Mnohoúrovňové (multiscale) počítačové modelování v oblasti chemie a fyziky pevných látek a v materiálových vědách

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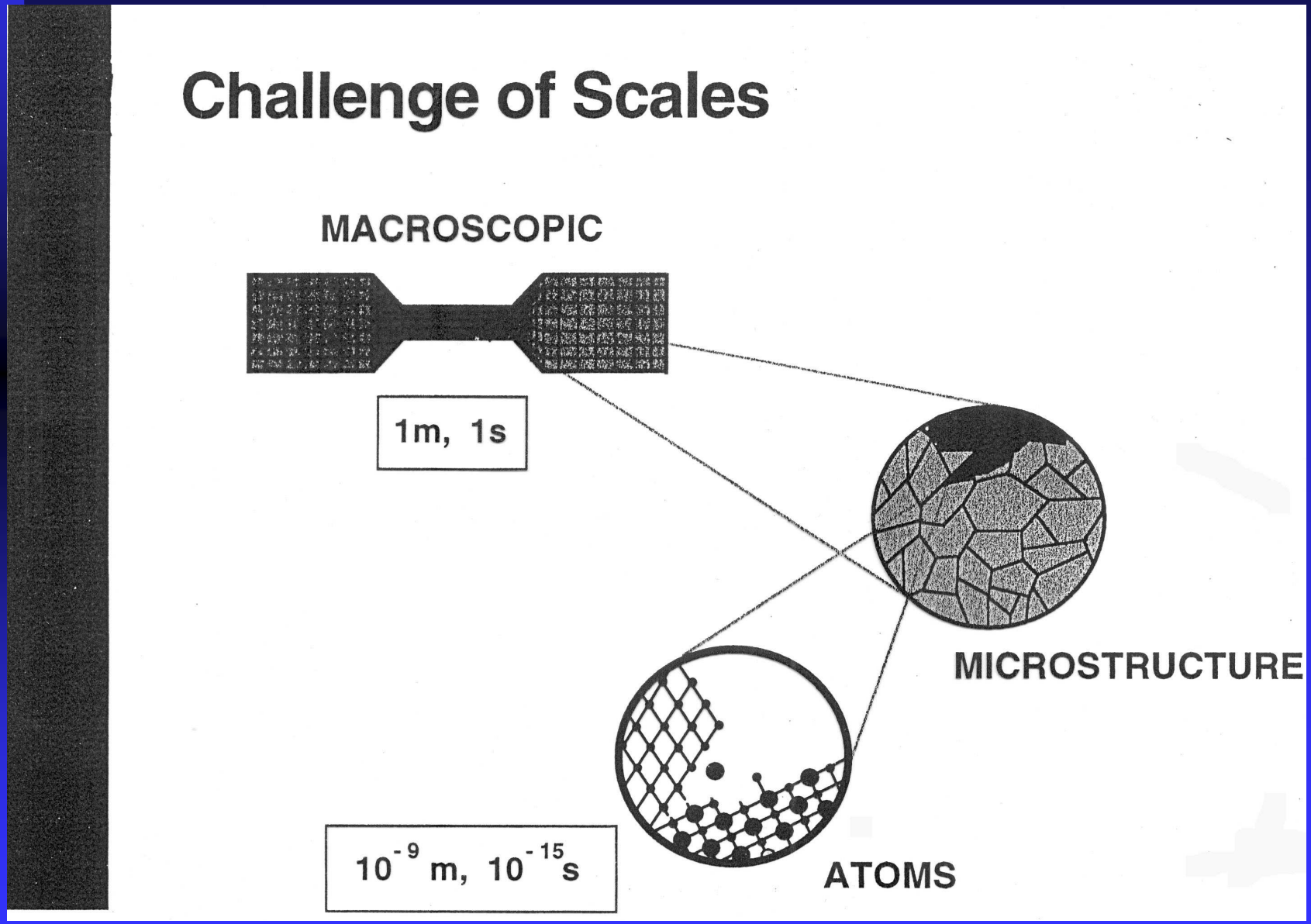
Stručný přehled presentace

1. Čím se zabýváme, kde leží zajímavé problémy
   - důležité jevy na různých úrovních
   - problém: přenos informace mezi úrovněmi
2. Úloha elektronové struktury
3. Ilustrativní příklady
4. Finanční zajištění výzkumu, podpora doktorandů

A typical fracture problem



Molasses, Liberty Ships, Titanic...

New York Times, Sept. 16, 1993

New Idea on Titanic Sinking Faults Steel as Main Culprit

Researchers studying the Titanic now suggest that its catastrophic rupture occurred not just because of hitting an iceberg but because the hull's metal plates were made of low-grade steel that was made brittle by the cold waters of the North Atlantic. Shattering plates caused the ship to plummet, they say.

By WILLIAM J. BROAD

A new analysis by maritime experts has concluded that the disastrous loss of the Titanic was caused not so much by an iceberg as by structural weaknesses in the ship's steel plates that caused them to fail catastrophically.

A better grade of steel, the analysis concludes, would have reduced the extensive fracturing and allowed the ship to remain afloat or to flood more slowly, perhaps saving many lives if rescue ships had arrived before the sinking. About 1,500 people died when the Titanic went down in the North Atlantic in 1912 on her maiden voyage.

The new analysis is based on physical and photographic clues gathered by five expeditions to the shattered hulk of the luxury liner, which lies in waters more than two miles deep. It also draws on a study of the fates of the Titanic's sister ships, the Olympic and the Britannic.

Weak Plates Cited

The culprit was found to be a process known as brittle fracture, in which low-grade steel breaks violently when chilled rather than bending.

from other companies and institutions are presenting their analysis today at the centennial meeting of the Society of Naval Architects and Marine Engineers in New York City.

"The real tragedy of the Titanic," the team concludes in its paper, is that better construction techniques and "a better quality of steel plate might have averted her loss or resulted in an even slower rate of flooding that may have saved more passengers and crew."

In a twist, the analysis holds that the rumbles and roars heard by survivors on the night of the sinking were caused not so much by shifting gear

crack that starts in one part of a welded steel hull can pass completely around it, causing a large ship to break in two.

Speculation still abounds as to why the Titanic met disaster. In recent years, five expeditions equipped with minisubmarines and advanced undersea robots have succeeded in viewing Titanic debris on the sea floor. The site was discovered in 1985 by Dr. Robert D. Ballard of the Woods Hole Oceanographic Institution, who revisited the ship in 1986. While Dr. Ballard took only photographs, expeditions in 1987, 1991 and 1993 took samples and artifacts. The ship lies in two large chunks some 2,000 feet apart.

No Evidence Yet of Gash

Contrary to the long-held belief that a gash was ripped in the Titanic when she struck the iceberg, Dr. Ballard and his colleagues found no gash in their limited time of searching, deepening the mystery of what sank the ship. He speculated that the collision loosened or buckled seams in the hull, thereby flooding the liner. Many other theories have been put forward in a flood of books and articles.

The ship clearly fractured where it split in two, but the new analysis believes there were many other fractures, having been probably started by hitting the iceberg, that played a more important role in the sinking.

In addition to Mr. Garzke, the new analysis is by Dana R. Yoerger of the Woods Hole Oceanographic Institution on Cape Cod; Stewart Harris of Marquest Inc., a marine manufacturer in Bourne, Mass., Robert O. Dulin of the Basic Technology Corporation, naval consultants in Newington, Va., and David K. Brown, a former naval architect with the British Navy.

Cracking Like Glass

When cooled and stressed, some types of relatively primitive steel fracture much like glass rather than bending or stretching as ductile materials do. Moreover, this type of breakage takes place with a very small expenditure of energy, which can be administered by an external blow or internal stress. The phenomenon is well known in shipbuilding and is avoided as a grave danger.

Most aspects of materials science involve multiple length and/or time scales:

- Elastic properties
  - of polycrystals and other composites
- Plasticity in crystalline materials
  - dislocation plasticity
  - creep
- Phase transformations
  - reconstructive (diffusional)
  - recovery and recrystallisation
  - displacive (martensitic)
- Processing of materials
  - precipitation, hardening etc.
  - grain size through thermo-mechanical processing
  - deformation and recrystallisation textures
  - rolling, extruding, forging, pressing

