	Force-Based
Coupled Atomistics and Discrete Dislocations	CADD	[47, 48] section 6.1	Linear Elasticity	None	Strong Compatibility	Force-Based
Hybrid Simulation Method	HSM	[28] section 6.2	Non-Linear Elasticity	atomic averaging for nodal B.C.	Weak Compatibility (average atomic positions)	Force-Based
Concurrent AtC Coupling	AtC	[19, 4, 5, 35] section 6.3	Linear Elasticity	Linear mixing of stress and atomic force	Strong Compatibility	Force-Based
Ghost-force Corrected Concurrent AtC Coupling	AtC-GFC	unpublished section 6.3.1	Linear Elasticity	Linear mixing of stress and atomic force	Strong Compatibility	Force-Based
Cluster-Force Quasicontinuum	CQC(m)-F	[24] section 6.4	Averaging of atomic clusters	None	Strong Compatibility	Force-Based

Table 1: Summary of the methods discussed in this presentation.

14 leading multiscale methods

The intended audience of the paper is mainly developers of these and related methods; we hope that it will help guide future improvements. It will also be somewhat useful to potential *users* of these methods, but less so. By users, we imagine researchers that are already experienced with molecular dynamics and other atomistic methods, and who are trying to determine whether implementing a multiscale method will be worth the trouble: to understand if multiscale methods have a chance of solving their particular problem of interest. Such a user should be less interested in our comparison of the performance of the methods, focussing instead on the discussion of the details of the various methods presented and on the actual code used to perform these tests (which is available at [51]). This will give a sense of the effort required. Finally, in assessing the overall capabilities of these methods,



http://www.qcmethod.com/

You can download two code packages on this page:

- Multibench Test Suite version 1.0 (May 2009)
- Quasicontinuum Method Distribution version 1.3 (May 2007)

Dynamic effects

Although many of the methods discussed here were developed with dynamics in mind, we focus only on the static limit. As such, we are putting aside questions of wave reflections, thermostats and others that remain open challenges to the development of dynamic multi-scale models [31]. Our goal is to focus on the accuracy and efficiency of just the *coupling method itself*. Any errors or inefficiencies present in the static implementation of a coupling method will remain in the dynamic setting. Dynamics may introduce new challenges, and indeed some of these methods may be better suited than others to address these dynamic issues, but on this matter our study will be unable to opine.

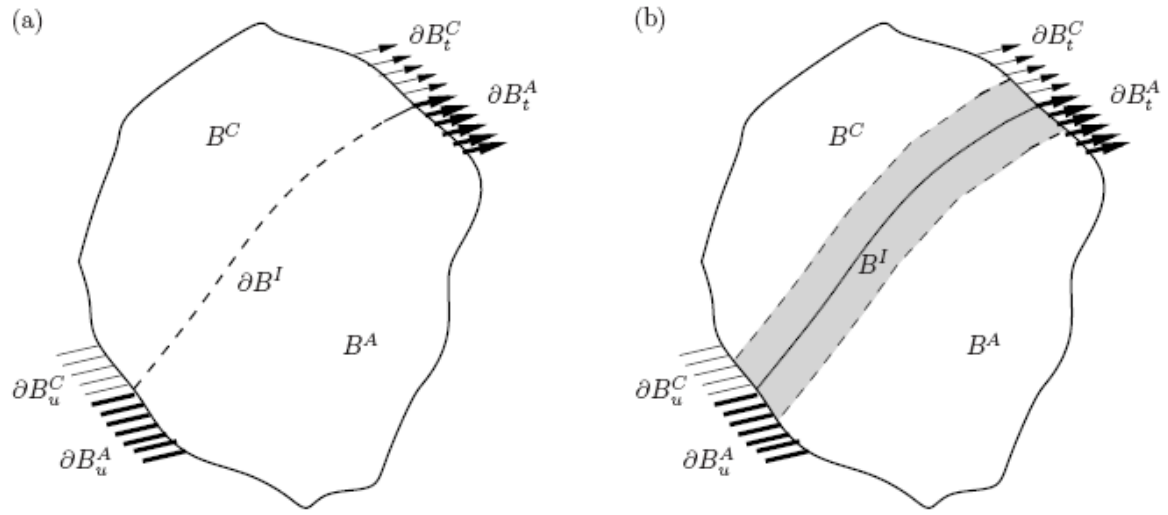


Figure 1: (a) A general partitioned domain problem. B^C is modeled as continuum while all atoms in B^A are explicitly treated as discrete degrees of freedom. (b) Some methods require a finite interfacial region, B^I, where the atomistic and continuum features must coexist.

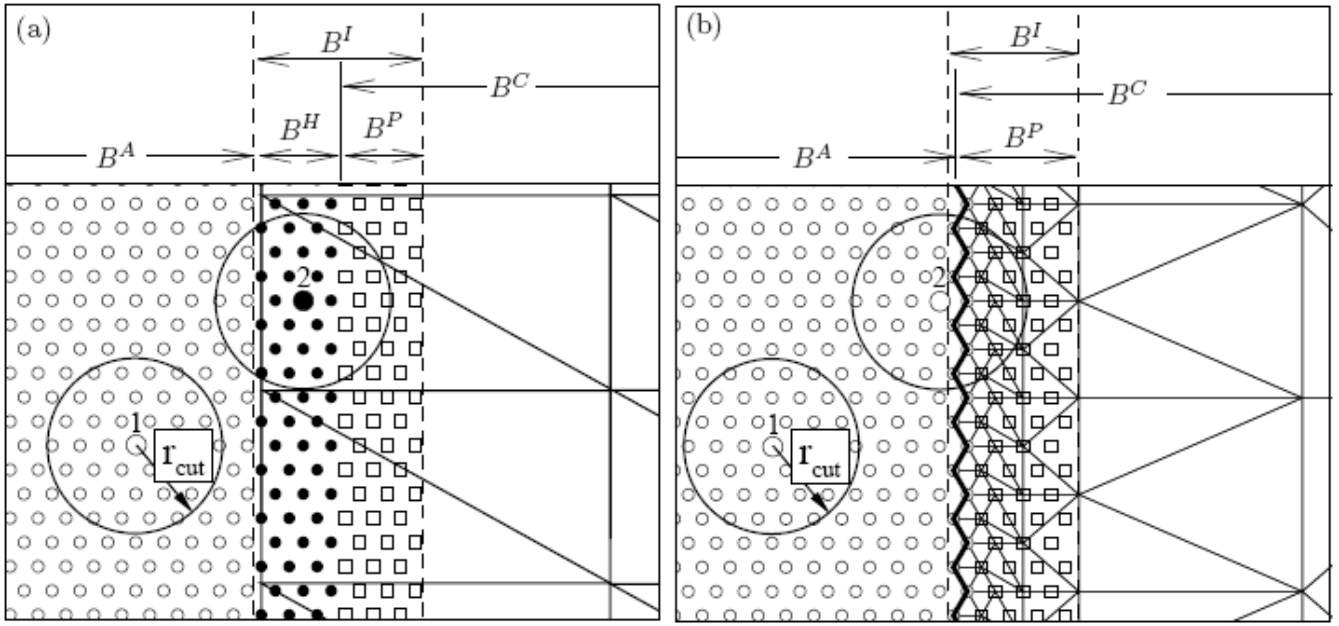


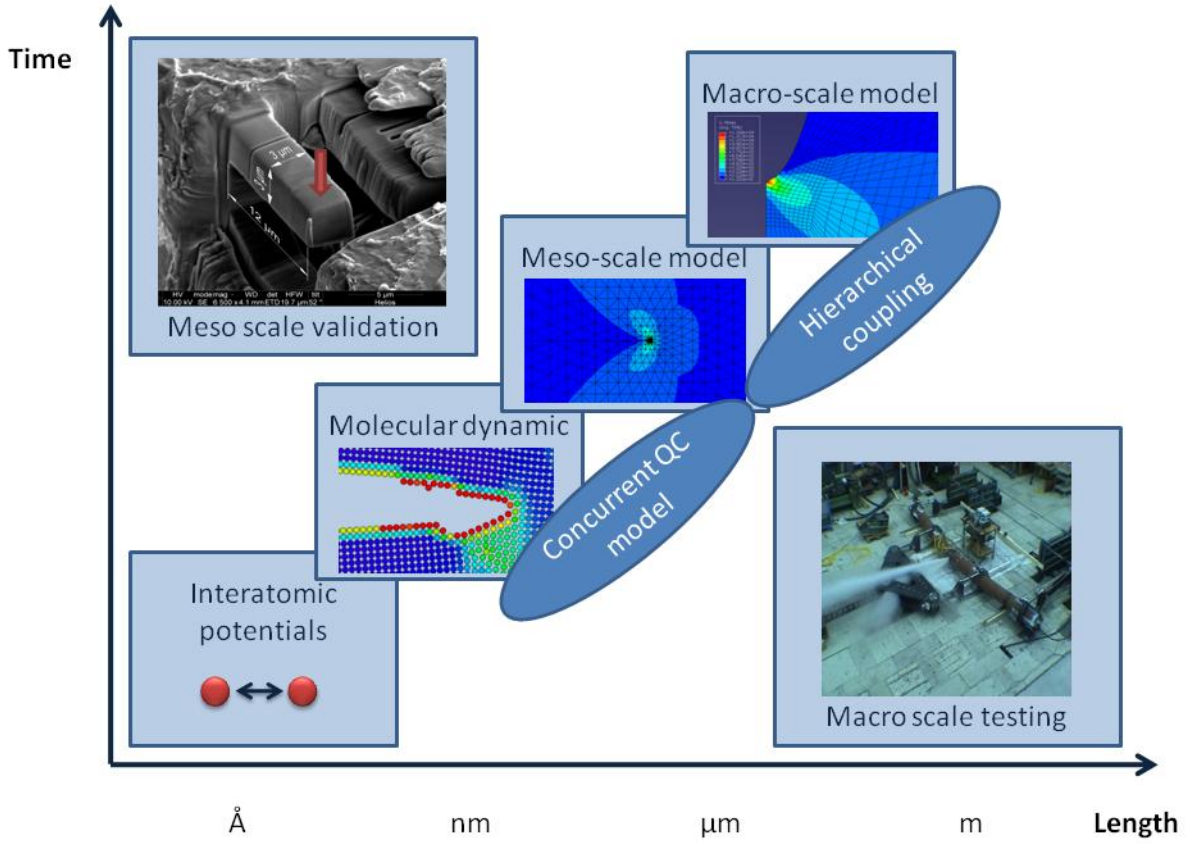
Figure 2: A generic interface in a coupled atomistic/continuum problem. The finite cut-off radius of the atoms mean that an atom like 1 cannot "see" into the continuum, while atom 2 can. Thus the need for a "padding" region as discussed in the text. The model on the left includes includes a handshake region, B^H, while the model on the right does not. Padding atoms are shown as open squares, handshake atoms as black circles and regular atoms as white circles. See the text for the discussion of frames (a) and (b).

- B^A region treated atomistically
- B^C region modeled as a continuum, FE
- B^I interface region, further subdivided in handshake region (H) and padding (fyll) region (P)

Multiscale Materials Modeling of Fracture

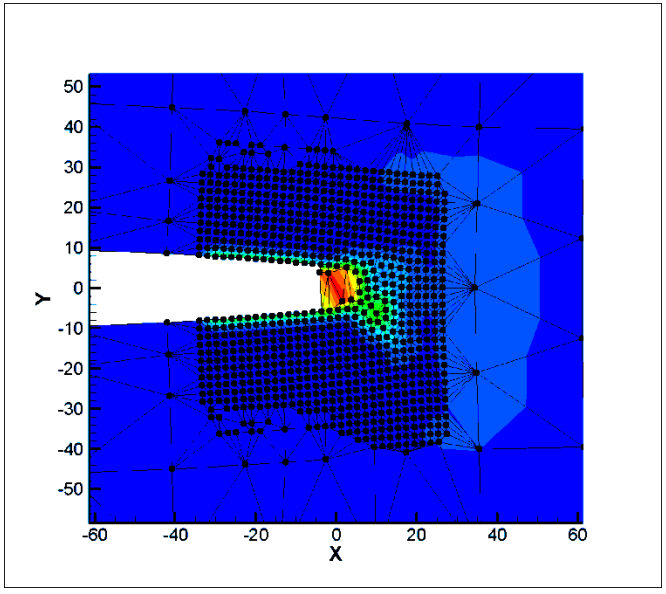
Work done at the Department for Engineering Design and Materials, NTNU

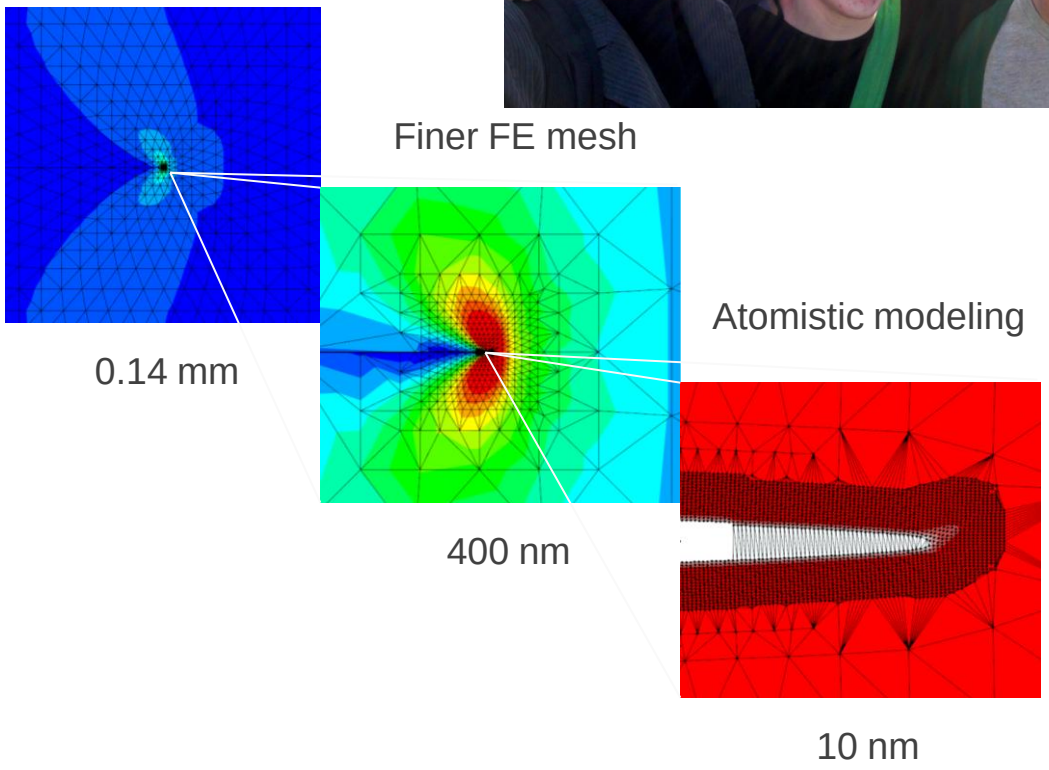
- Compared different crystallographic orientations
- Modified boundary layer (MBL) with different T – stresses
- Anisotropic vs. isotropic MBL
- Simulations with mixed mode loading (mode I and II, mode I and III)



Inga Ringdalen Vatne, PhD Arctic Materials
Multiscale Material Modeling of Fracture in bcc-Fe

QuasiContinuum model

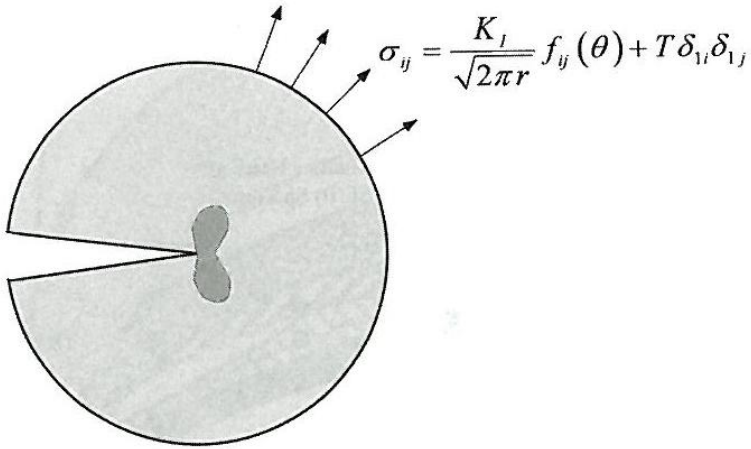


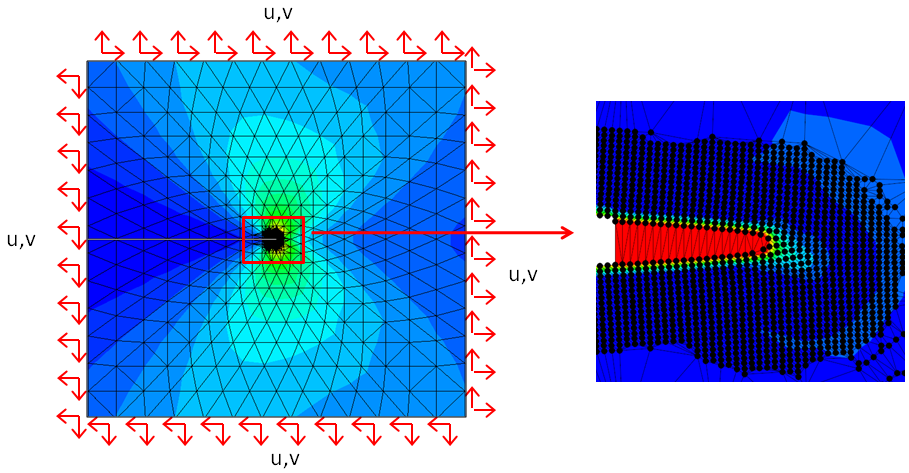


I R Vatne, E Østby and C Thaulow, “Multiscale Material Modeling of Fracture in Fe using Modified Boundary Layer(MBL)” Presented at ECF18, Dresden, Germany, Sept 2010.

