A multiscale model for fracture and radiation damage in tungsten

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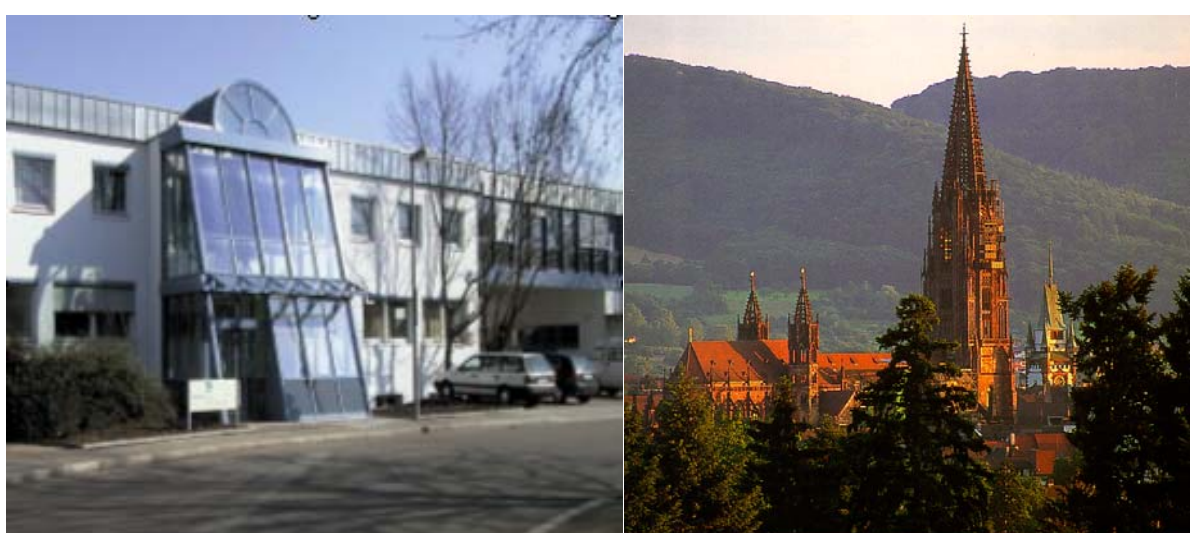
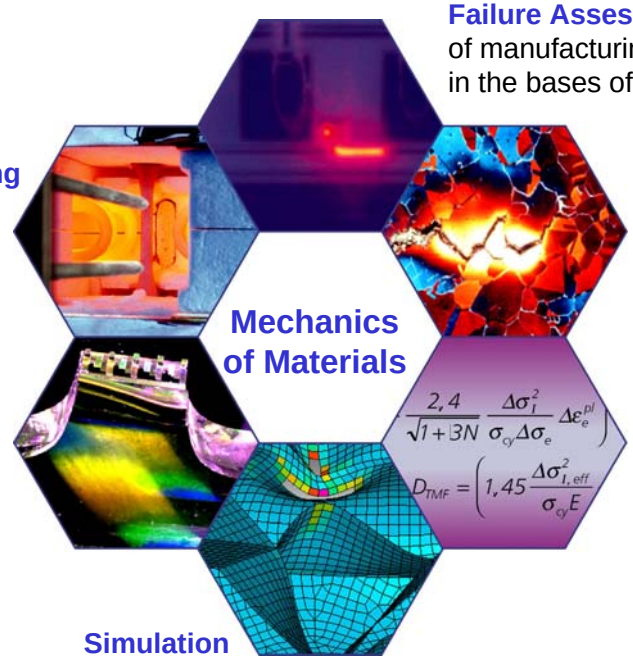


IWM
Fraunhofer Institut Werkstoffmechanik

Fraunhofer IWM Freiburg and Halle - Core Competencies

Failure Assessment
of manufacturing or in-service related faults in the bases of safety and lifetime concepts

Materials and Component Testing
under condition of use (temperature, wear, pressure ...) yield significant results for assessment and simulation



Microstructural Analysis
by high resolution diagnostics and ion beam technologies lead to a sound understanding of the materials microstructure

Forming
Specific methods to improve forming processes: hot embossing of glass, springback during sheet forming, rolling of wires, forging, powder pressing and sintering

Modelling
Development of micromechanical models for damage, brittle fracture and thermocyclical stress