- Failure of materials
  - brittle fracture
  - ductile fracture
  - fatigue

- Electrostatic properties
  - piezoelectricity, ferroelectricity

- Magnetic properties
  - ferromagnetism

- Synthesis of materials
  - from the vapour
  - from the liquid
  - sintering

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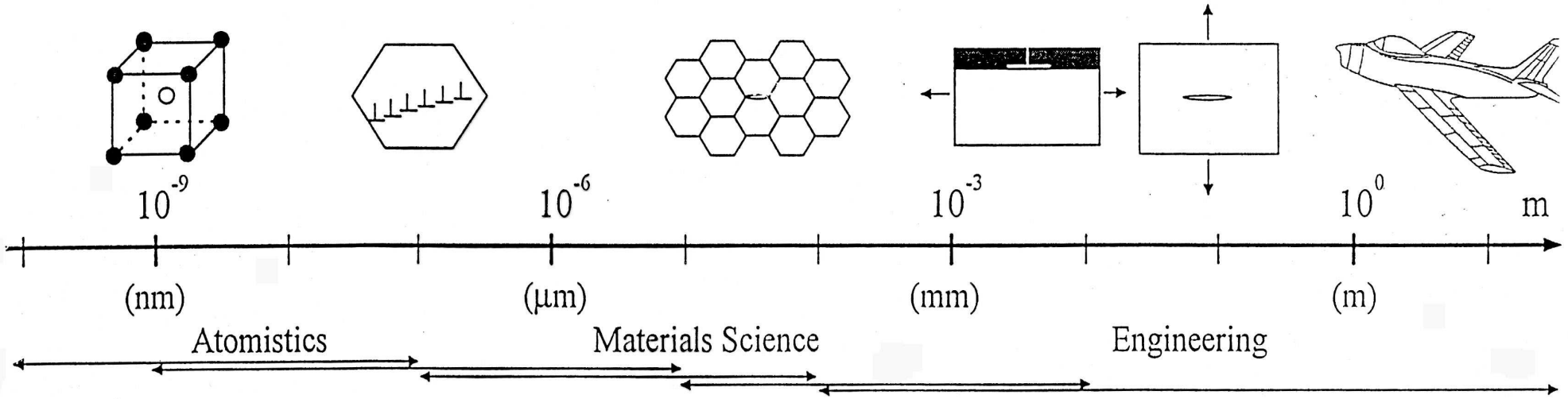
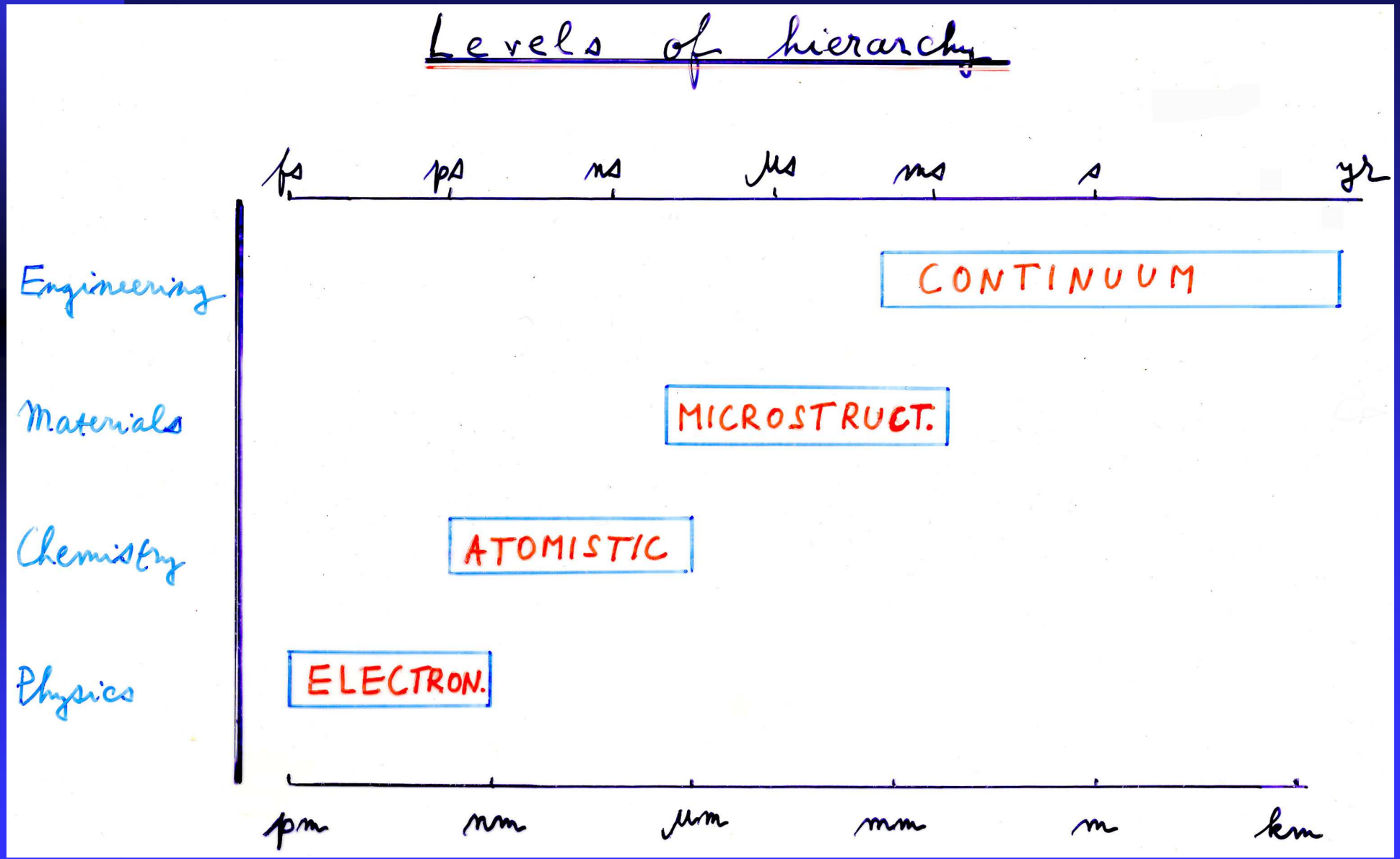
Dimensions of Mechanical Modelling



Nano	Meso I	Micro	Meso II	Macro
Nano simulation	Dislocation model	Microstructure model	Mesoscopic fracture aspects	Meso-macro-coupling
Atomic bonds	Dislocations	Microstructure	Coating	Specimen, Component
Molecular Dynamics	Dislocation theory	Micromechanics	Mesomechanics	Structural mechanics
		L o c a l a p p r o a c h		
Fracture of atomic bonds	Dislocation movement	Microcrack	Delamination	Macrocrack
		Void formation at inclusions		Plastic deformation
FEAT	Dislocation/particle-interaction	Real microstructural model	Layered model	Structural model
(Finite Element/ Atomistic-coupling)	Orowan-Model	Self-consistent embedded cells		

Multiscale modelling



What does *multi-scale modelling* mean?

1) modelling a problem at different length/time scales *separately* and passing information between *distinct* simulations at the separate scales.

2) modelling a problem at two or more length/time scales *simultaneously* so that the scales are linked within the *same* simulation. embedding.

- (1) is often difficult information transfer
- (2) is likely to be much harder compatibility

- (1) could be called "series multi-scale modelling"
- (2) could be called "parallel multi-scale modelling"

Electronic level

Most of the properties of solids:

- can be traced to the behavior of **electrons**,
  - the "**glue**" that holds atoms together to form a solid

A lot of properties of solids

- can be predicted accurately from

  ab initio (first - principles) ES calculations

  i.e. from fundamental quantum theory

  (Schrödinger equation)

Most ES calculations:

- routinely performed within the framework of density functional theory (Hohenberg- Kohn-Sham 1964)
- complicated many-body motion of all electrons replaced by an equivalent but simpler problem
    - * of a single electron
    - * moving in an effective potential

Walter Kohn and John Pople-Nobel Prize in Chemistry 1998

Zaměření naší skupiny:

- magnetické a mechanické vlastnosti materiálů z prvních principů (teoretická pevnost, magnetismus tenkých vrstev, magnetické vlastnosti rozlehlých defektů - hranice zrn, antifázové hranice, chemie segregace)
- fázové diagramy slitin se složitými fázemi, vytváření databází
- vytváření databáze pro konstrukci semiempirických meziatomových potenciálů
  - segregation of Bi at GB in Cu (combined approach)
  - GBs in nanocrystalline Ni (combined approach)
- počítačové experimenty („měření“ v počítači)

SEMI-EMPIRICAL SCHEMES FOR DESCRIPTION OF INTERACTIONS BETWEEN ATOMS

Working rule:

Such schemes should capture the physics necessary for the studied phenomena and materials considered

BUT SHOULD NOT TRY TO BE ALL-EMBRACING

Results of ab initio electronic structure calculations may be utilized as an 'empirical' data base

- pair potentials
- many-body central-force potentials –
  - -- embedded-atom method
  - -- Finnis-Sinclair potentials
- potentials with non-central interactions (Tersoff, Brenner)
- parametrized tight-binding and bond-order potentials

ESSENTIAL INGREDIENTS

- adjustable parameters fitted to the material properties
- ab initio results constitute an important part of the data base
- resulting potentials are tested by ab initio calculations

Copper-bismuth alloy

(D.E. Luzzi, M. Yan, M.Š., V.V.)

Very suitable model material for investigation of segregation and embrittlement phenomena

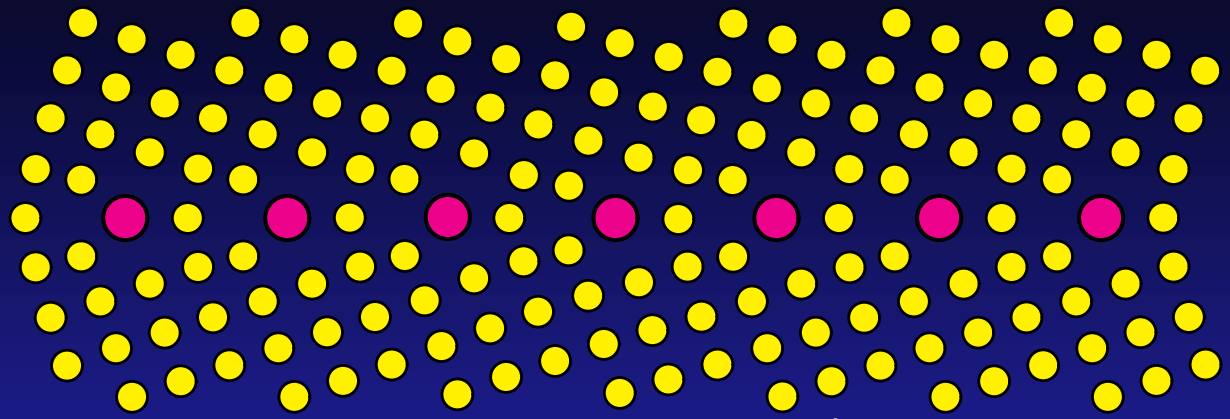
FS-POTENTIALS FOR Cu-Bi CONSTRUCTED BY FITTING

- Equilibrium lattice parameter
- Bulk modulus
- Tetragonal and trigonal shear moduli