Multiscale modeling of fracture in bcc-Fe

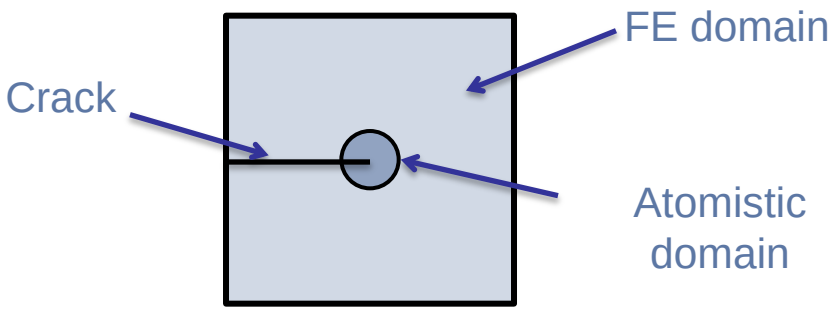
- Using the Quasicontinuum method.
- Atomistic description at the crack tip. (adaptive)
- Continuum mechanical description in the rest (Cauchy Born)
- Using modified boundary layer analysis with different T-stress and mode I and II. Isotropic and anisotropic.
- Investigated three different crystallographic orientations.

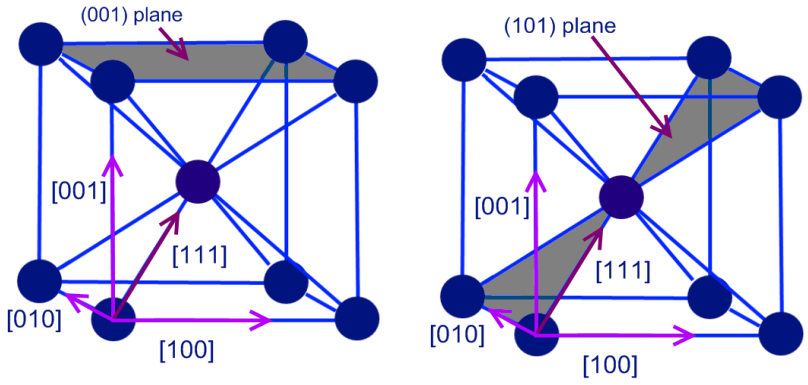




Method and model

- Quasicontinuum method – adaptive atomistic where high accuracy is needed, FE with Cauchy Born elsewhere.
- Square model, 1500 x 1500 Å
- 0 K, static simulations, 2D
- EAM potential by Mendelev et. al.





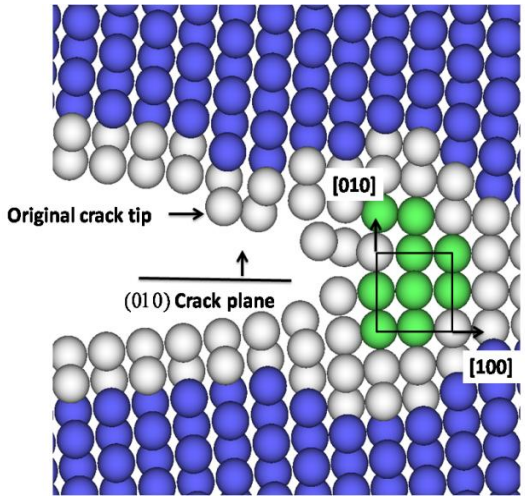
Orientation	Crack plane/ Crack front
1	(010)[101]
2	(110][001]
3	(011)[011]
4	(010)[001]

Mendelev, M.I et. al. *Development of new interatomic potentials appropriate for crystalline and liquid iron* Phil. Mag. 2003

Miller, R.E et al. *The Quasicontinuum method: Overview, applications and current directions* J. comp. mat. Des. 2002

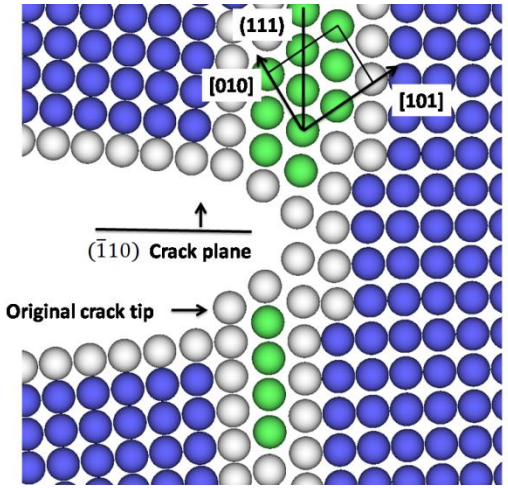
Crack tip mechanisms

Details of mechanisms at crack tip with pure mode I loading. Visualized in Ovito with common neighbor analysis (cna). Blue – bcc, green – fcc, red – twinning, white – other



Orientation 1

Crack growth on {001} plane. Creation of fcc area at crack tip with Bain orientation relationship.



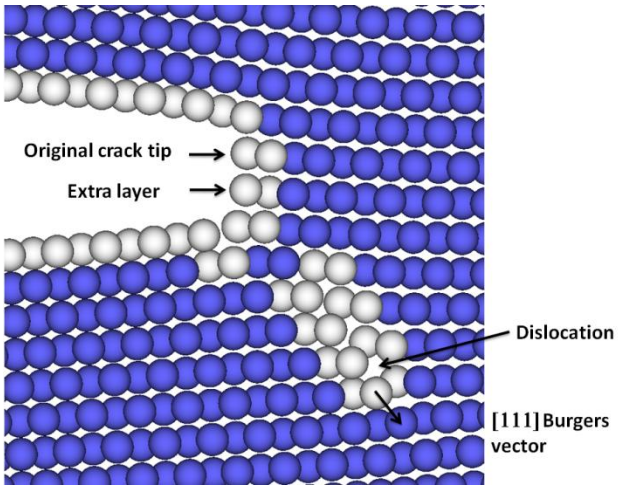
Orientation 2

Crack growth on {011} plane (which have lowest surface energy for potential). Creation of fcc area at crack tip with Nisishima-Wassermann orientation relationship.

Stukowski, A. *OVITO – the Open Visualization Tool* Mod.and Simul. In Mater. Sci. and Engineering, 2010

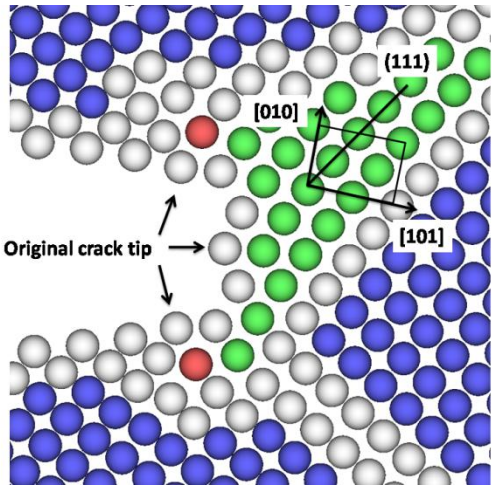
Crack tip mechanisms

Details of mechanisms at crack tip with pure mode I loading. Visualized in Ovito with common neighbor analysis (cna). Blue – bcc, green – fcc, red – twinning, white – other



Orientation 3

Emission of edge dislocation with ½[111] Burgers vector on the {112} plane



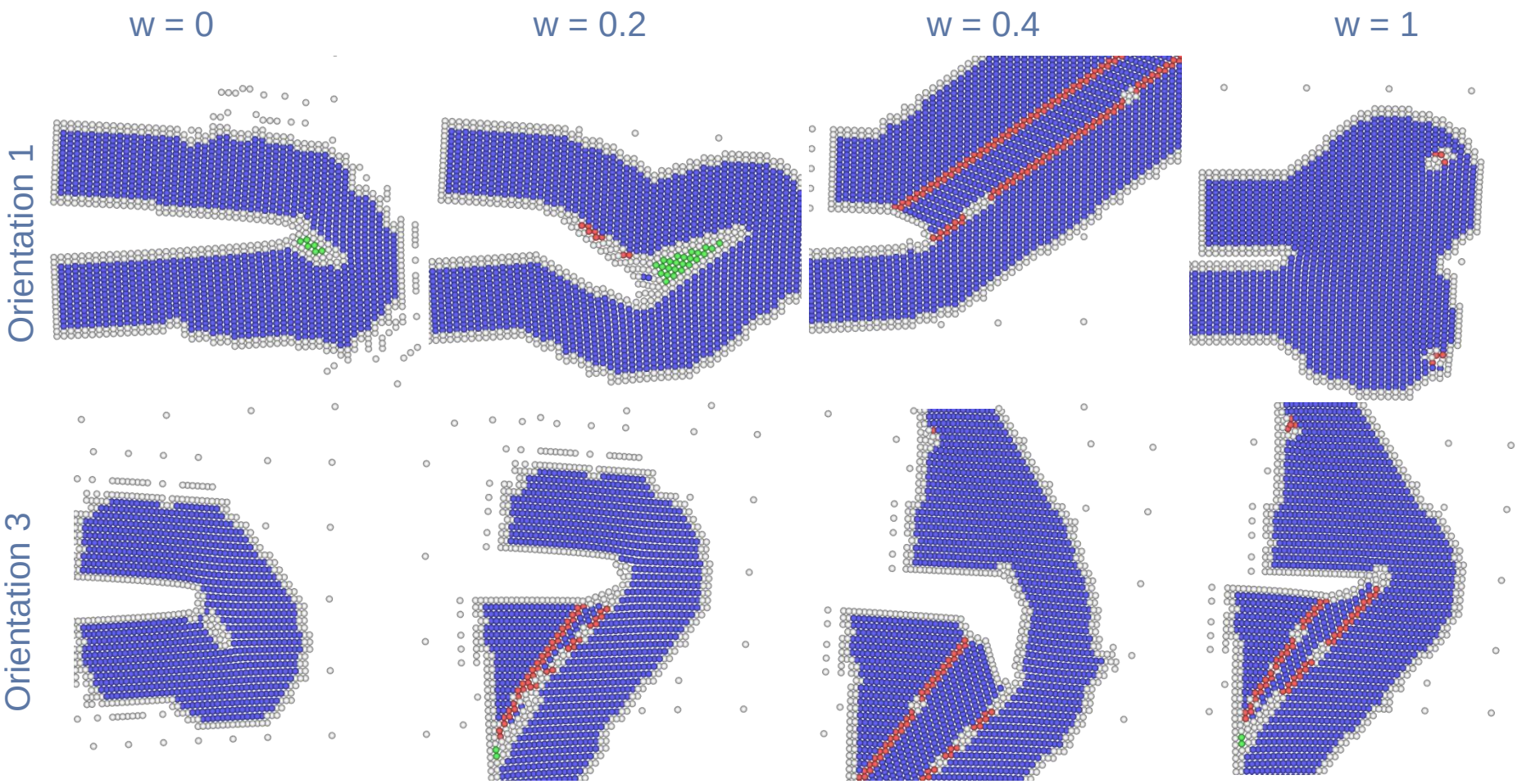
Orientation 4

Crack propagation on a {011} plane and creation of fcc area with a Nisishima-Wassermann orientation relationship like orientation 2.

Stukowski, A. *OVITO – the Open Visualization Tool* Mod.and Simul. In Mater. Sci. and Engineering, 2010

Mixed mode simulations (mode I and II)

Stress intensity factors given by w through: $K_I=K*(1-w)$, $K_{II}=K*w$

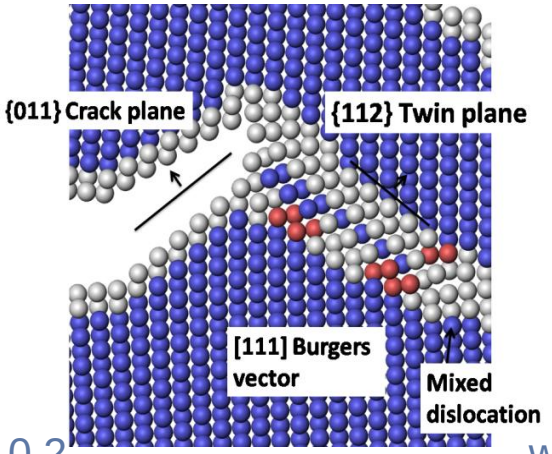


Mixed mode simulations (mode I and III)

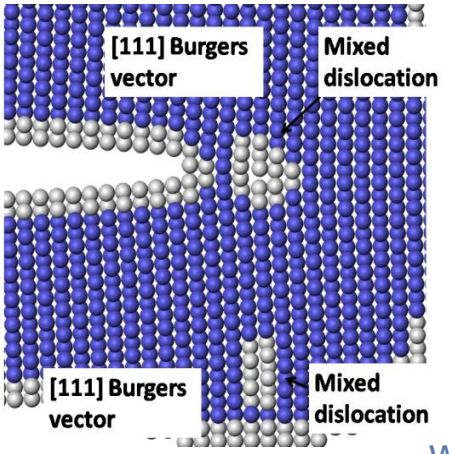
Stress intensity factors given by w through: $K_I=K*(1-w)$, $K_{III}=K*w$