Simulation
The linking of testing and simulation is significant for the outstanding position of Fraunhofer IWM in the simulation of materials, processes and components

Fraunhofer society invested 3 Mio. € into development of MMM-Tools

TG_hel_00802e.ppt

our current interest in tungsten:

drawing of wires

understanding crack nucleation
and crack propagation

by atomistic modelling

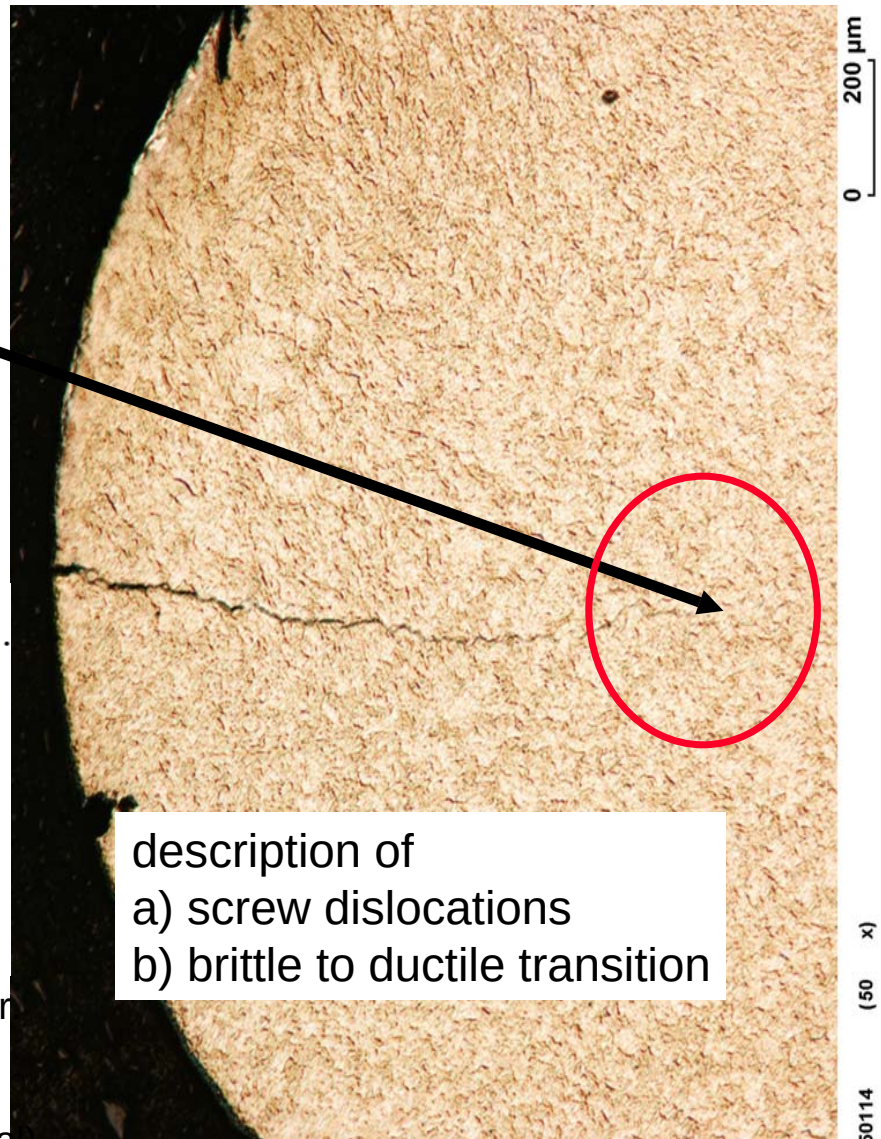
Fracture toughness of tungsten in MPa $m^{1/2}$.