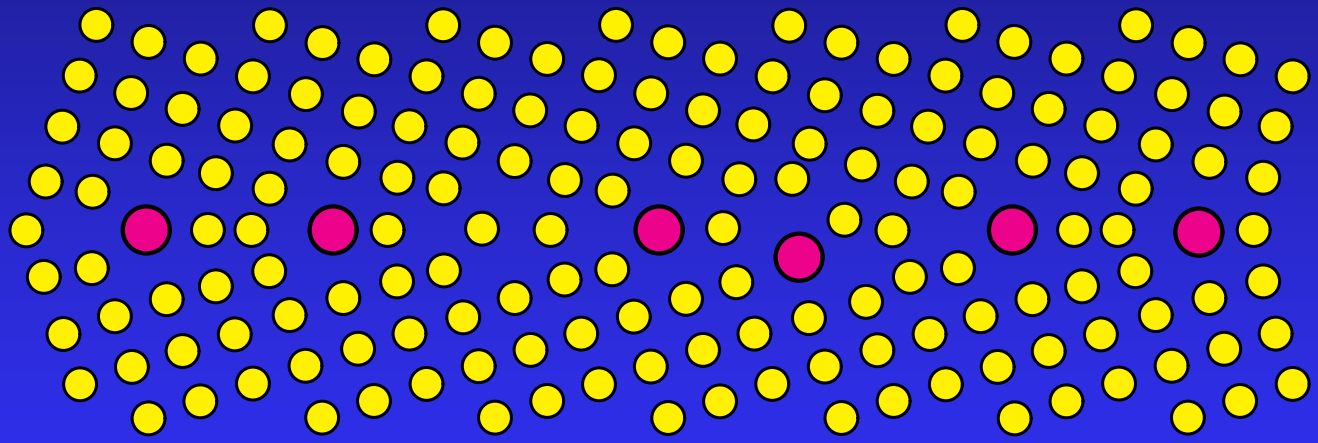
OF A HYPOTHETICAL COMPOUND Cu_3Bi WITH THE $L1_2$ STRUCTURE CALCULATED AB-INITIO USING FP-LMTO CODE

Size of the Bi atom embedded in Cu has been correctly estimated by this approach

Σ=5(310) symmetrical tilt boundary



Molecular statics

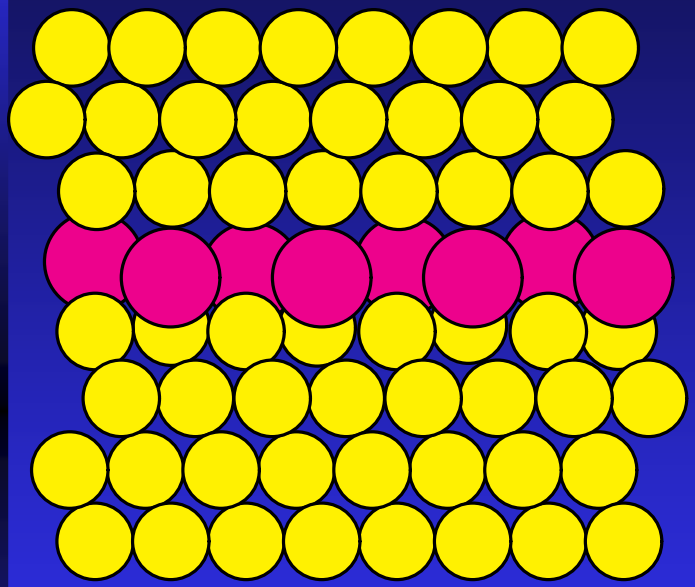


Monte-Carlo 300K

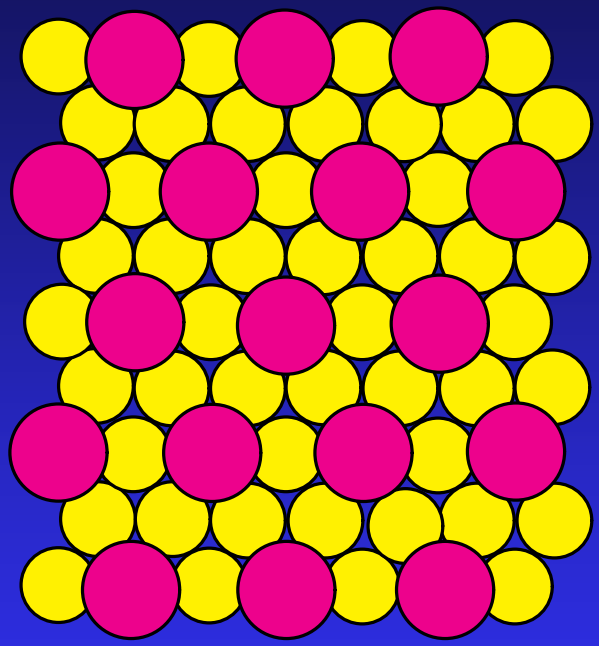
EXCELLENT AGREEMENT WITH HIGH-RESOLUTION Z-CONTRAST IMAGING

(Alber, Mullejans, Rühle, 1999, Acta Materialia 47, 4047)

Σ=3 (111) symmetrical tilt boundary



[11$\bar{0}$] projection

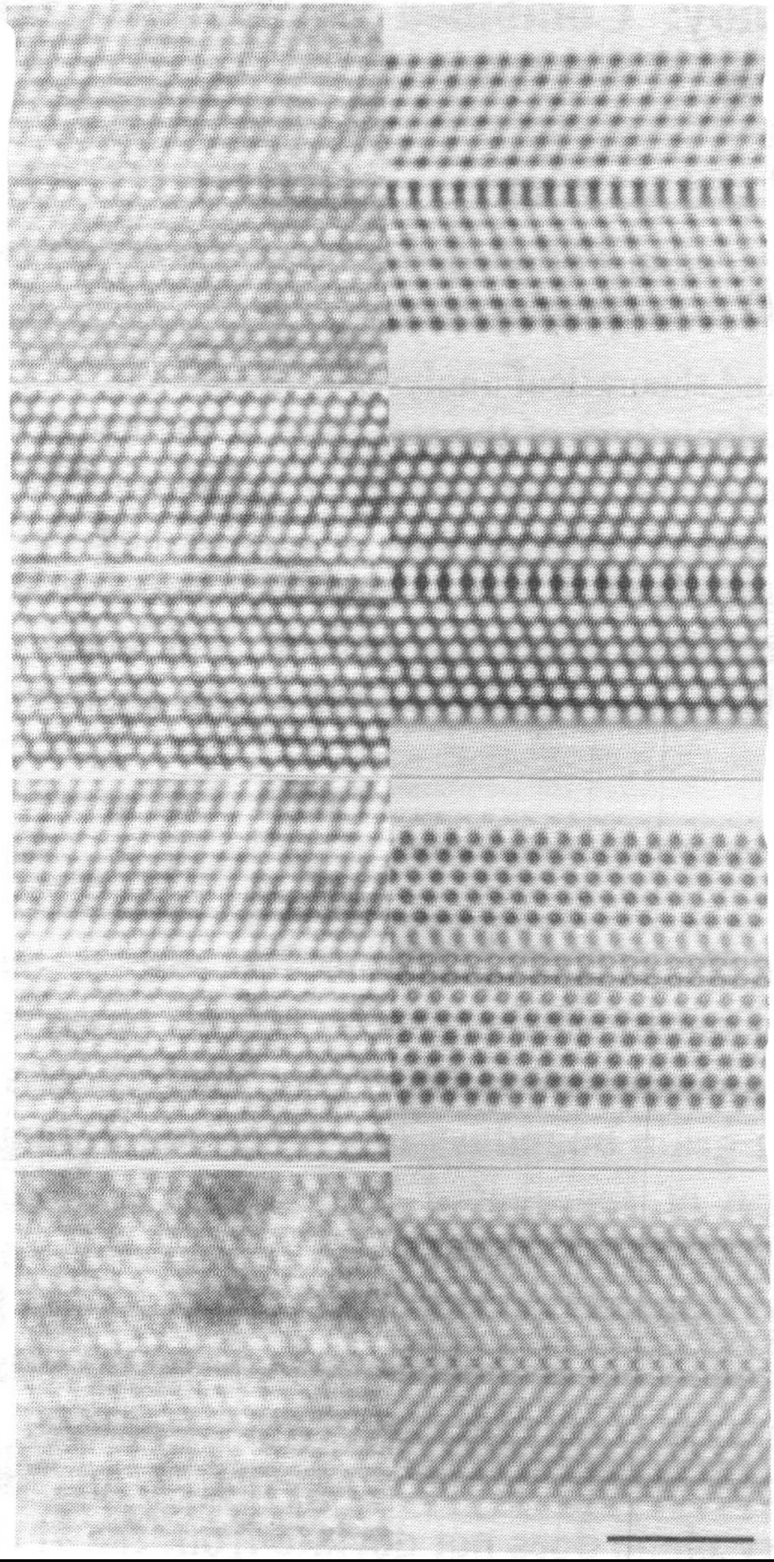


[111] projection

STRUCTURE FOUND BY MOLECULAR STATICS

HIGH-RESOLUTION TEM IMAGE OF THE Σ = 3 (111) BOUNDARY WITH BISMUTH

Comparison of the observation with image simulated using the structure obtained in the atomistic modeling



Grain boundaries in nanocrystalline Ni

Motivation: to understand the signal from the positron annihilation spectroscopy in nanocrystalline metals

- positrons probe open-volume defects such as vacancies, their clusters, grain boundaries etc.
- the electronic density in these regions is “less-than-average”
- they are attractive for a positron, their lifetime is longer there

Basics of positron annihilation

- positron is an antiparticle of an electron
- theoretically predicted 1928 (Dirac), experimentally discovered 1932 (Anderson)
- positrons have the same mass and lifespan as electrons, but opposite electric charge
- if a positron meets an electron: annihilation process takes place:
- $e^+ + e^- \Rightarrow 2\gamma$
- $E(2\gamma) = 2\, m_0c^2 + E(e^+) + E(e^-)$
- $m_0c^2 = 0.511$ MeV
- m_0c – rest mass of the electron (and of the positron)
- in our world, high density of electrons attracted to a positron=> the typical positron lifetime is 100-1000 ps