Orientation 1

w = 0.3

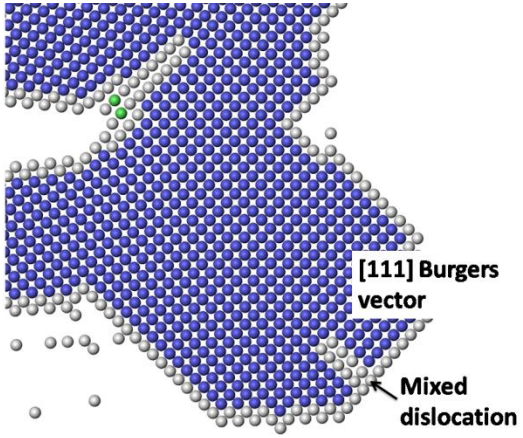


w = 0.5

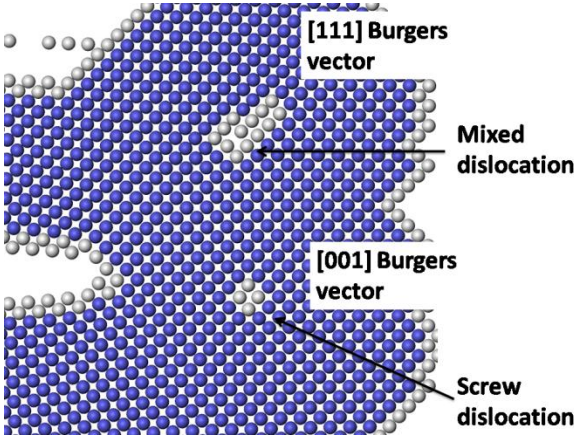


Orientation 4

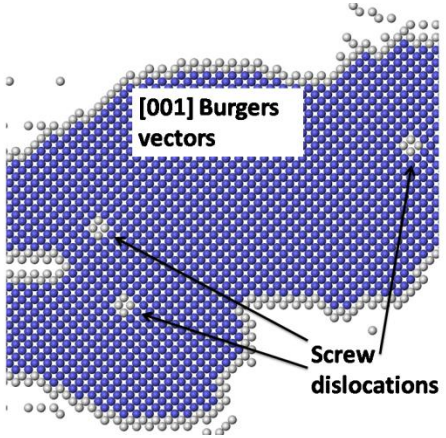
w = 0.2



w = 0.6



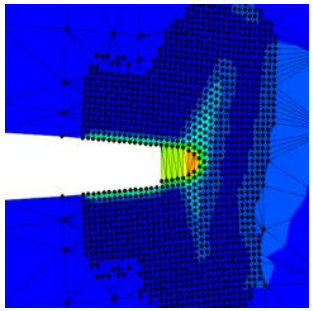
w = 1



Concurrent Multiscale Methods

Challenges with multiscale methods:

- Timestep
  - Limited by atomistic vibrations also in continuum domain
- Temperature
  - How to account for kinetic energy
  - What to do with waves
- Interface
  - How to enforce compability and equilbrium across interface
  - Can cause spurious forces



Fifth International Conference

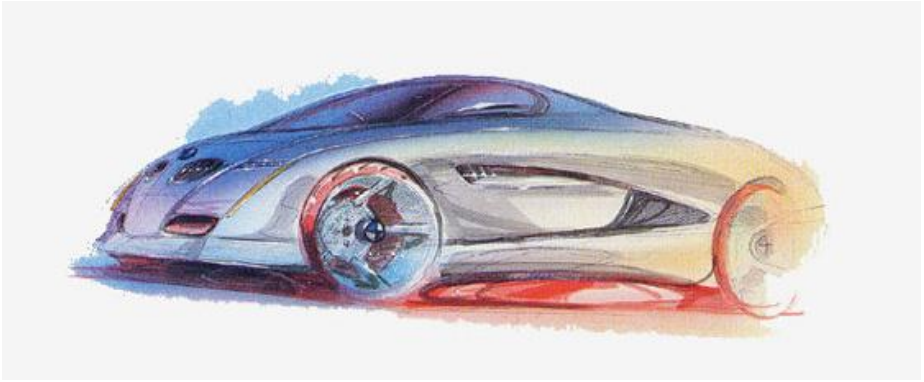
MMM 2010

Multiscale Materials Modeling

October 04 - 08, 2010, Freiburg, Germany

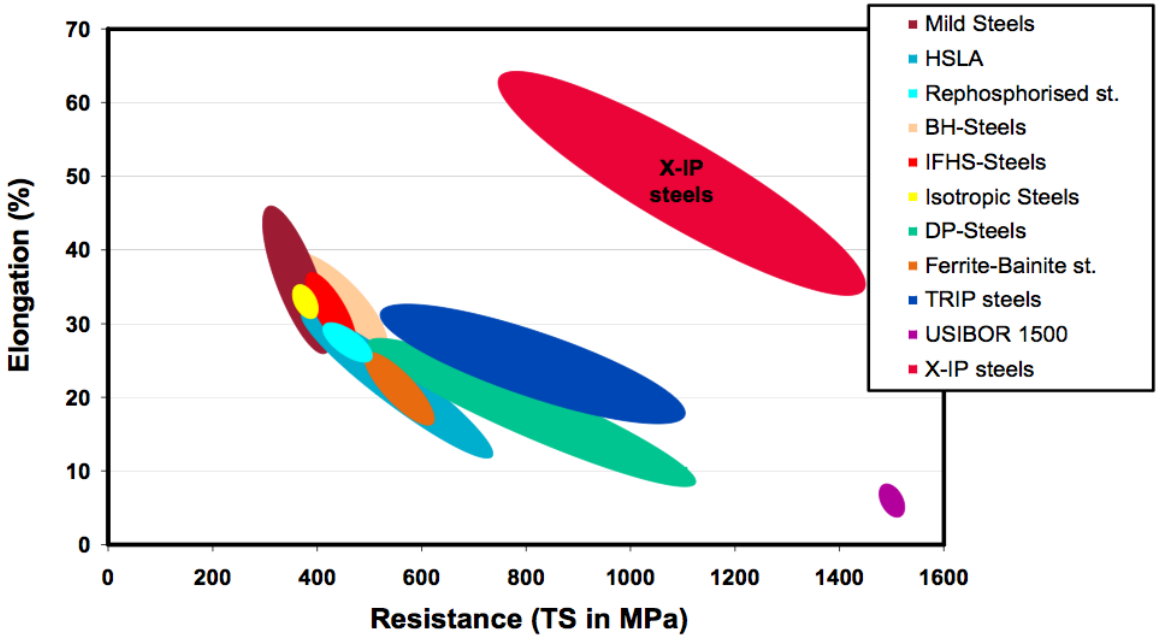
PROGRAM

DEVELOPMENT OF NANOTECHNOLOGY BASED STEELS



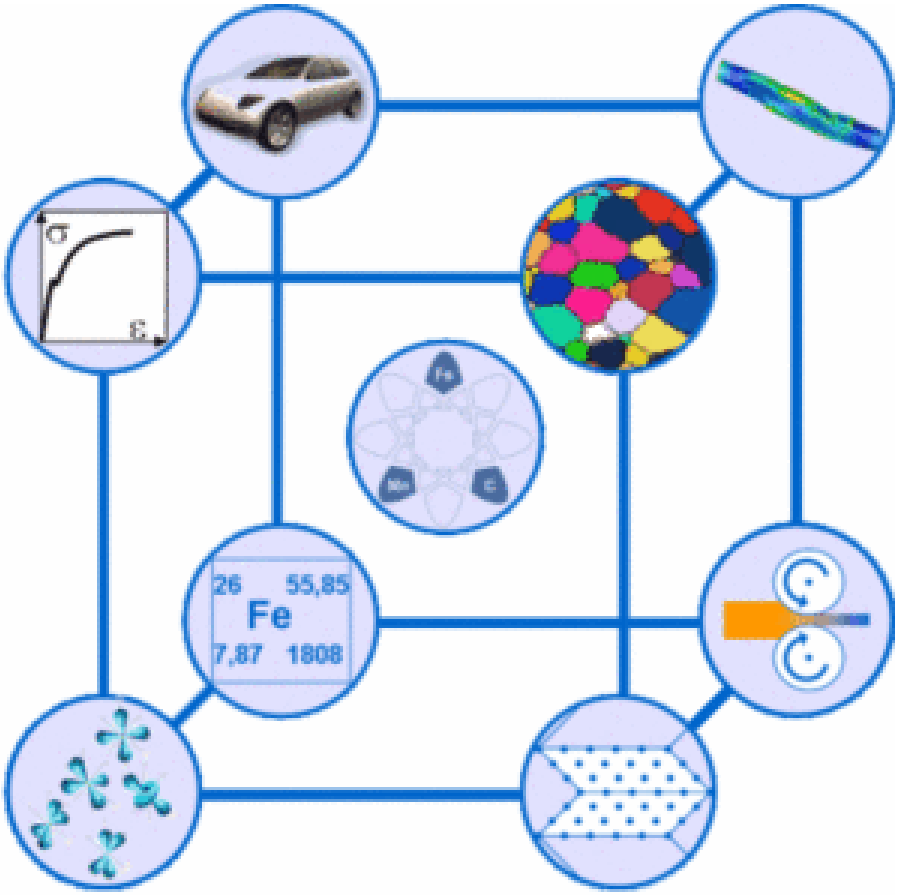
CYBER STEEL 2020 USA

STAHL AB INITIO GERMANY



Stahl ab initio - Germany

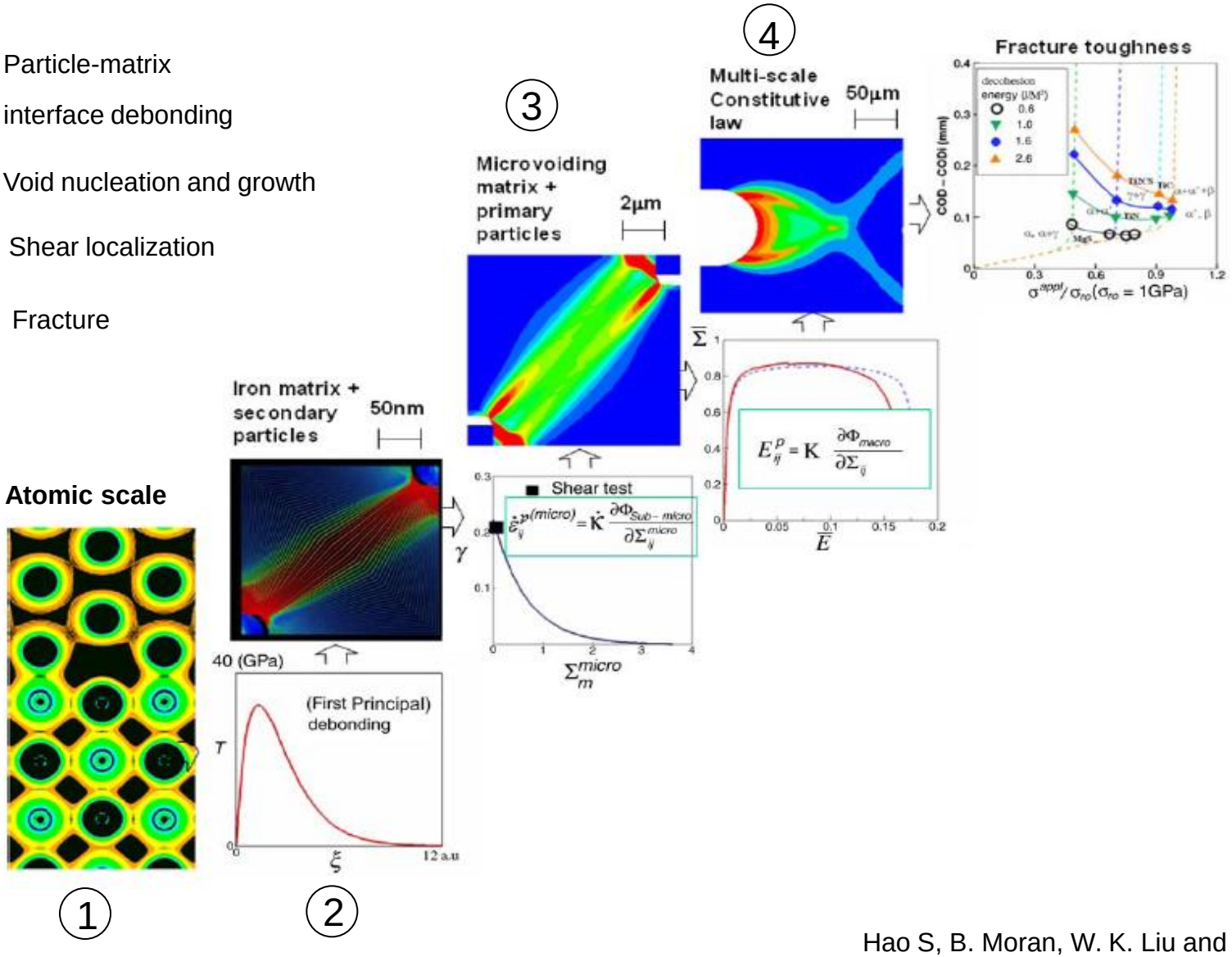
Quantum mechanics-guided design of new Fe based materials: Fe-Mn-C



Neuer Ansatz: Parallelität von
Werkstoffentwicklung und Modellierung

Multiscale material modelling of ductile fracture in steel

1. Particle-matrix interface debonding
2. Void nucleation and growth
3. Shear localization
4. Fracture

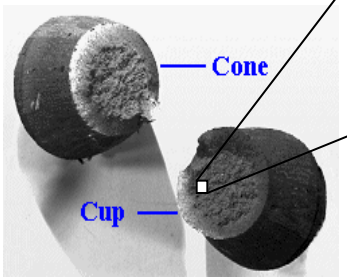


Hao S, B. Moran, W. K. Liu and G.B. Olson 2004

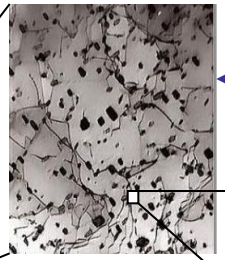
Microstructure of high strength and high toughness steel

Heterogeneous material

Interfacial strength between inclusions influence the strength and ductility

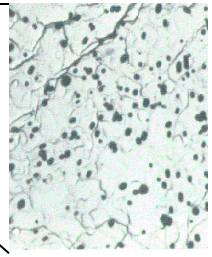


Macro scale



Micro scale

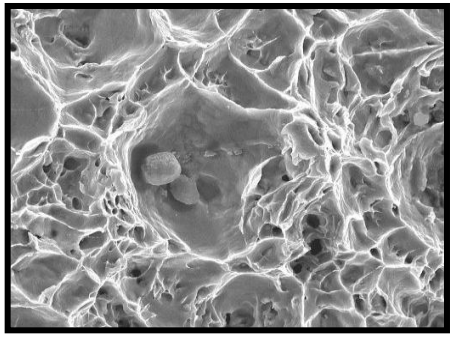
primary particles (~μm) – yield strength



Sub-micro scale

secondary particles (~0.1μm) – ductility

Fracture surface



• Deformation of microstructure at each scale is important in the fracture process

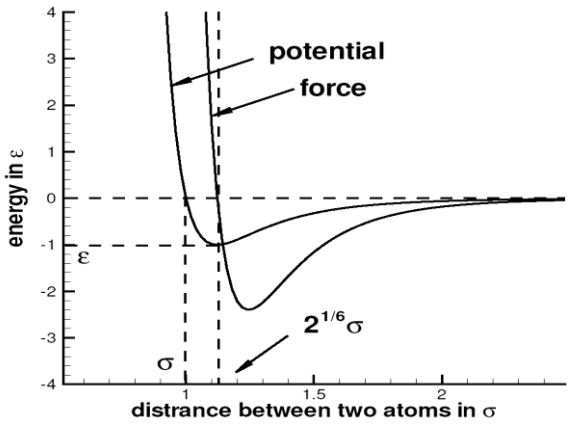
•Need a general **multi-scale continuum theory** for materials that accounts for microstructure deformation and interactions