Crack system	RT exp.	77 K exp.	Atomistic modeling
{100}⟨010⟩	8.7 ± 2.5	3.4 ± 0.6	2.05
{100}⟨011⟩	6.2 ± 1.7	2.4 ± 0.4	1.63
{110}⟨001⟩	20.2 ± 5.5	3.8 ± 0.4	2.17
{110}⟨1$\bar{1}$0⟩	12.9 ± 2.1	2.8 ± 0.2	1.56

{crack plane} <crack front>

Gumbsch J.Nucl.Mater
323, 304 (2003)

(using Finnis-Sinclair-potential)



description of
a) screw dislocations
b) brittle to ductile transition

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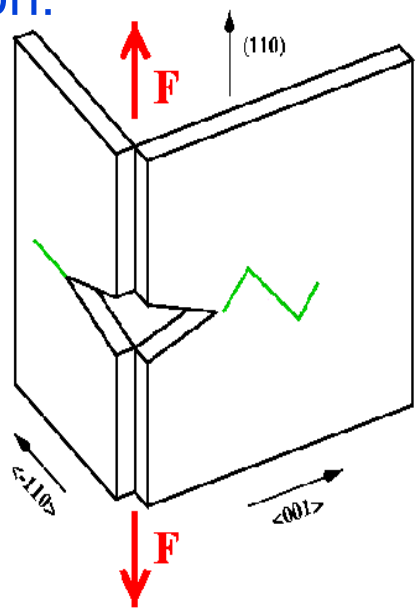
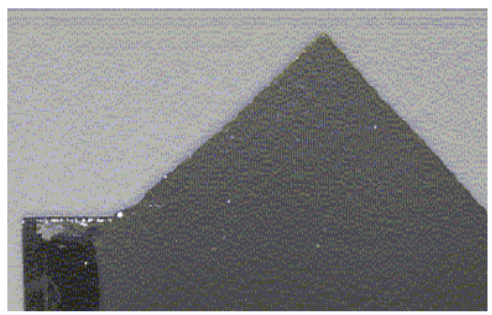
cleavage anisotropy in Silicon:

cracks on the {110} plane

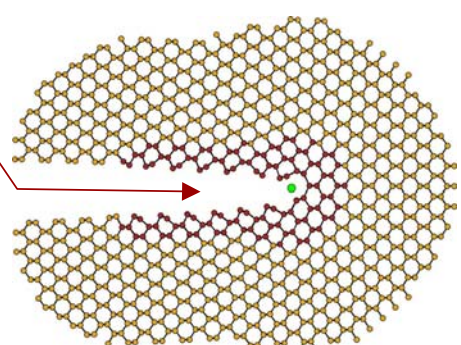
crack propagation direction:
[-110] easy
[001] not observed





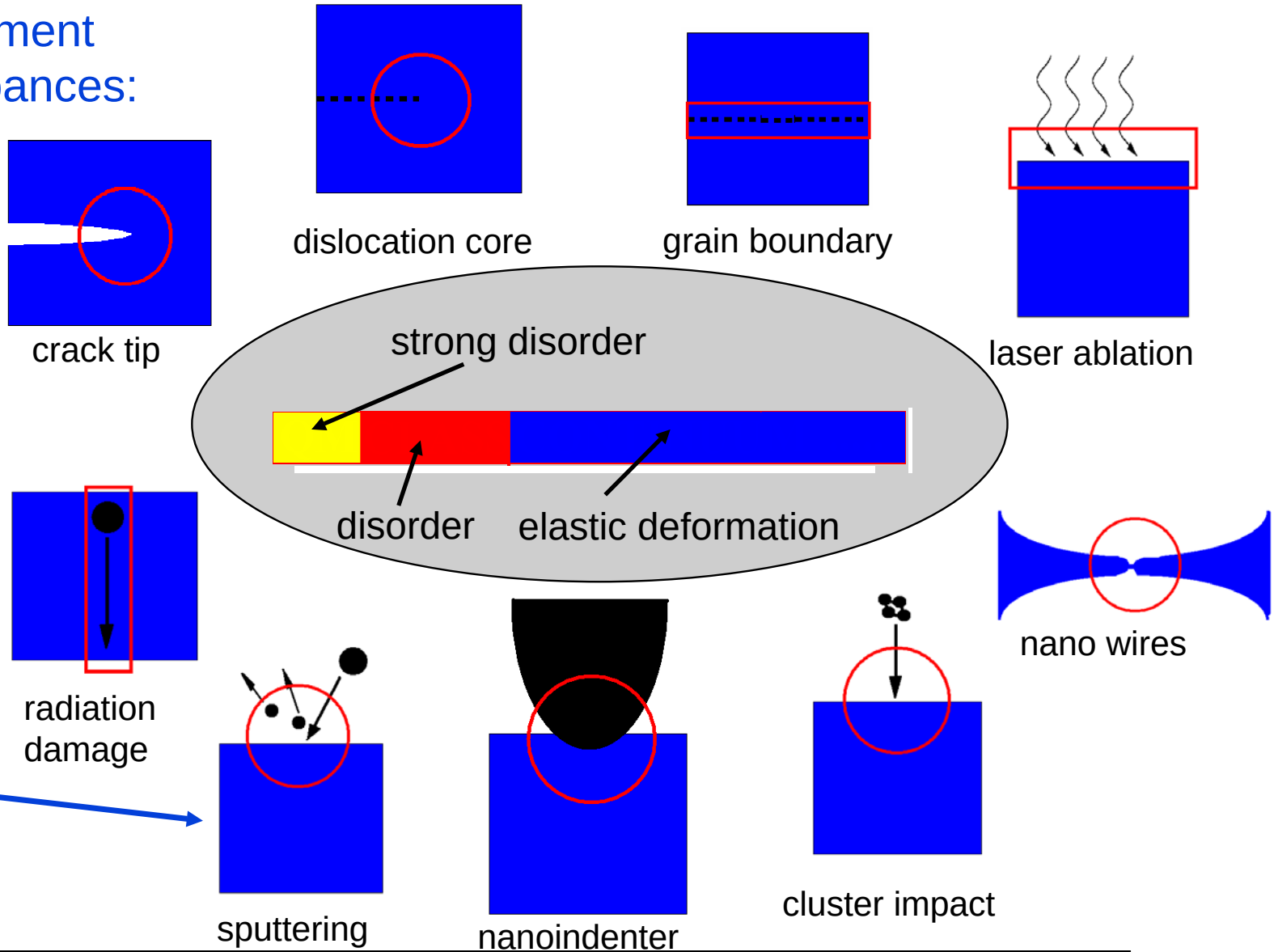
common classical potentials
(Stillinger-Weber, Tersoff)
give wrong predictions.