A positron in our world

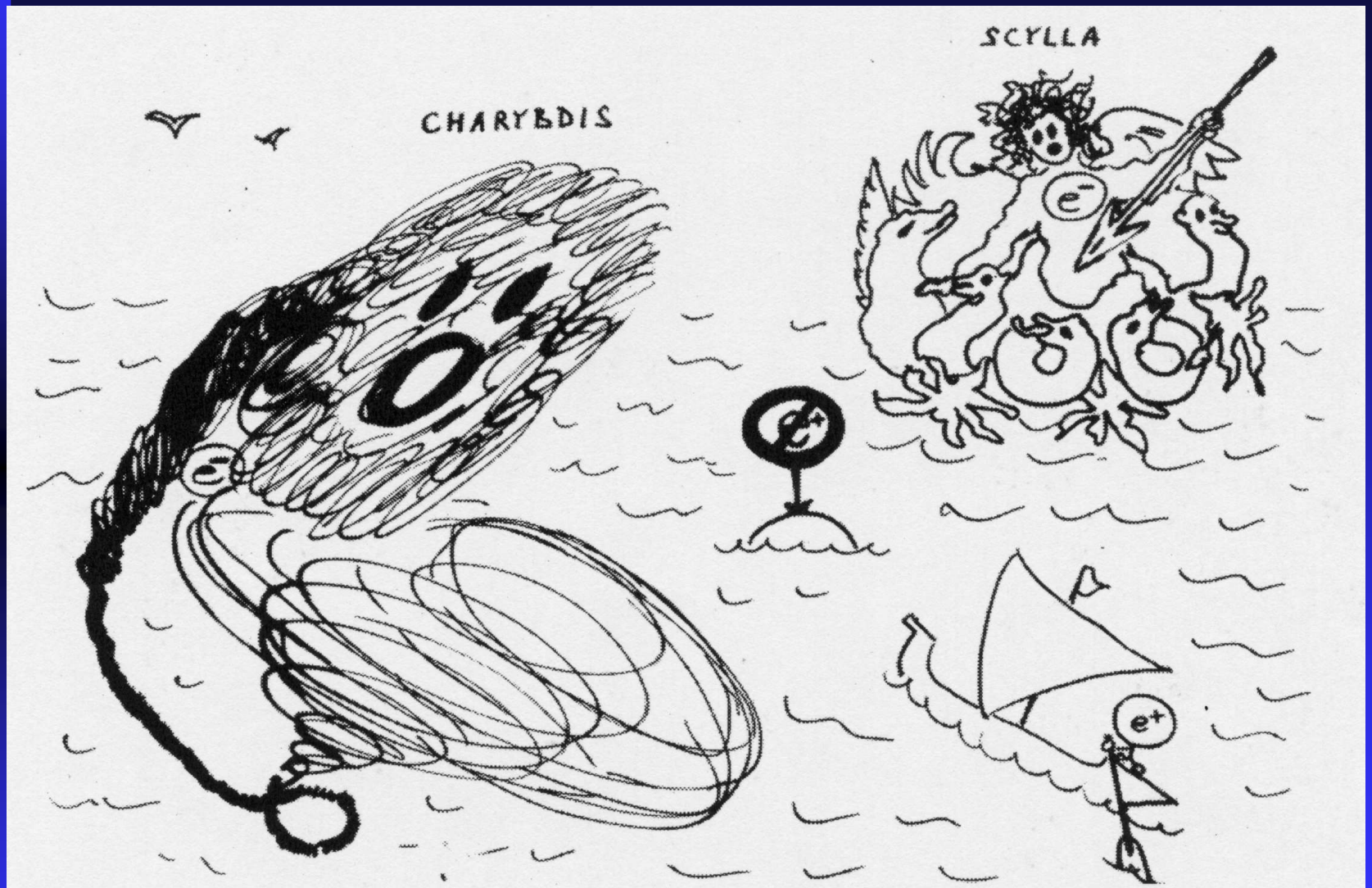


Fig. 1. The challenges a positron must face in our (non-anti)material world. For a positron, electrons constitute the same danger as Scylla and Charybdis for mythological Ulysses.

Electrons are attracted by a positron

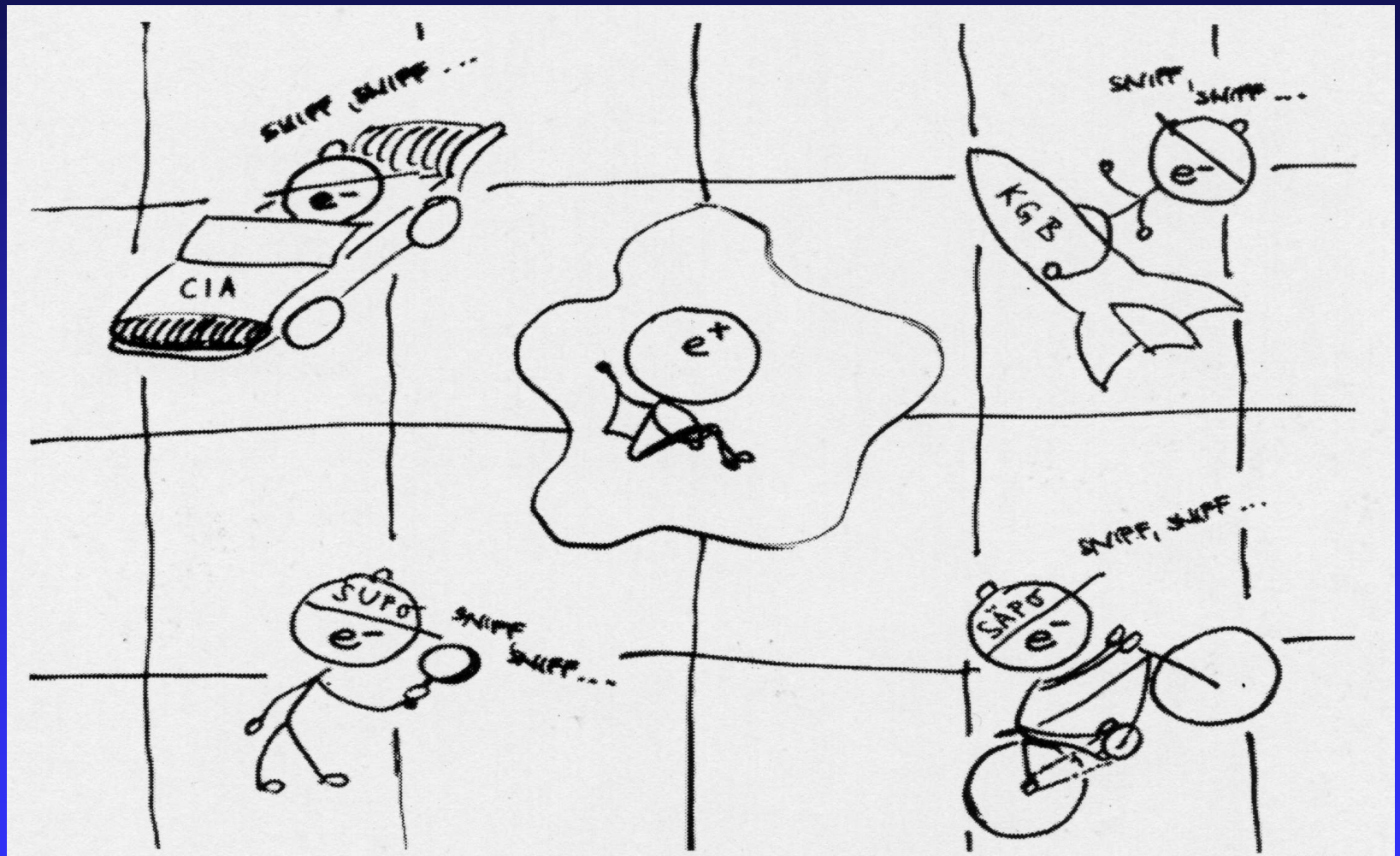


Fig. 2. A positron gathering information about its environment. The electron counter intelligence service is searching for it. Due to the strong Coulomb attraction, an electron screening cloud is formed around the positron. The positron's picoseconds are numbered.