Classical MD

- **Main point: calculate atomic interaction**

The force vector for each particle $\mathbf{f} = -\nabla E_{tot}$

Total energy of the system $E_{tot} = \sum_{i=1}^{N} \phi_i$

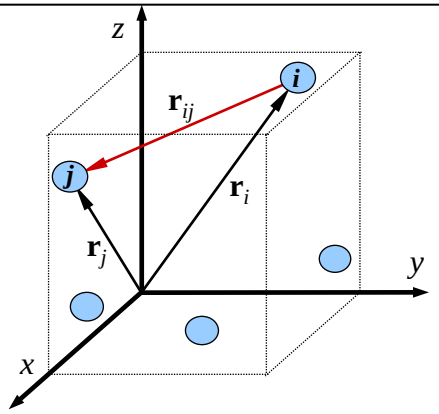


ϕ_i potential energy of a particle

Example: Lennard-Jones potential

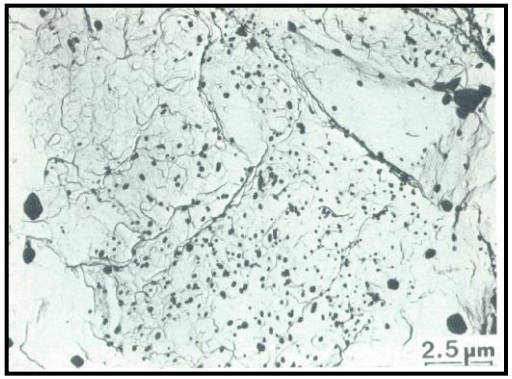
Pair potential $\phi_i(r) = \sum_{j=1}^{N_i} \phi_{ij}(r_{ij})$

$$\phi_{ij}(r_{ij}) = \sum_{j=1}^{N_i} 4\epsilon_0 \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right]$$

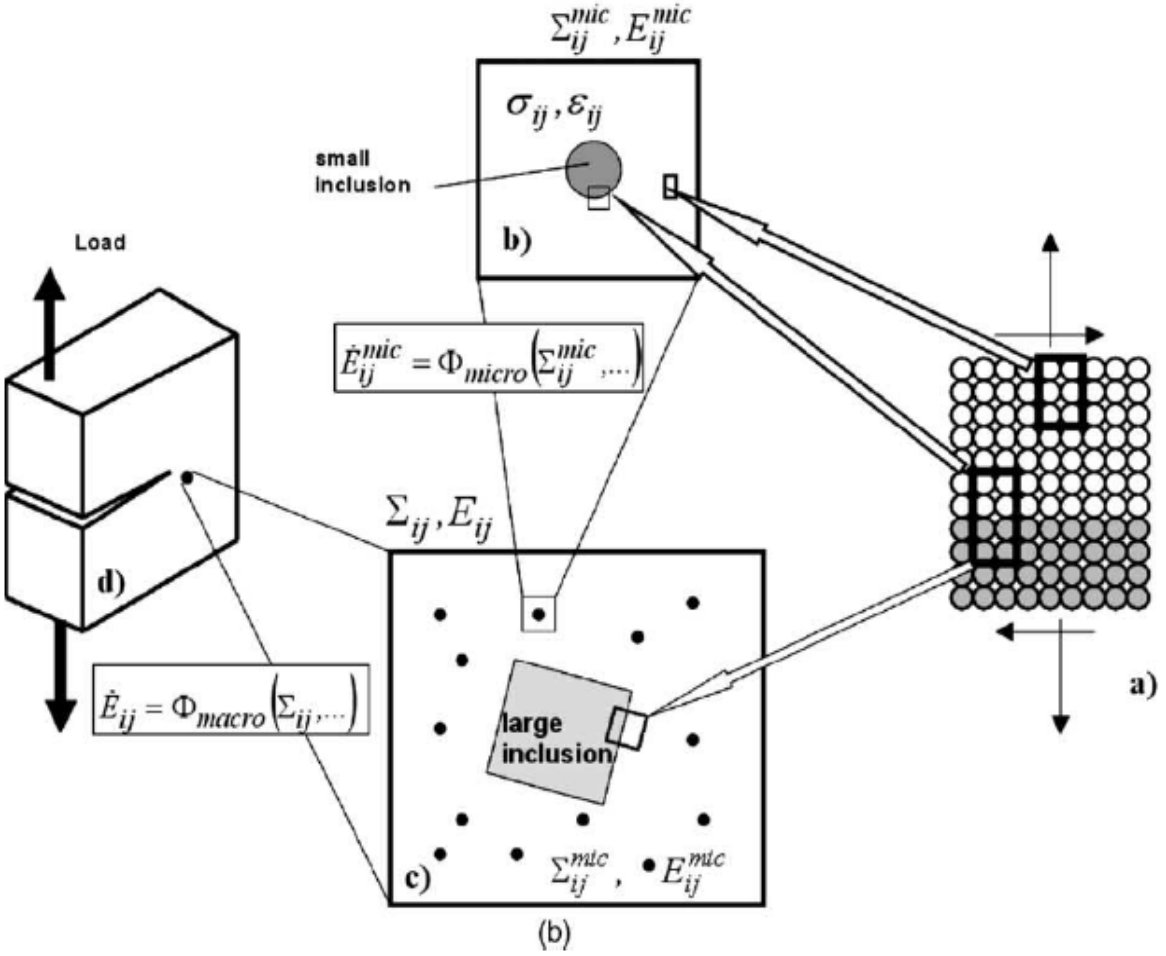


A hierarchical multi-physics model for design of high toughness steels

Bottom – up model



Micrograph of high strength steel

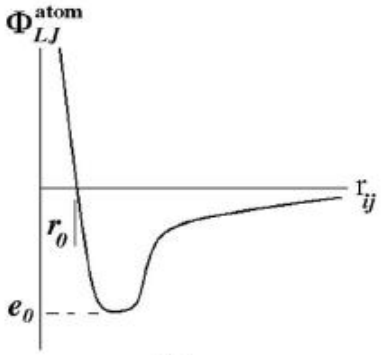


S. Hao, B. Moran, W. K. Liu and G.B. Olson, Journal of Computer-Aided Materials Design, 10, 99-142, 2003

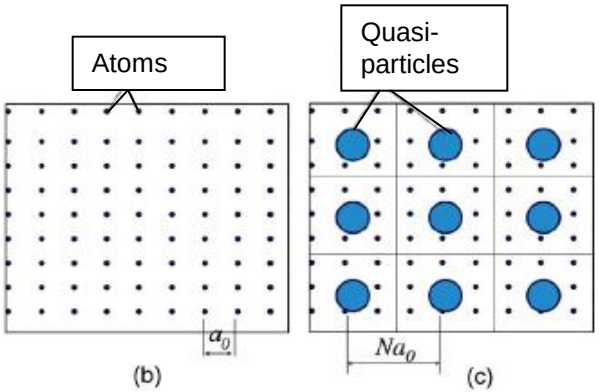
S. Hao, W. K. Liu, B. Moran, F. Vernerey and G.B. Olson, Comput. Methods Appl. Mech. Engrg. 193, 1865-1908, 2004

Quasi-particle dynamical approach – sub-microcell

- Molecular dynamics (MD) breaks down when a sufficiently large amount of atoms to represent the physics of interest.
- Quasi-particle dynamical approach: lumping of fixed number of atoms into ”super atoms” = ”quasi-particles”

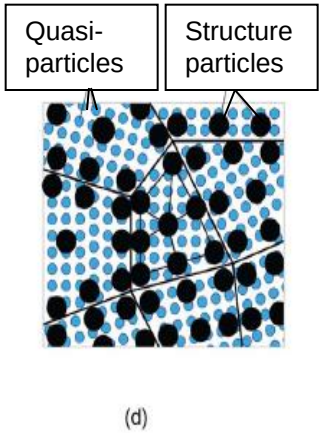


Lennard-Jones interatomic potential

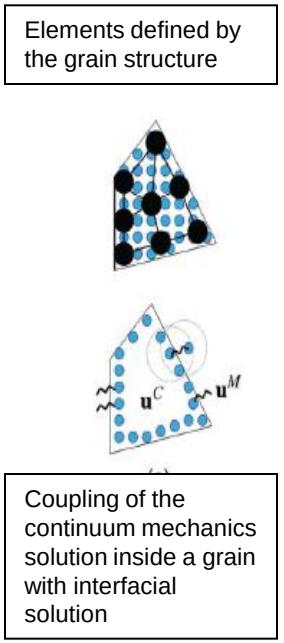


Atomic system: equilibrium interatomic distance a_0

Particle system: equilibrium inter-particle distance Na_0



Structural particle system



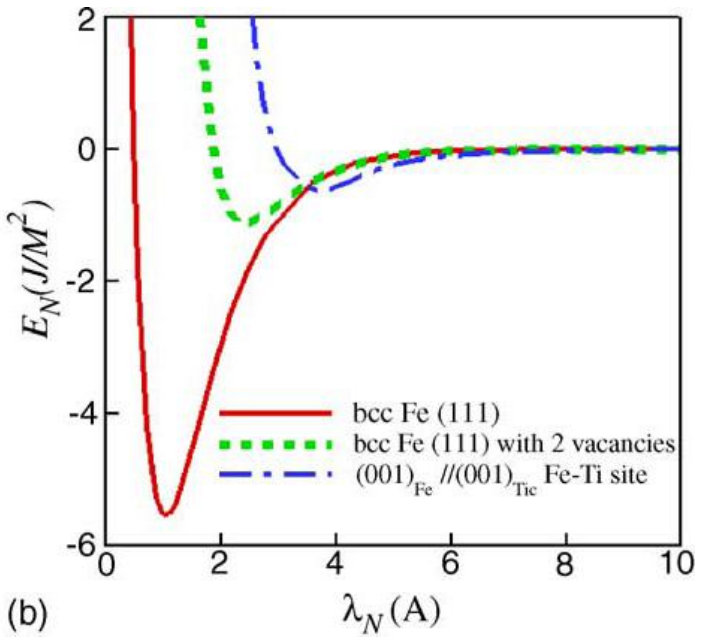
A quantum mechanical analysis has been performed to determine the constitutive relations for iron matrix and the interfacial behavior between the matrix and a TiC-inclusion.

FLAPW (full-potential spin-polarized linear augmented plane wave) was considered to be the most accurate scheme to determine the electron density distribution for metallic and intermetallic system. Hence, this method was used to compute both the generalized fault energy against dislocation sliding in a bcc-Fe crystal and to compute the interfacial debonding of Fe/TiC.

The primitive cell considered represented the interface of a periodically repeated Fe/TiC layered structure. The height of each layer is twice times of the atoms layers.

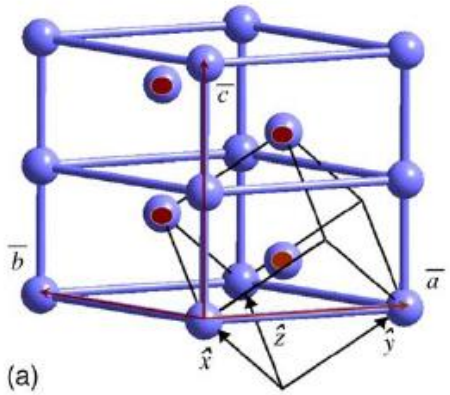
Surface energies and equilibrium separations – results of first principle calculations,

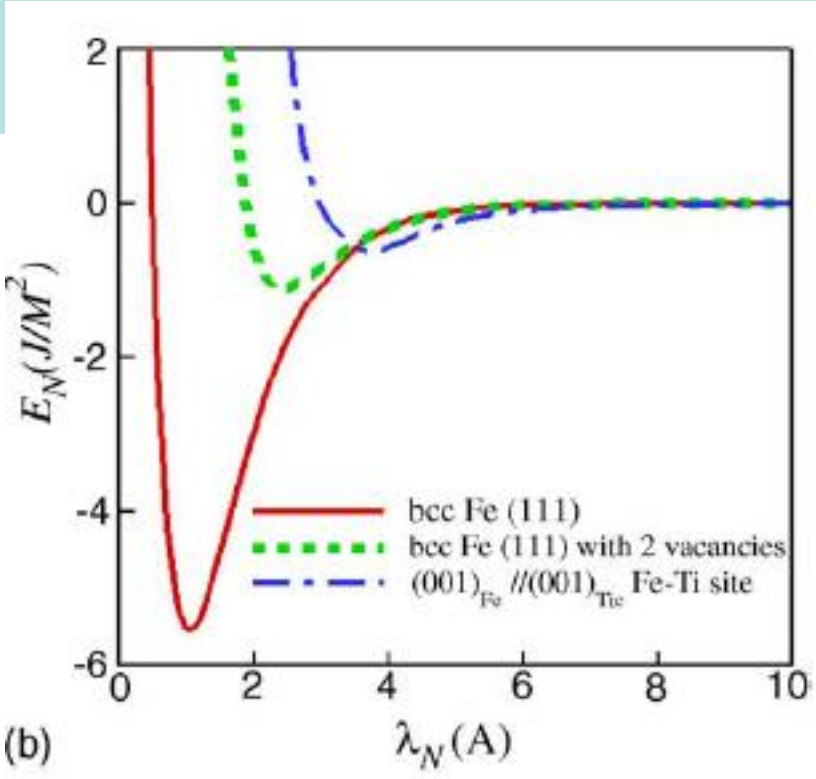
Decohesion surface	Interface	$2\gamma_F$ (J/M^2)	λ_{N0} (nm)
$\{001\}^{Fe}_{bcc}\|\{001\}^{TiC}_{fcc}$	Fe–C site	3.82	0.213
$\{001\}^{Fe}_{bcc}\|\{001\}^{TiC}_{fcc}$	Fe–Ti site	0.61	0.361
{1 1 1}	Perfect	5.43	0.094
{1 1 1}	Perfect	5.38	0.0809
{1 1 1}	Two-empty sites	1.1	0.241
$[\bar{1}\,\bar{1}\,1]$ stacking fault	Fe–Fe	$\gamma_{US} = 0.43$ (J/M^2)	



The present research concentrates on single crystal bcc-Fe, there are however also a few reports on more complex behaviour, including **diffusion of hydrogen**, effect of fracture **initiation from a TiC-particle** and development of **stainless steels**.

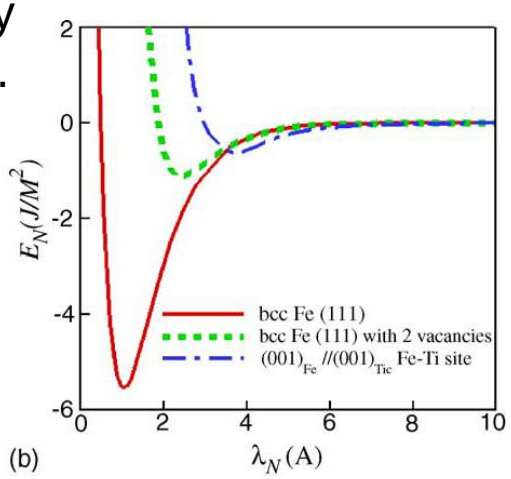
Development of potentials towards microstructures
- vacancies
- interstitials
- substitute alloying elements
- particles (islands of hard ceramics)
- low- and high angle grain boundaries.





S Hao, 2004

From the results it is clear that vacancies have a strong effect on the fracture mechanisms since they reduce the decohesion energy significantly, and thus can transform a ductile fracture to brittle.