The positron annihilation event

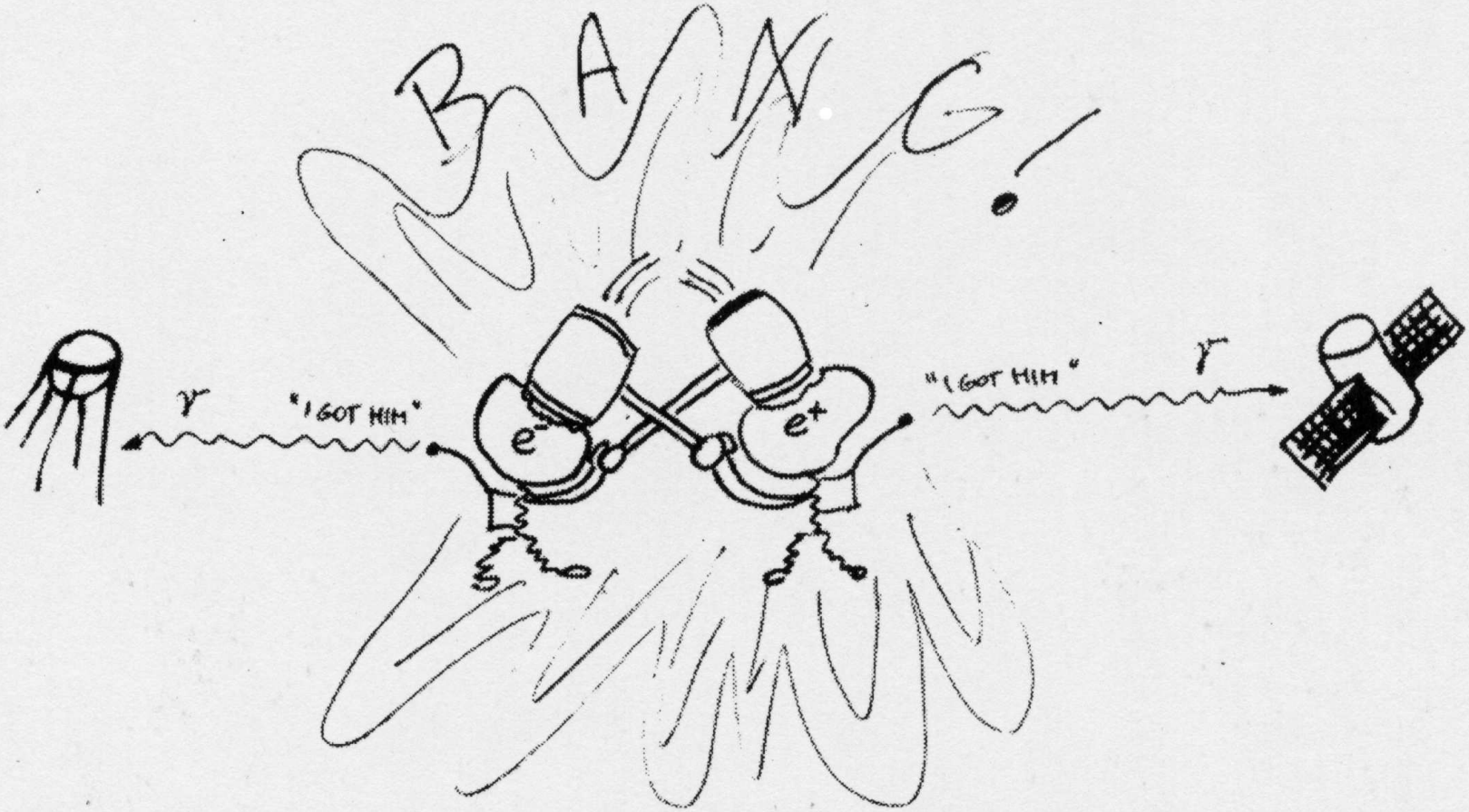


Fig. 3. The positron annihilation event. The information the positron has gathered is taken away by the pair of annihilation photons to our fast-electronics γ-ray detectors, where it is decoded and analyzed.

Scheme of a positron annihilation experiment

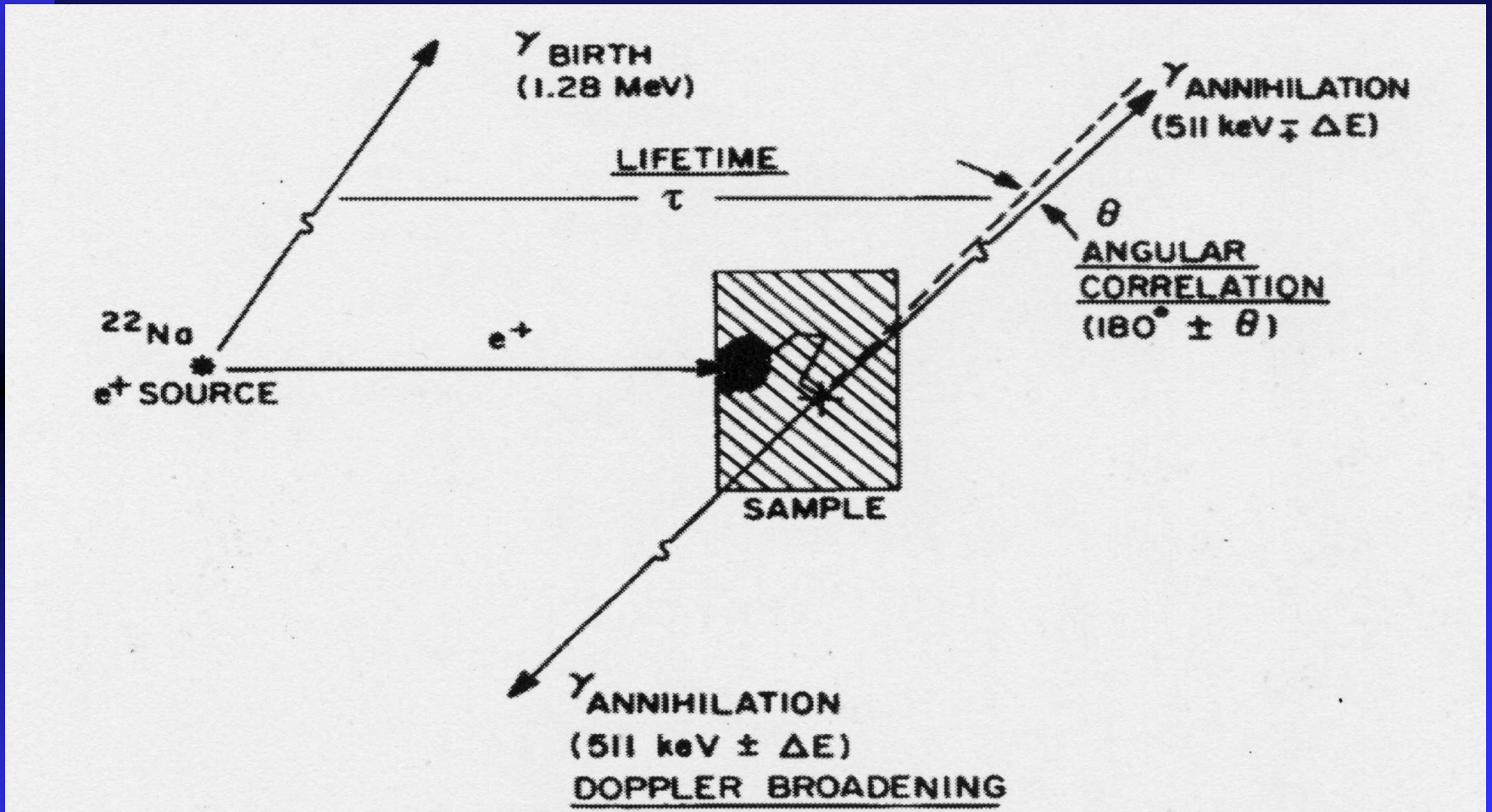


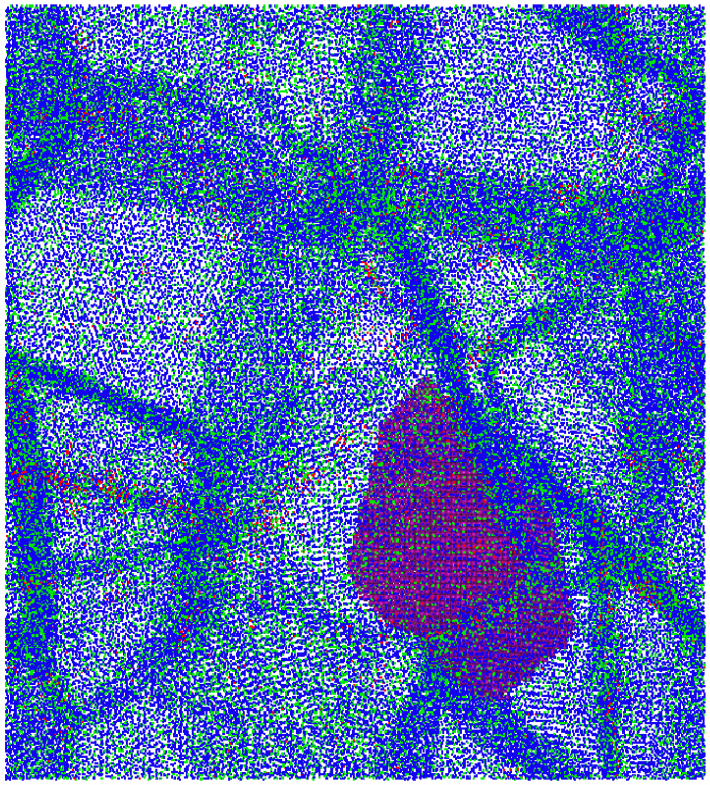
Fig. 4. Positron annihilation in a solid sample and basic positron annihilation experiments [9, 10].

Generation of a computer sample of nanocrystalline Ni:

(H. van Swygenhoven et al.)

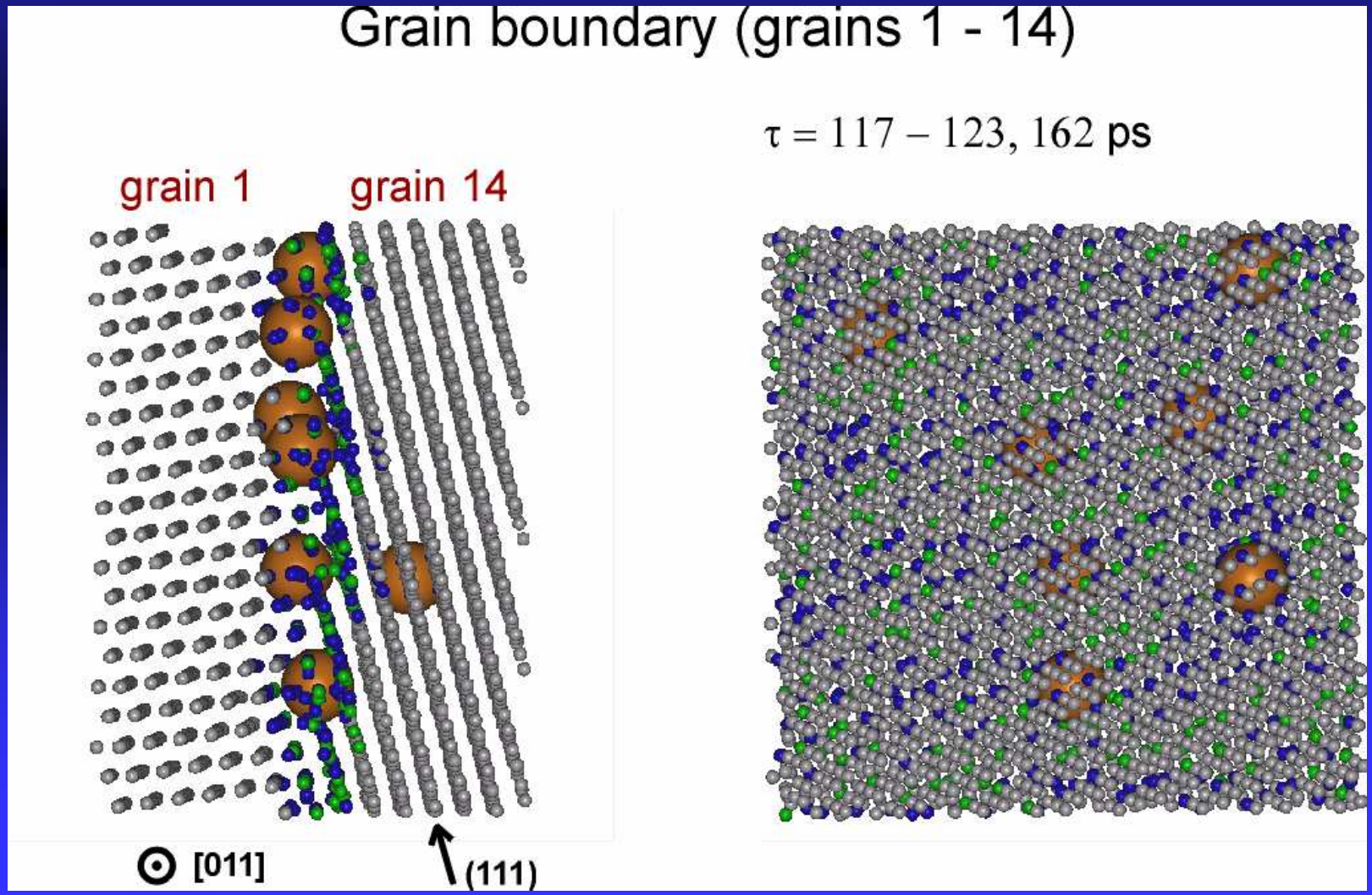
- simulation cell volume filled by nanograins (seeds) with random location and orientation
- grains allowed to grow until they touched
- sample relaxed by molecular dynamics for 50-100 ps at 300 K (central-force potentials, magnetism not included)
- => computer sample of n-Ni, 1.2 million of atoms, 15 grains, density 96 % of bulk Ni, high-angle grain boundaries present
- so far, only several GBs and one triple junction analyzed

n-Ni, 12 nm grain size, 300 K

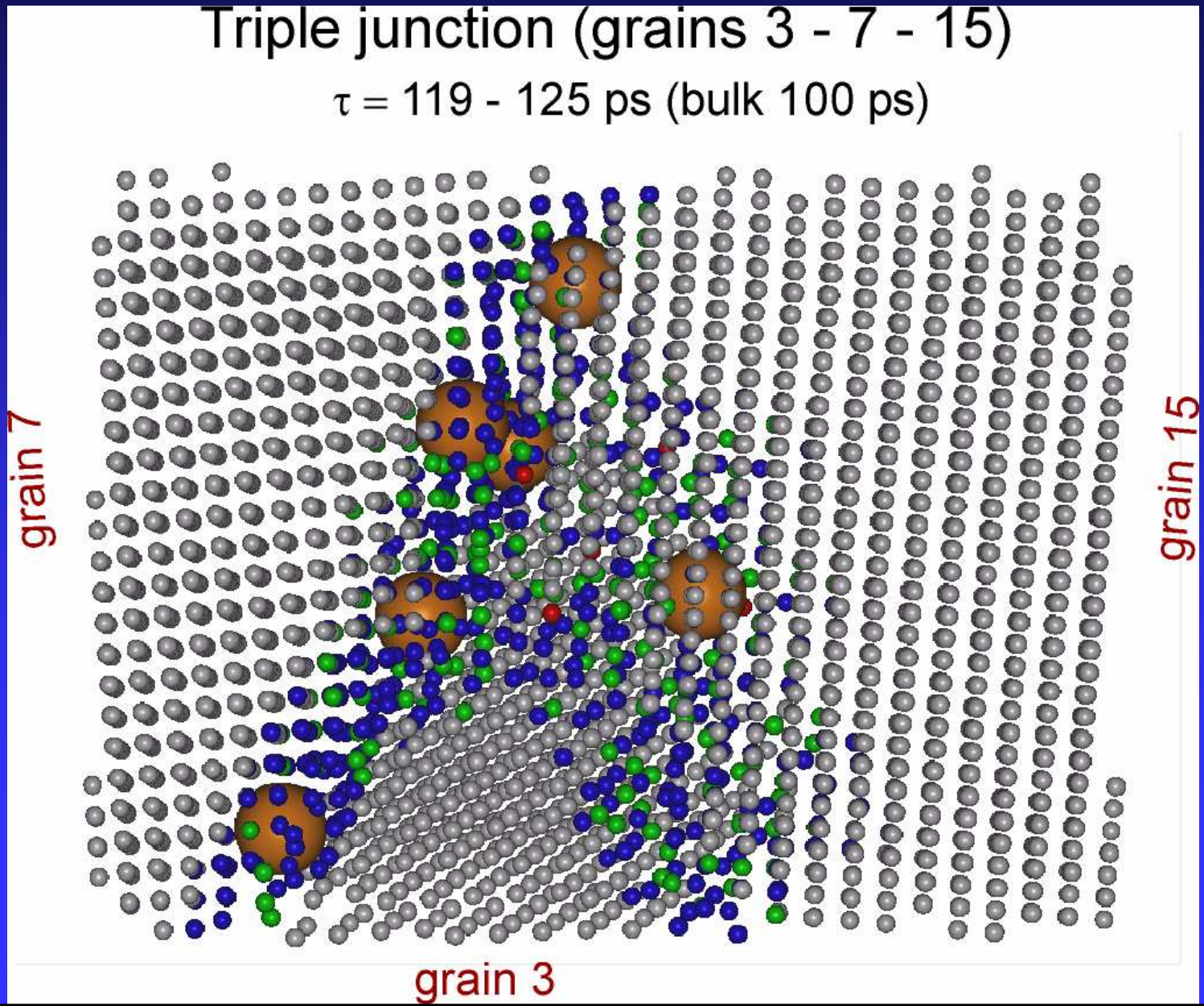


High-angle grain boundary in nanocrystalline Ni

-- calculated positron lifetimes only slightly higher than the bulk value (100 ps)
-- they correspond to shallow traps (marked by orange spheres)
-- one vacancy was found (=> vacancy concentration is about 1 ppm)