(b)

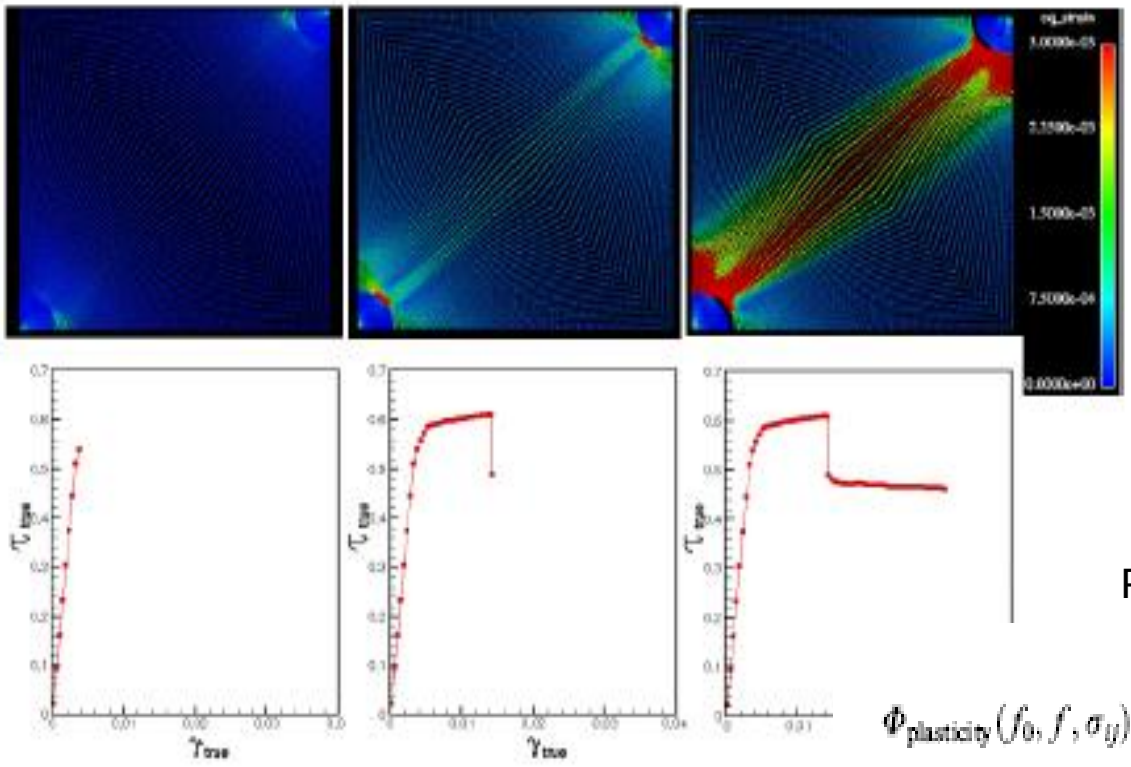
The paper also demonstrated the application of a so-called quasi-particle approach to bridge the above quantum physics calculations to continuum mechanical scale by molecular dynamics.

Each particle can be a “super-atom” containing several atoms, or represents an inclusion particle. As the particle system have fewer degrees of freedom than the atomistic system, the method can be used for bridging atomistic and continuum scales.

Multipotential models
An EAM potential was developed for the system, based on the principles of Daw and Baskes, where the potential reflected the quantum mechanical calculations performed.

Sub-microcell model – numerical simulation

Simulation of localization induced debonding process



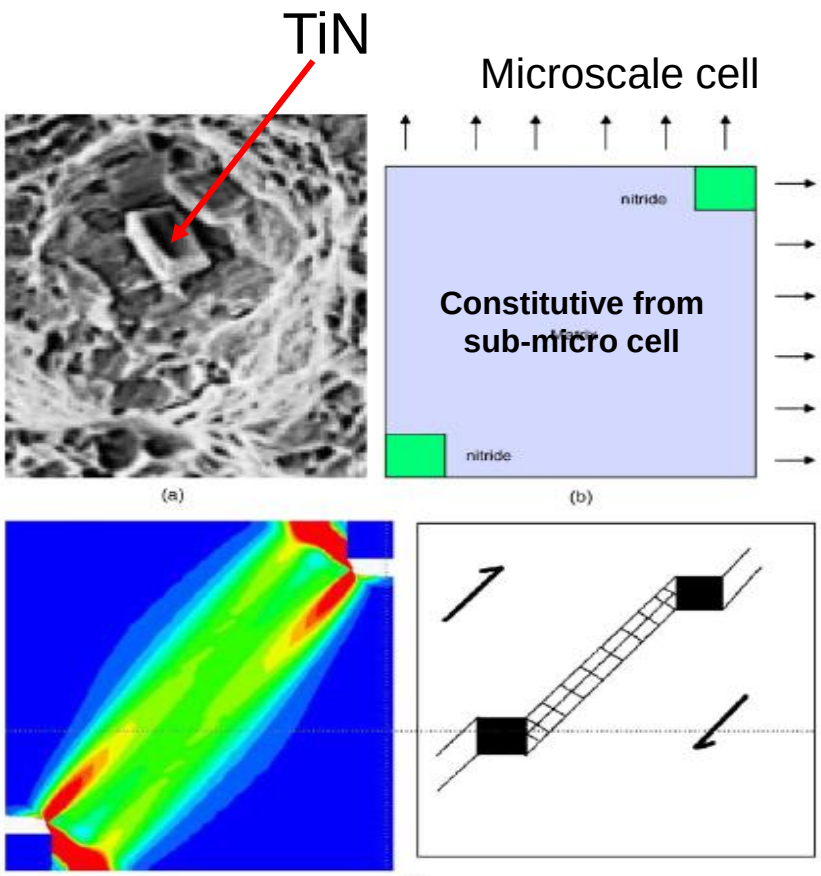
Shear band induces the coalescence

- Volume fraction of particles
- Orientation
- Distribution
- Stress state
- Decohesion energy

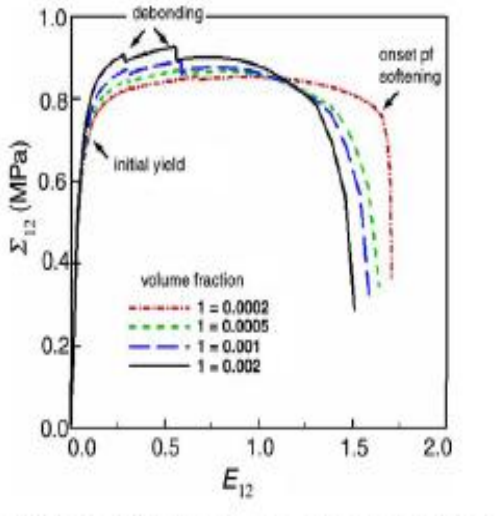
Plastic potential from the sub micro-cell:

$$\Phi_{\text{plasticity}}(f_0, f, \sigma_{ij}) = \left(\frac{\bar{\sigma}}{\sigma_{\text{intr}}}\right)^2 + A_0 \frac{\sigma_{\text{m}}}{\sigma_{\text{intr}}} + A_1 (f + g_1) \exp\left(-\frac{\sigma_{\text{m}}}{\sigma_{\text{intr}}}\right) + A_2 (f + g_2) \exp\left(\frac{\sigma_{\text{m}}}{\sigma_{\text{intr}}}\right) - (q_0 + q_1 (f)^2) = 0,$$

Microscale cell simulations



Macroscale stress-strain response with varying volume fraction of nitrides



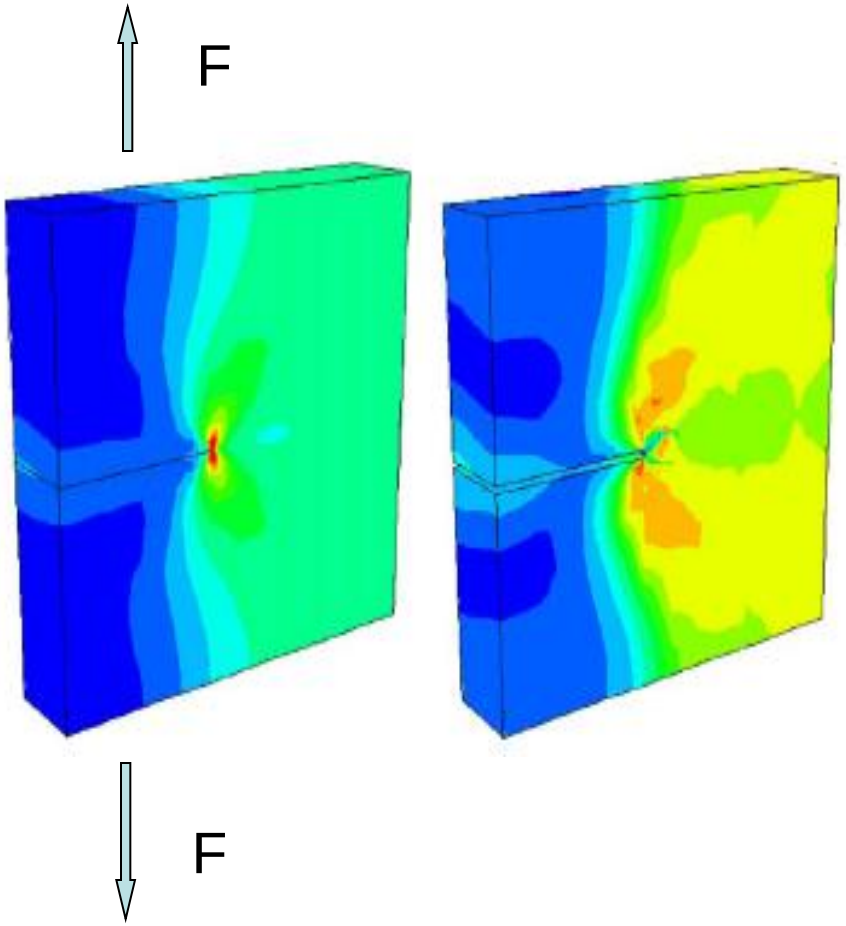
- Volume fraction of particles
- Shape, size and distribution
- Decohesion energy

Localization induced decohesion

Plastic potential:

$$\Phi_{\text{micro}}(f_0^{\text{II}}, f^{\text{II}}, \Sigma_{ij}^{\text{micro}}) = \left(\frac{\bar{\Sigma}^{\text{micro}}}{\sigma_{\text{flow}}}\right)^2 + (f^*(f^{\text{II}}))^g g_0 \exp(\chi_1) - \frac{3\sigma_{Y0}}{\sigma_{\text{flow}}}(1 + (f^*(f^{\text{II}}))^g q) = 0$$

Fracture: crack growth simulation



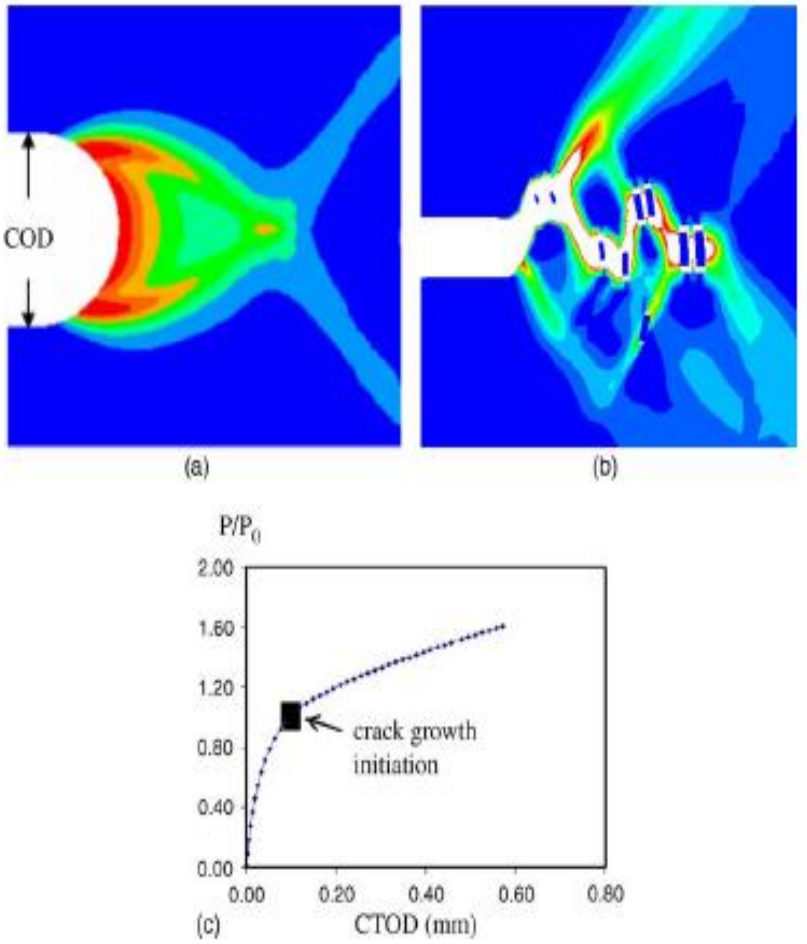
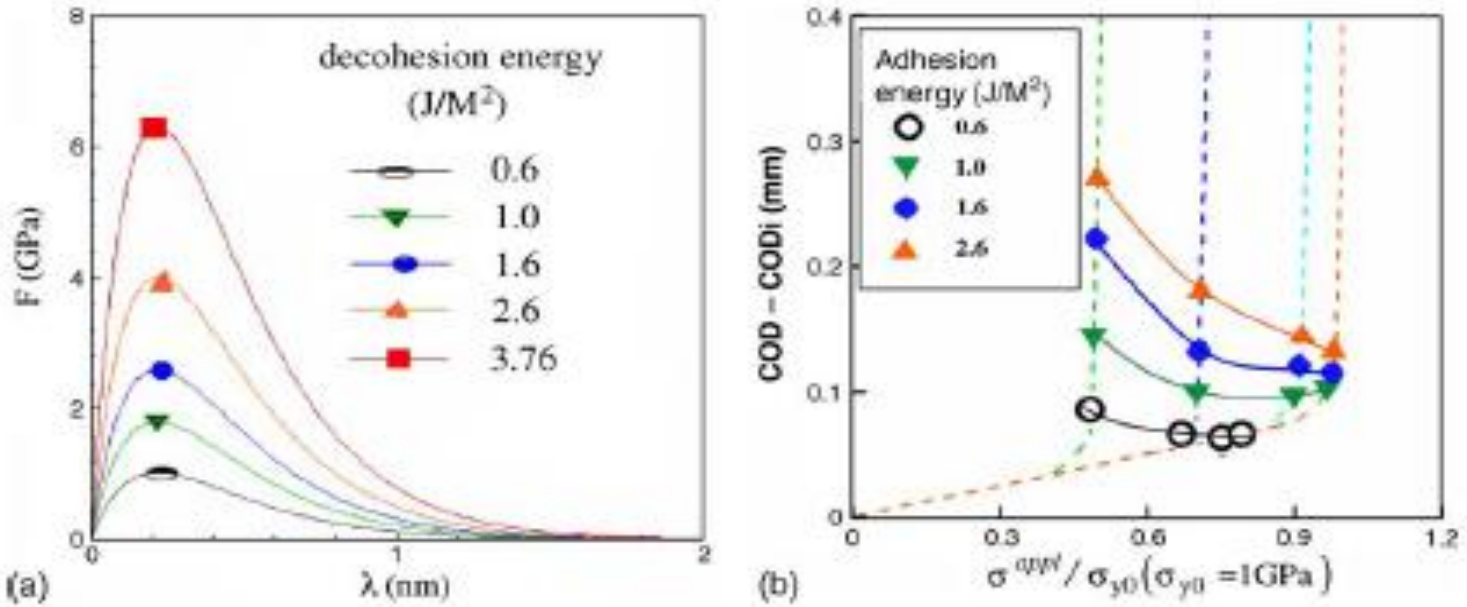


Fig. 21. A simulation of crack growth: contours of equivalent stress and load–CTOD curve