Triple junction in nanocrystalline Ni

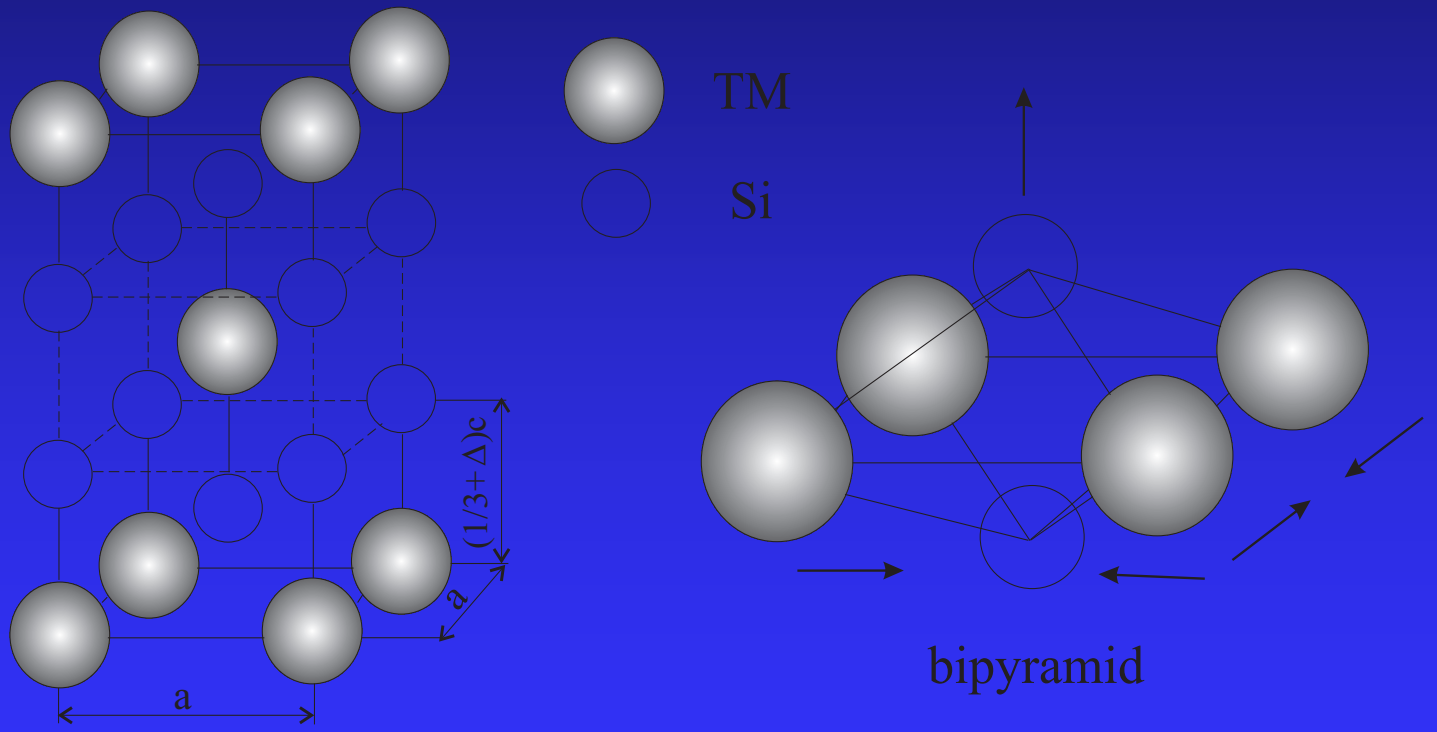


Transition-metal disilicides

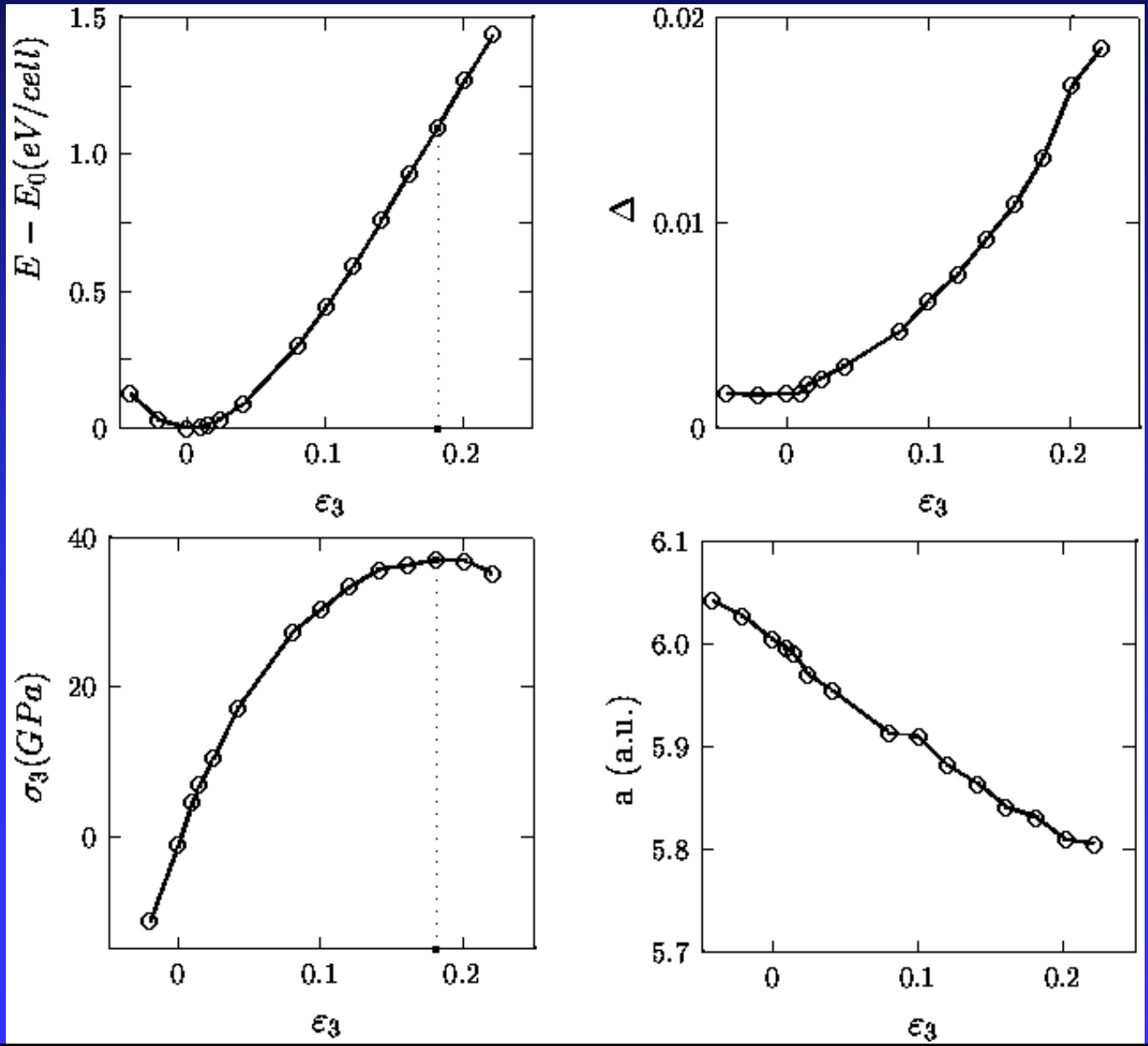
- promising in structural applications
- bonding has mixed metallic and covalent character
- brittle
- various structures: tetragonal $C11_b$ ($MoSi_2$, WSi_2), hexagonal C40 ($NbSi_2$, $TaSi_2$, VSi_2, $CrSi_2$), orthorombic C54 ($TiSi_2$)


A380
A380

C11$_b$ structure; the internal parameter Δ is defined as a small deviation from the ideal value of 1/3



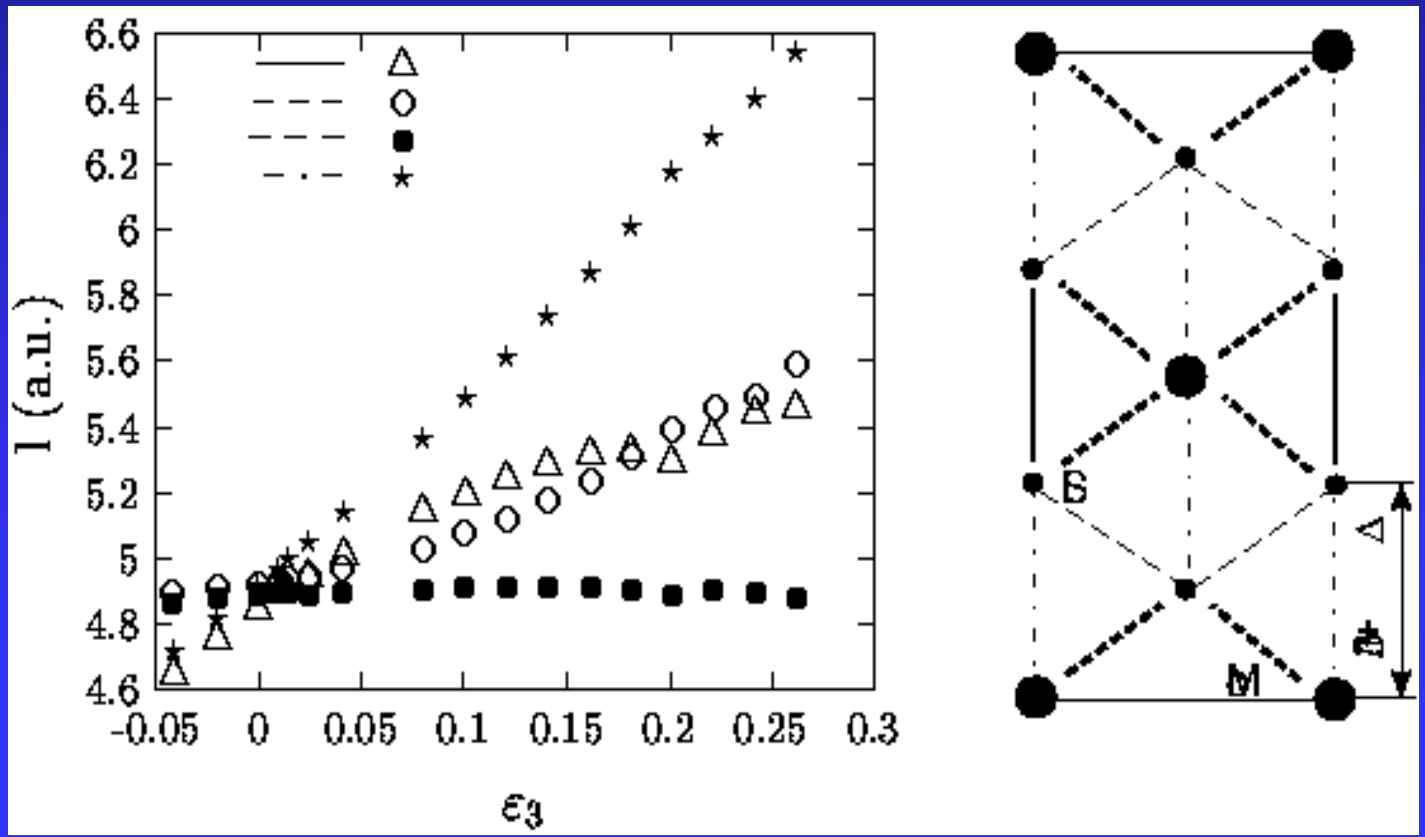
Tensile test for $MoSi_2$ ([001] loading)



Behavior of bond-lengths during a tensile test in $MoSi_2$ along the [001] direction

**** weak Mo-Si bonds

●●● strong Mo-Si bonds (nearly constant)



Calculated theoretical tensile strength for [001] loading:

$MoSi_2$: 37 GPa

WSi_2 : 38 GPa

Dohledné perspektivy studia soustav kovů a jejich slitin (nové materiály)

Úkoly nyní řešitelné vyžadující čas, lidské a finanční zdroje

- Rovnovážné stavy
  - Pokračování ve vývoji konzistentních termodynamických databází (ekonomický zájem, společenská objednávka, progresivní skupiny materiálů,…).
  - Plánovaný experiment (ověřování predikcí fázových diagramů)
- Kinetika
  - Tvorby kinetických databází, experiment
  - 3D simulace (zahrnutí distribuce velikosti, tvar fází, …)
  - Zahrnutí jiných mechanismů difůze (nizké teploty, dráhy vysoké difúzivity,..)

Tvůrčí úkoly

- Rovnovážné stavy
  - Výpočty fázové stability z prvních principů
  - Propojen fázový diagram, fázová mikrostruktura a fyzikální vlastnosti
- Kinetika
  - Nerovnovážný potenciál na mezifází
  - Nukleační mechanismy, stavy a procesy za nízkých teplot

Současné směry společenské objednávky v sledované oblasti

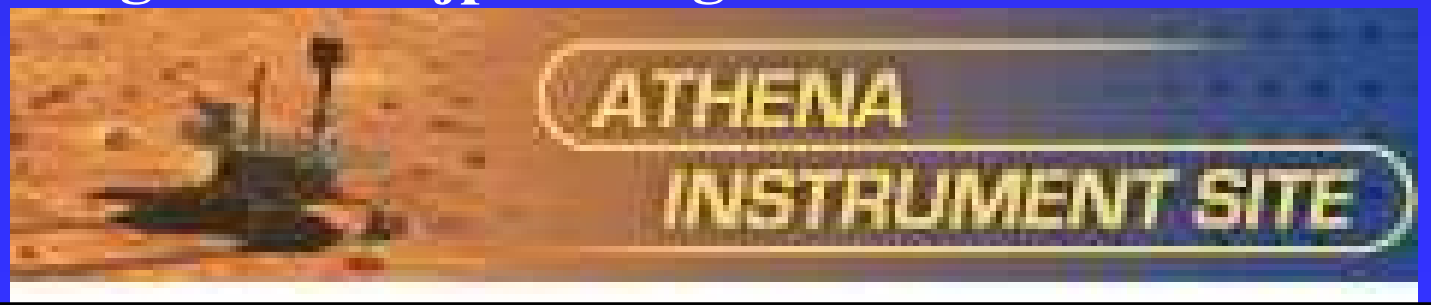
- Niklové superslitiny (letecký průmysl)
- Materiály pro energetiku (mikrostrukturní stabilita fázových a pevnostních vlastností
- Odhady zbytkové životnosti technologií – turbíny elektráren, chemické a nukleární reaktory, sváry,

- Ekologické projekty (bezolovnaté pájky, kontejnery pro radioaktivní odpad,…)
- Speciální materiály ….