Toughness – strength – adhesion diagram

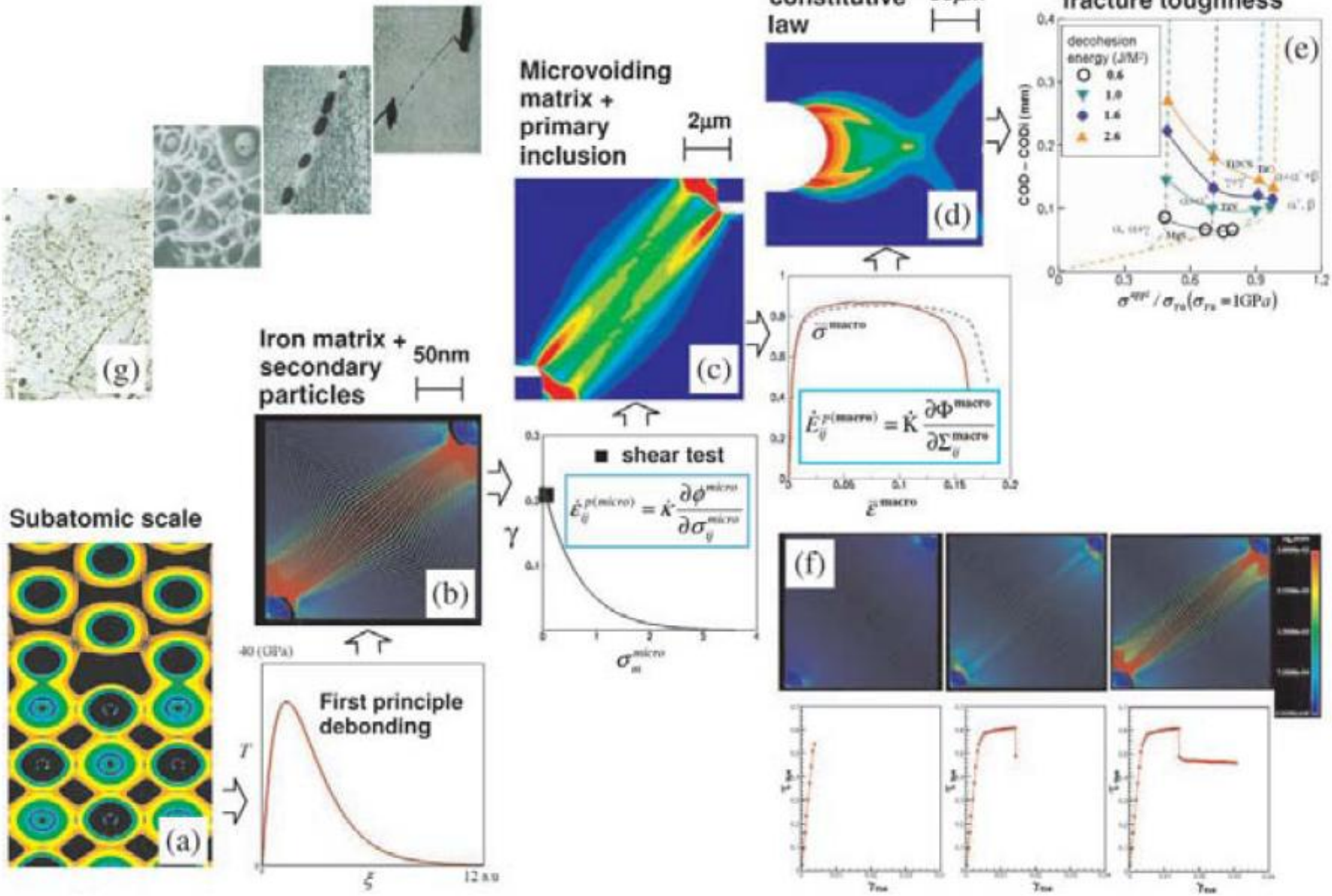
”..a guideline to assist for future engineering design and materials development”



Examine the effect of size and type of inclusions, dechoesion between inclusion and matrix, lattice orientation etc

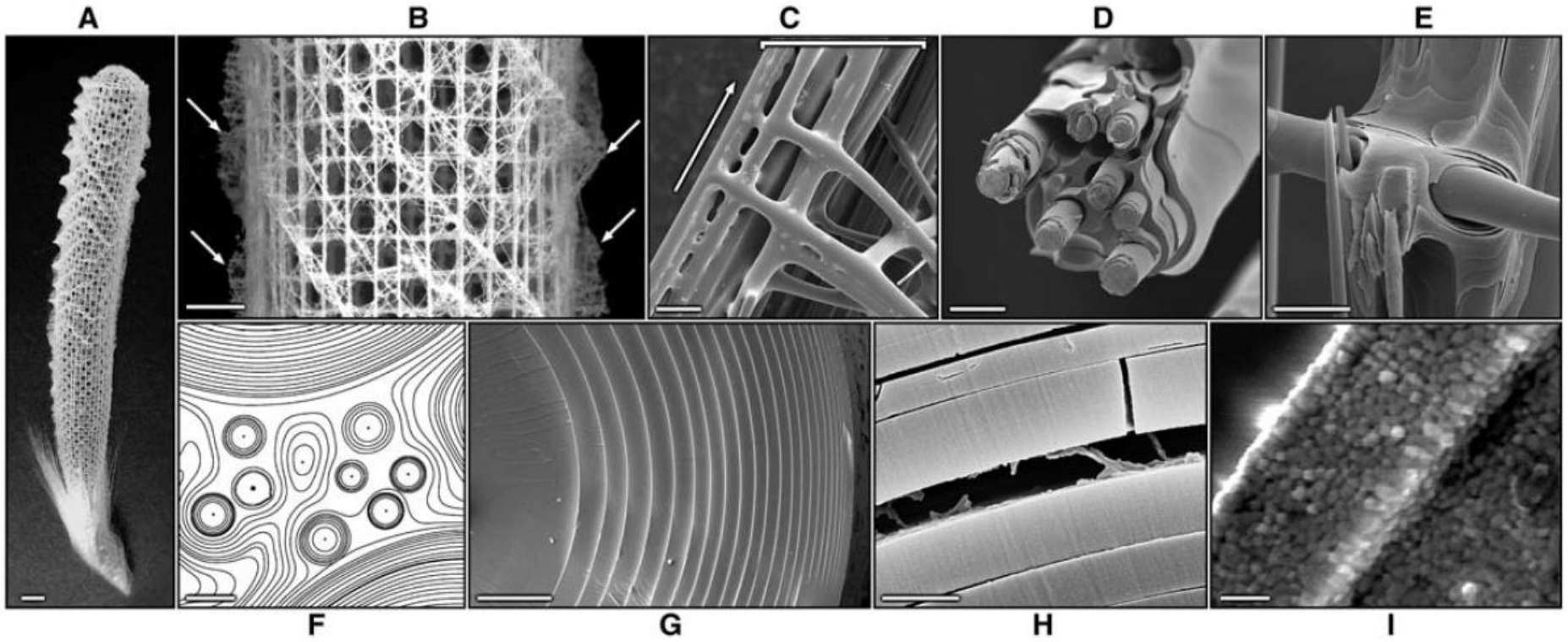
S. Hao, B. Moran, W. K. Liu and G.B. Olson, 2004

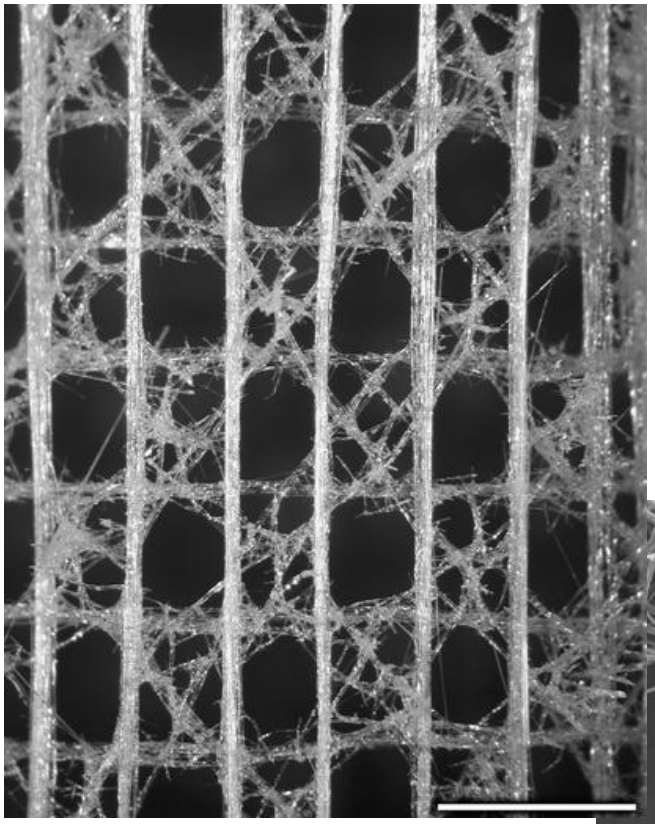
Cybersteel 2020
Multiscale modeling of ductile fracture



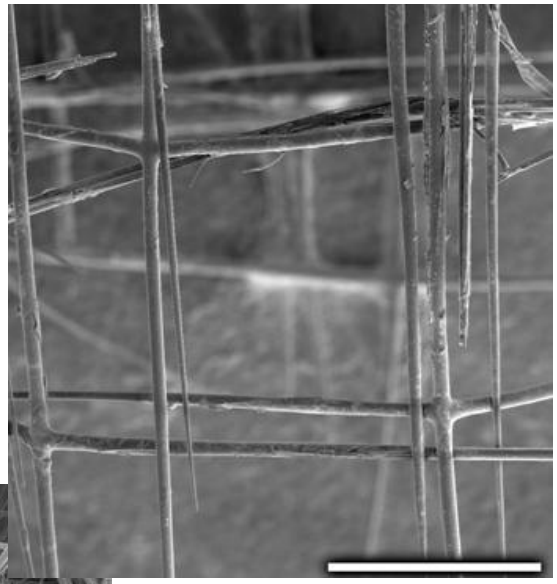
Hao S, B. Moran, W. K. Liu and G.B. Olson 2004

DEEP SEA SPONGES
Seven levels of structural hierarchi

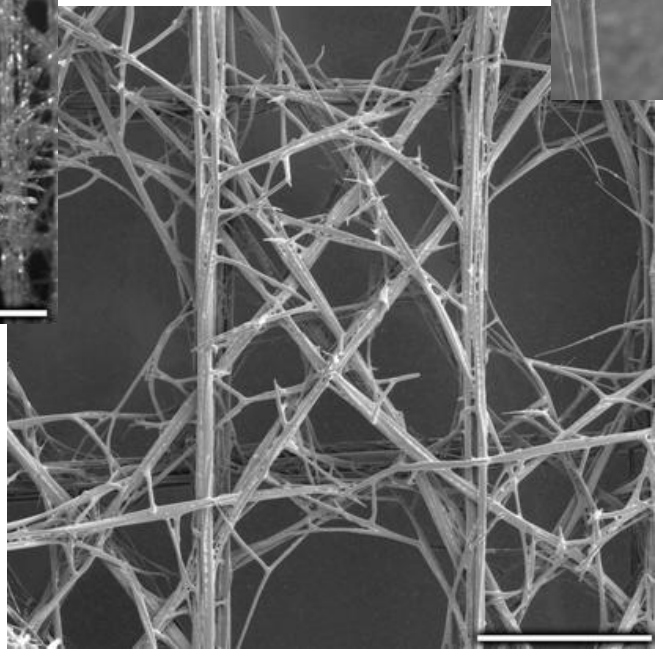




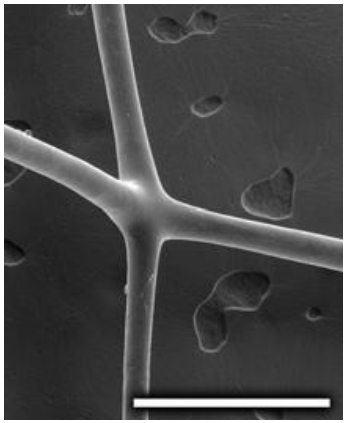
5 mm



1 mm



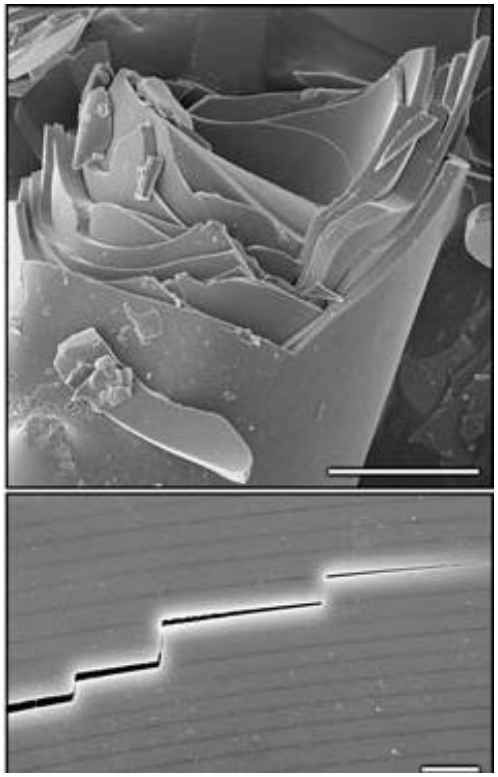
2 mm



0.5 mm

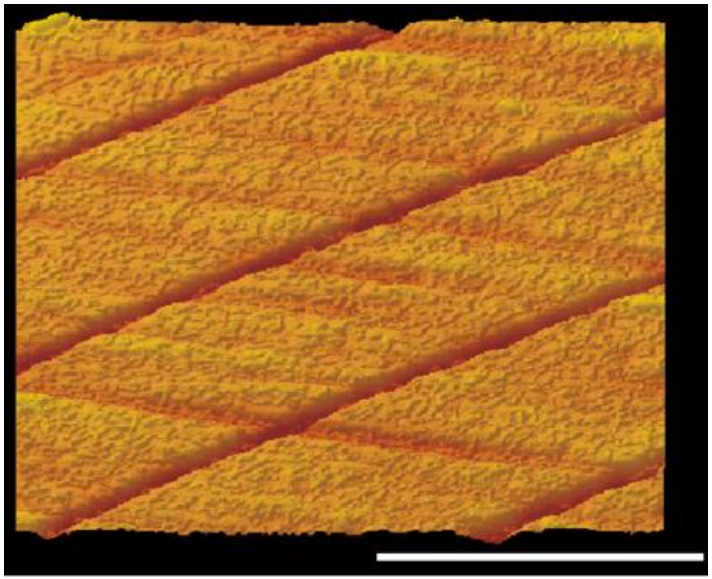
Skeletal lattice

Fracture of the laminated spicule:
Brittle fracture in silica arrests in the protein layers

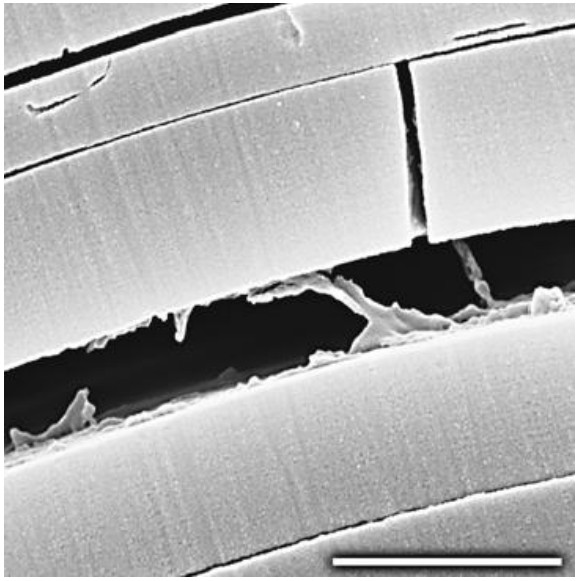


10 μm

Organic layers: 5-10 nm thick

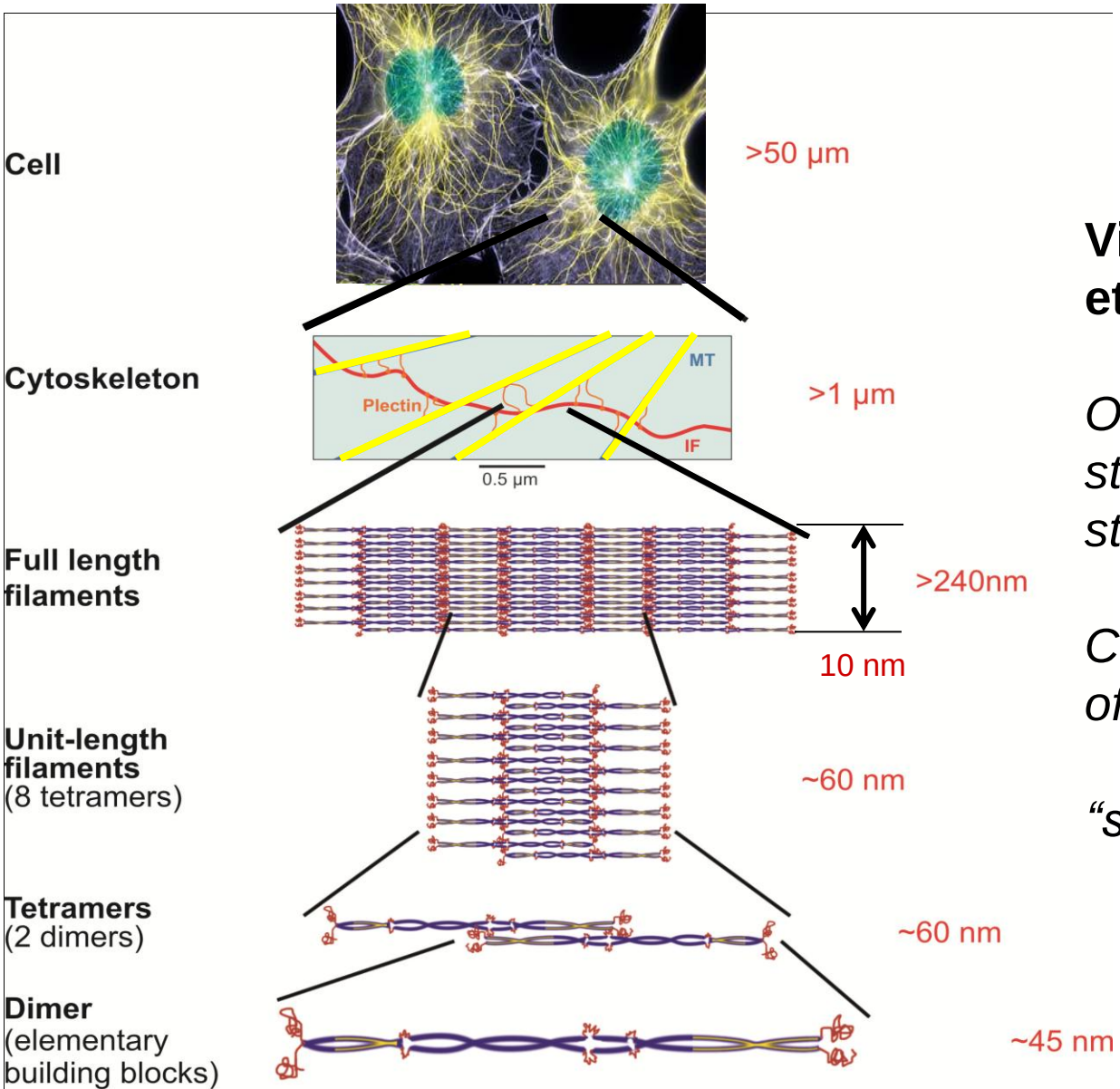


0.5 μm



0.5 μm

Intermediate filament (IF) proteins of cells



Vimentin, lamin, desmin etc.

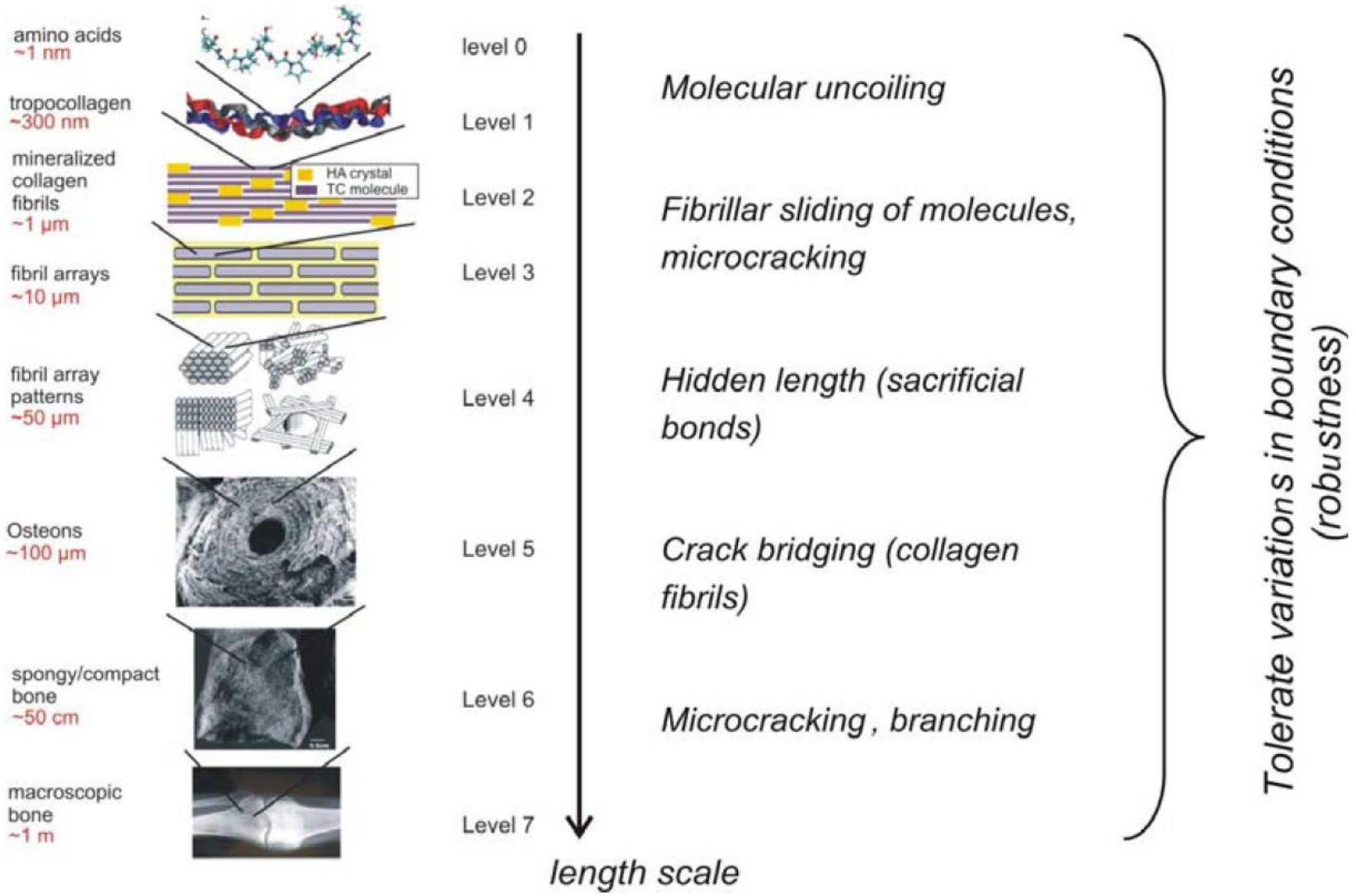
Organize the internal 3D structure of the cell, provide strength

Common structural support of many cells

"safety belt of cells"

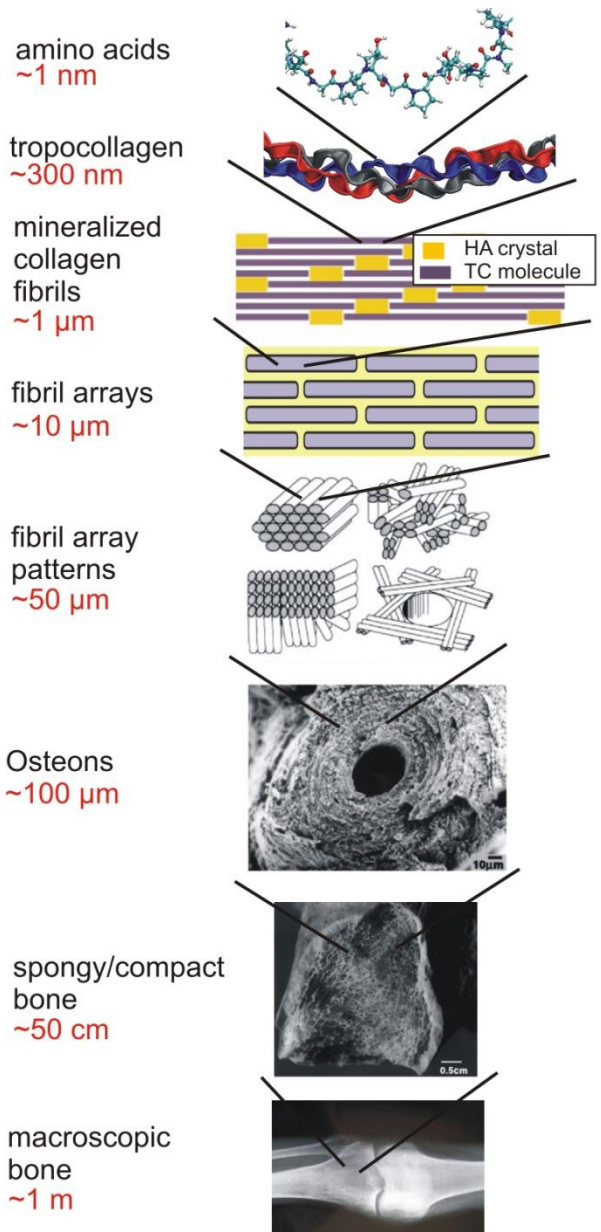
Buehler and Ackbarow, *Materials Today*, 2008

The key for bone's properties? Multi-scale structures and mechanisms, from nano to macro

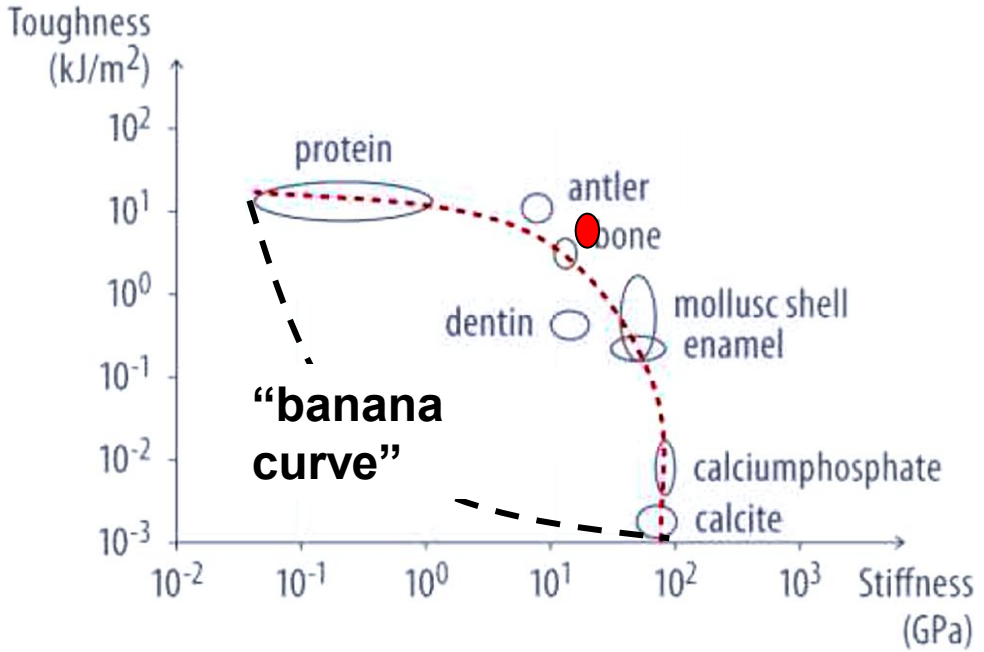


R. Ritchie, M. Buehler, P. Hansma, *Physics Today* (in submission)

Bone – hierarchically structured adaptive material



- *Strong and tough*
- *Stiff*
- *Lightweight*
- *Adaptable (remodeling, healing)*

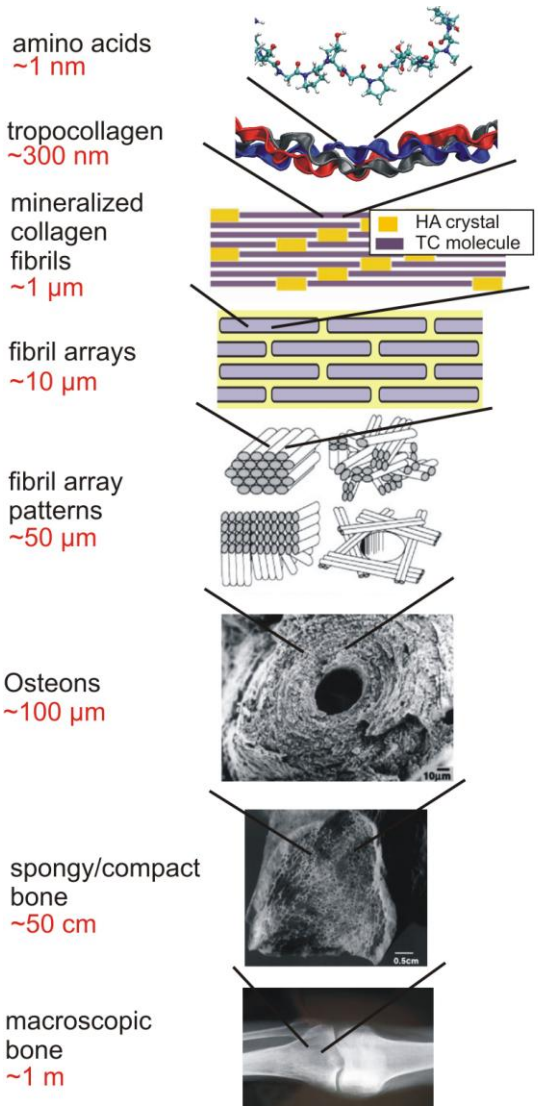


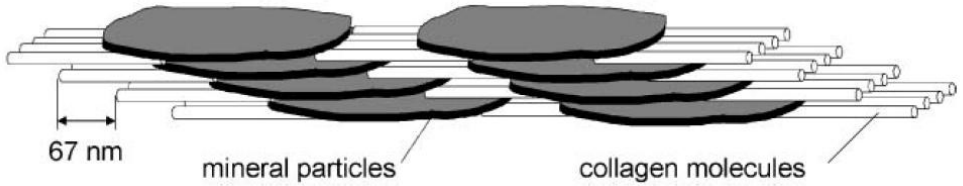
R. Ritchie, M. Buehler, P. Hansma, *Physics Today* (in submission)

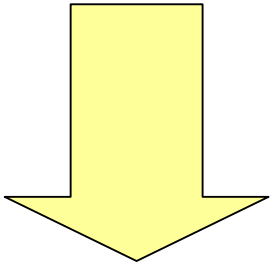
Bottom –up approach

Bone – hierarchically structured adaptive material

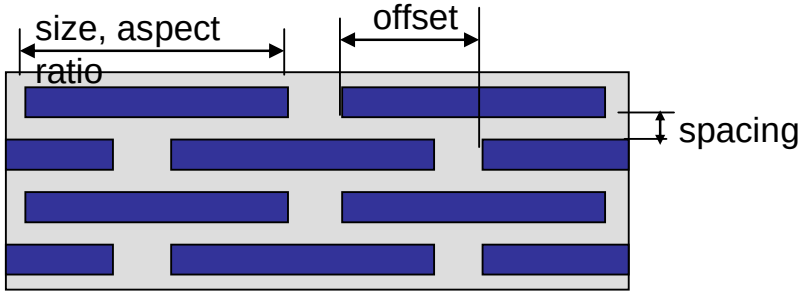
Stiff – Lightweight – Strong – Tough – Adaptable (healing)