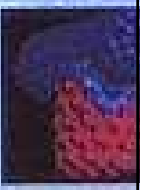
Další aplikace

- speciální materiály pro extrémní teploty teploty (viz kosmický program)
- Izolační materiály
- Speciální elektrotechnické materiály
- Extrémní struktury

- http://origin.mars5.jpl.nasa.gov/home/



What is Nanotechnology?



Nanotechnology is the creation of functional materials, devices and systems through control of matter on the nanometer length scale and exploitation of novel phenomena and properties (physical, chemical, biological) at that length scale

"If I were asked for an area of science and engineering that will most likely produce the breakthroughs of tomorrow, I would point to nanoscale science and engineering."

-Neal Lane
Assistant to the President for Science
And Technology

Simulation of nanoindentation process I
(semiempirical potentials)

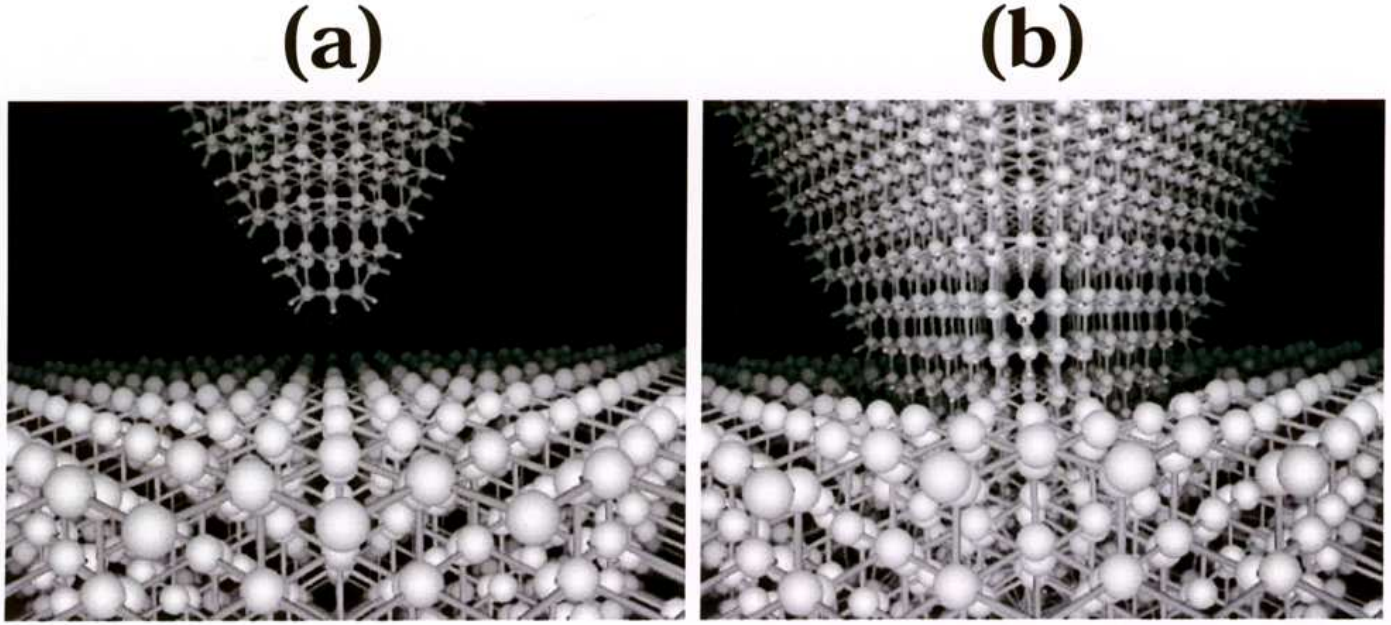
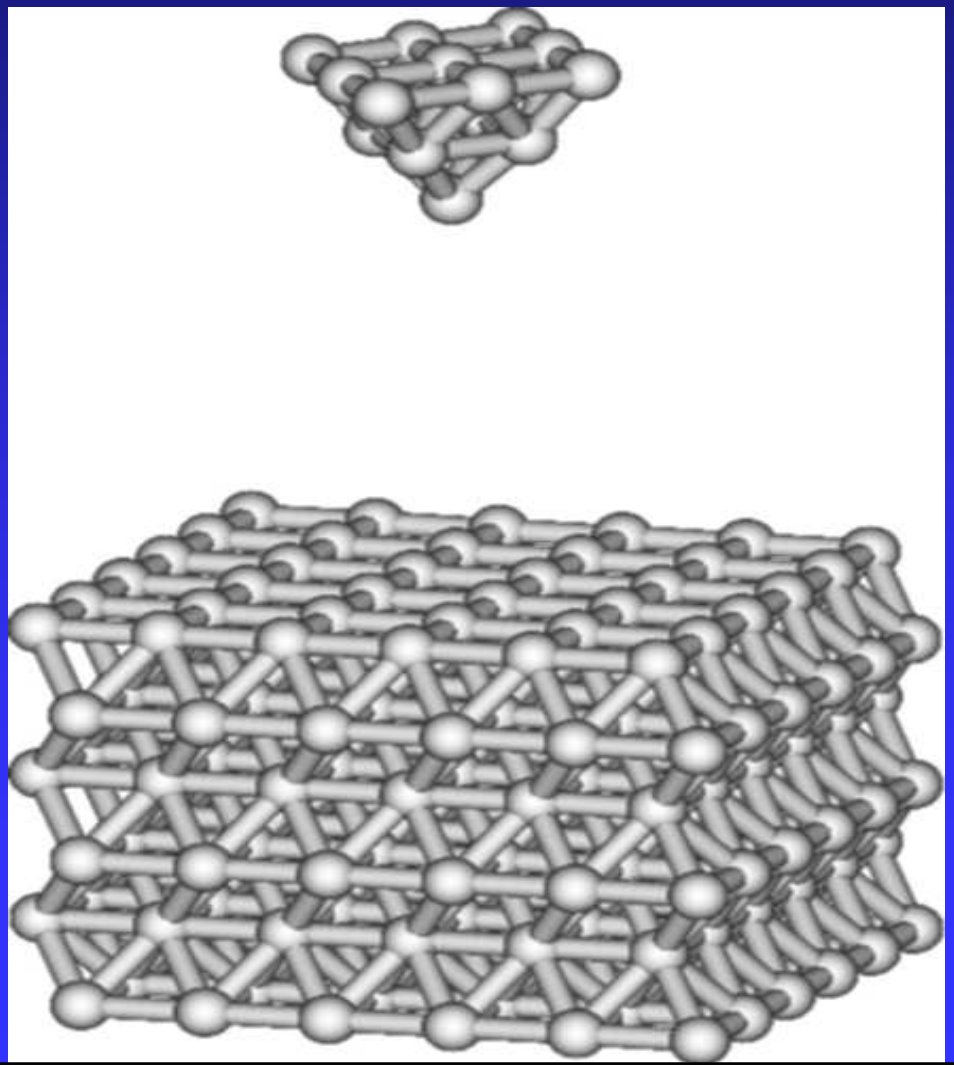


Figure 1: Snapshots illustrating the surface region during indentation. The small spheres on the diamond tip are hydrogen atoms. a) Initial configuration. (b) Indentation of 1.2 nm.

Simulation of nanoindentation process II

(ab initio)



Finanční zajištění výzkumu

- výzkumný záměr MŠMT, výzkumný záměr AV ČR (2005-2011)
- 3 projekty GA ČR (2005-2008)
- 1 projekt GA AV (2003-2007, požádáme o nový)
- 2 projekty COST (2006-2009)
- mezinárodní spolupráce:
  - University of Pennsylvania, Philadelphia, USA
  - Max-Planck-Institute for Iron Research, Duesseldorf, SRN
  - Tohoku University, Sendai, Japonsko
  - University of Vienna, Rakousko
  - Evropské projekty (COST)

Celková částka cca 2,2 MKč ročně

Podpora spolupracujících studentů

- speciální doktorský projekt od GA ČR určený výlučně pro materiální podporu doktorandů; na každého doktoranda vychází
  - až 40.000 Kč dodatečného stipendia ročně
  - až 30.000 Kč dodatečného cestovného ročně
    - typicky 2 mezinárodní akce ročně
- další odměny (až 10.000 Kč ročně) z běžících grantových projektů
- zahraniční studijní pobyty během doktorského studia
  - půlroční na některých spolupracujících pracovištích
  - short-term scientific missions (1 týden – 1 měsíc) po celé Evropě
- výborné pracovní uplanění po ukončení magisterského a doktorského studia
  - post-doktorátní pobyty na předních světových pracovištích
    - University of Uppsala, Švédsko
    - University of Louvain, Belgie
    - Max-Planck-Institute for Iron Research, Duesseldorf
    - Imperial College, London,
    - University of Vienna

The role of ab initio calculations in multiscale modeling (I)

- the importance of ab initio methods consists in
  - high predictivity
  - no adjustable parameters
  - benchmarks for less accurate but faster methods

but they are

  - computationally intensive
  - less than 1000 non-equivalent atoms may be included

The role of ab initio calculations in multiscale modeling (II)

- for full understanding of various phenomena: combination of
  -- ab initio calculations & simpler approaches
  . **(multiscale modelling)**
  -- checking with experimental data

- **main goal:** developing predictive methods and algorithms to understand the properties of realistic materials (e.g. strength, plasticity, creep, fracture)