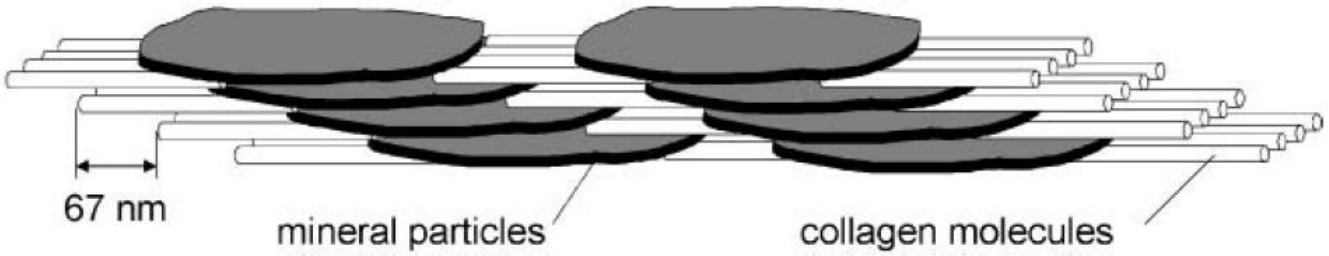


Transfer biological structures to engineering design



Adapted from M J Buehler, MIT

Biomimetic Ni-Al nanostructured composite



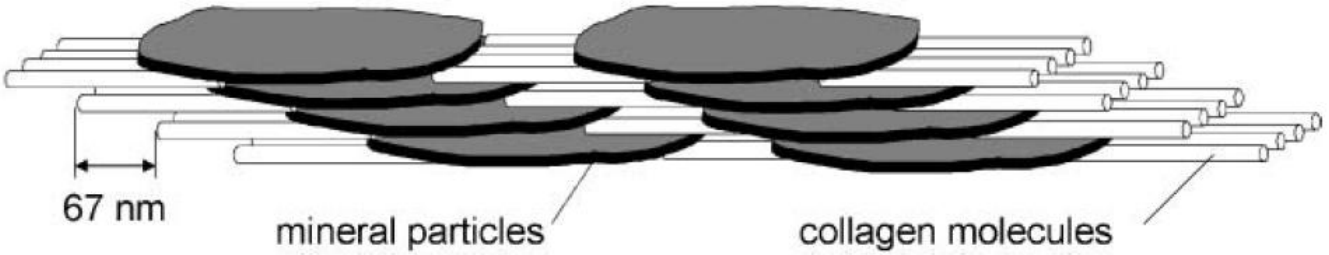
Bone: nanocomposite of rigid “brittle” and plastic “soft” materials
Arranged at nanoscle, in characteristic pattern (staggered molecules with embedded mineral particles)

Concept for technological innovation: mimic structure of bone by combinations of metals, where metallic constituents mimic bone’s material constituents (that is, combination of soft-protein and stiff-mineral particles)

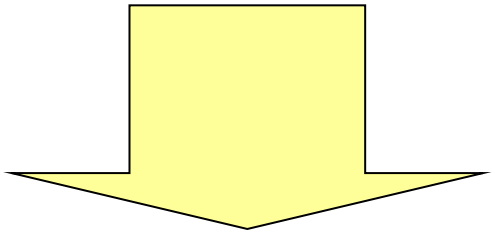
N. Broedling, M.J. Buehler *et al*., *JMPS*, 2008

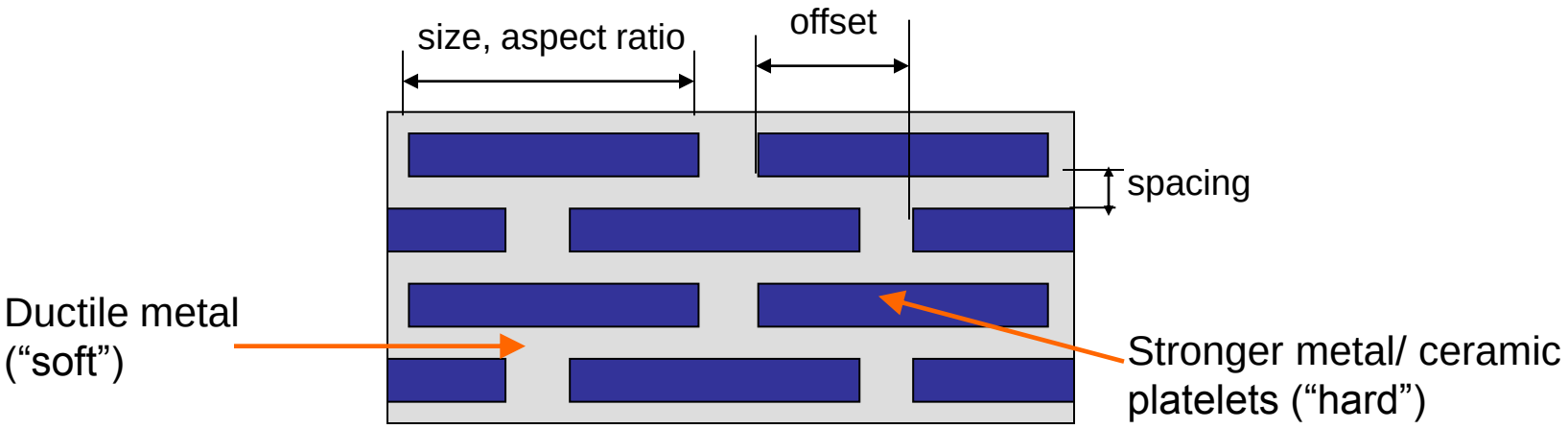
Transfer to metallic nancomposite analysis & design

Bone: Composite of rigid/plastic materials

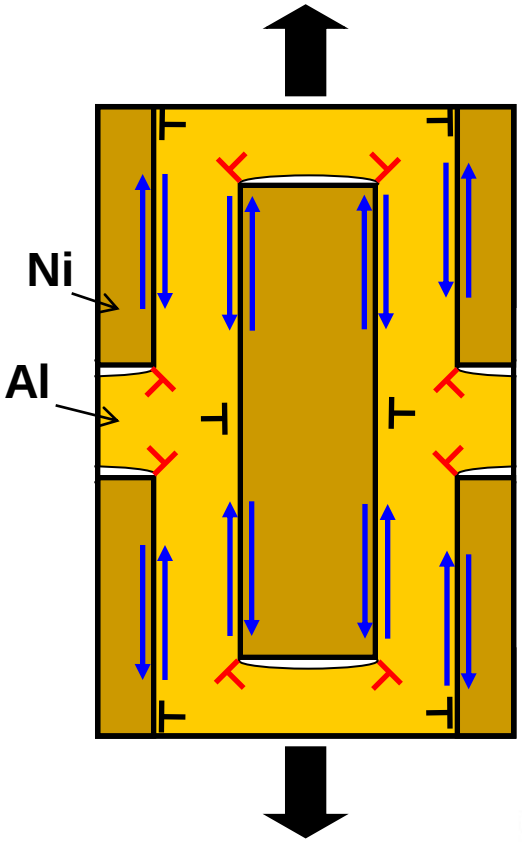


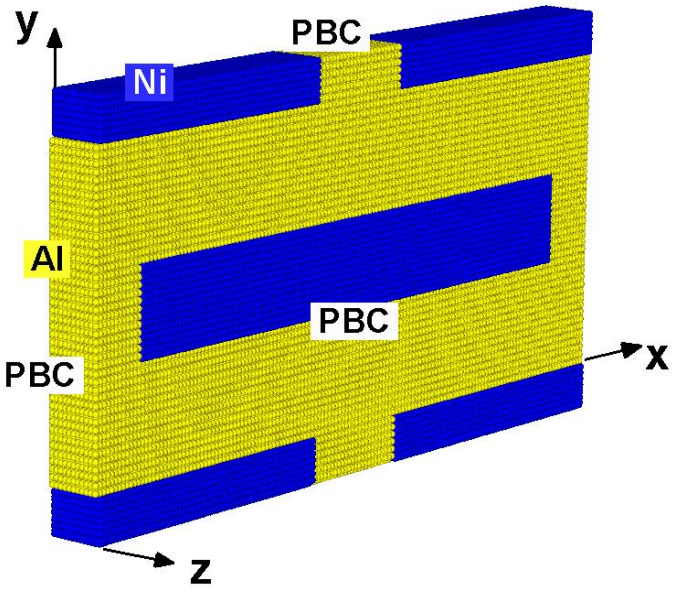
Transfer biological structures to engineering design "metal nanocomposite"



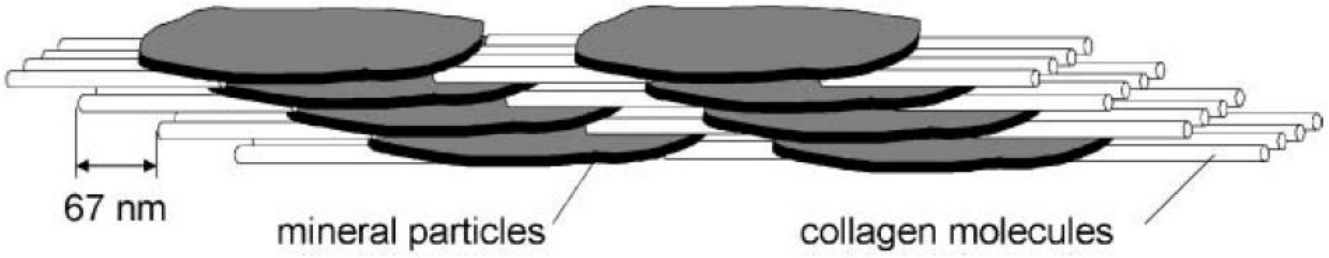


Biomimetic Ni-Al nanostructured composite





Bone: Composite of rigid/plastic materials

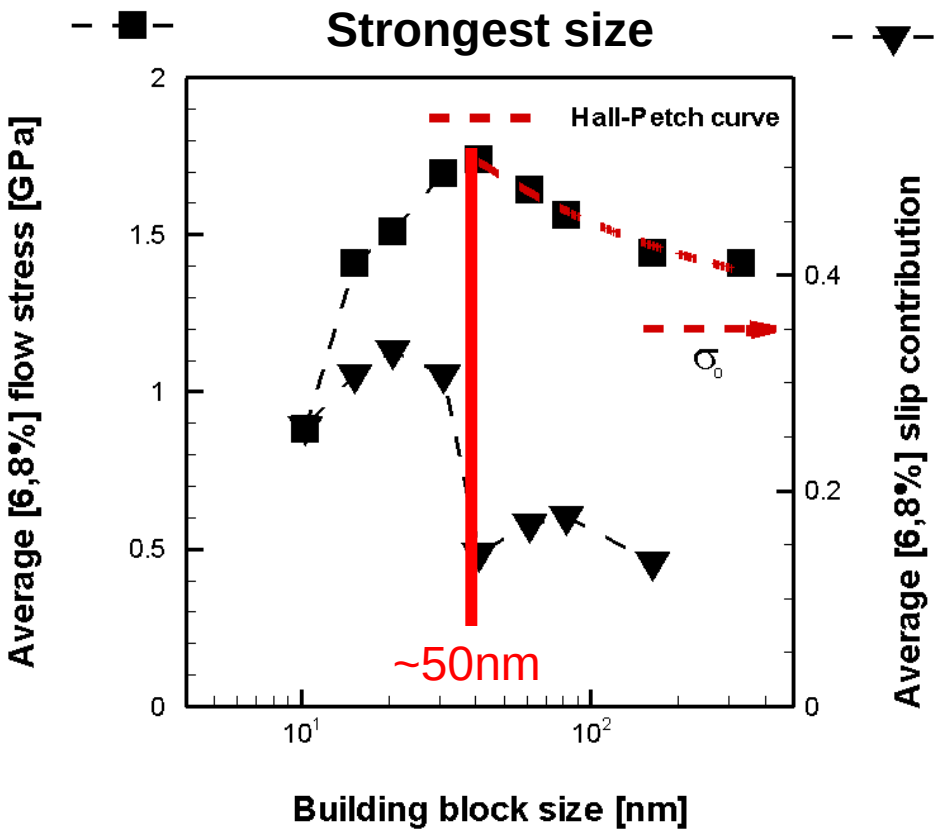


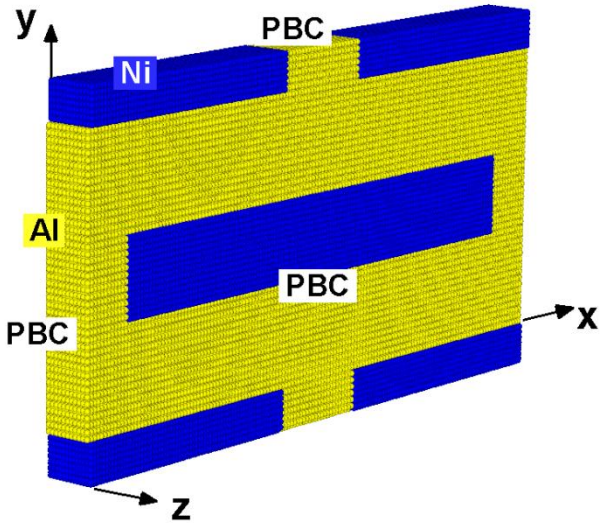
Nickel: Hard platelets

Aluminum: Soft, ductile matrix material

N. Broedling, M.J. Buehler *et al*., *JMPS*, 2008

Bio-inspired nanocomposite: the strongest size



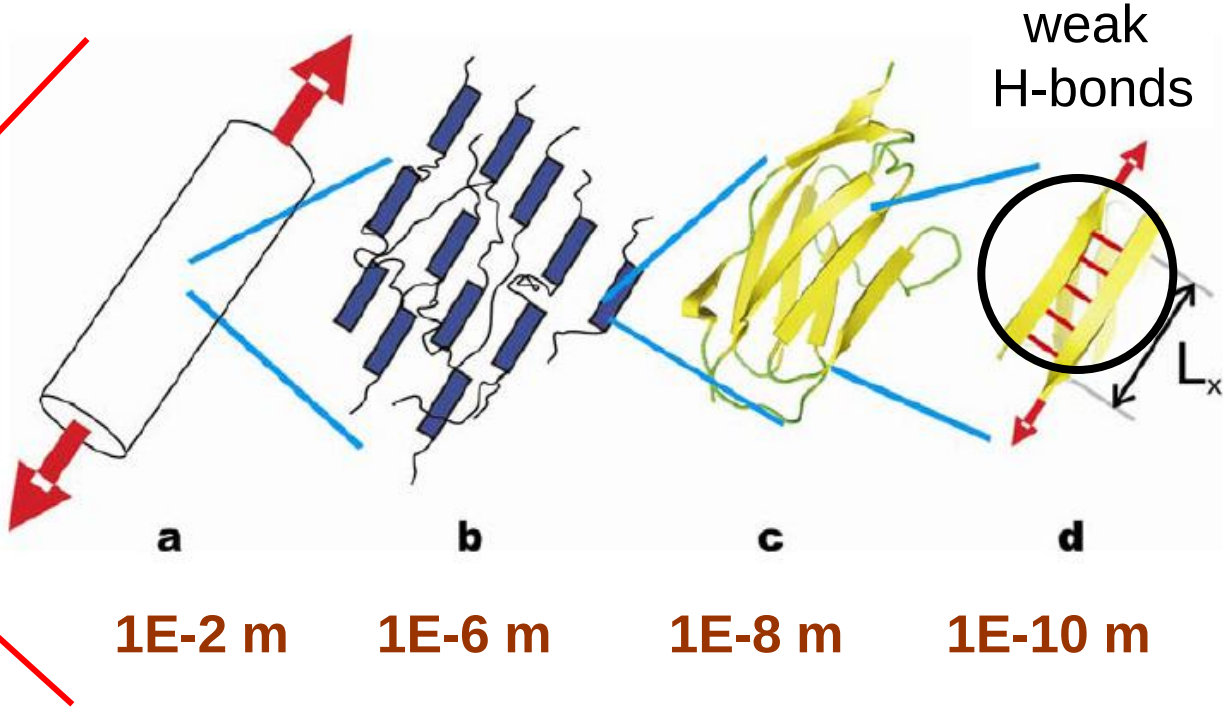


Nanoscale structure can be used to tune "overall" mechanical strength

At optimal size – balance of dislocation strengthening and sliding

N. Broedling, M.J. Buehler *et al*., *JMPS*, 2008

Structure: hierarchical structure of spider silk



Identify the strength of spider silk: Comparable to steel cables (very light weight, elastic, robust), despite extremely "weak"