quantum-forces



R.Perez and P.Gumbsch,
PRL **84**, 5347 (2000)

atomistic treatment of local disturbances:



Salonen, Nordlund, Keinonen, Wu
J.Nucl.Mater. **313-316**, 404 (2003)
Sputtering of divertor Materials C and W

a multiscale problem

→ atomistic processes in nano- and microscale regions

- far from equilibrium → quantum treatment
- close to equilibrium → semi-empirical potentials

→ macroscale prescription of Dirichlet or von Neumann boundary conditions (BC) far away from the atomistic zone

- asymptotic stress field or strain field
- asymptotic temperature field

→ physics outside the atomistic region is only relevant concerning the atomistic BC

- micro stresses, micro strains
- nonreflecting BC
- heat sink
- thermostat

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a multiscale model

→outline of the talk:

A) coupling of the three different zones
B) choice of the potentials

A: coupling schemes

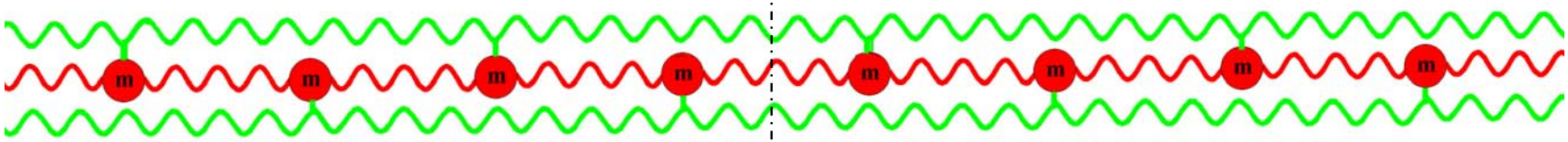
FEAt: Kohlhoff, Gumbsch, Fischmeister, Phil.Mag.A **64**, 851 (1991)
QC: Tadmor, Ortiz, Phillips, Phil.Mag.A **73**, 1529 (1996)
SMA: Moseler, Nordiek, Haberland, PRB **56**, 15439 (1997)
CLS: Broughton, Abraham,Bernstein, Kaxiras, PRB **60**, 2391 (1999)

model for atomistic zone: 1-D solid

V(x)

- atoms interact via 1st and 2nd neighbour potential:

$$E_{pot} = \tfrac{1}{2} \sum_i [V(x_i - x_{i-1}) + V(x_i - x_{i-2})]$$

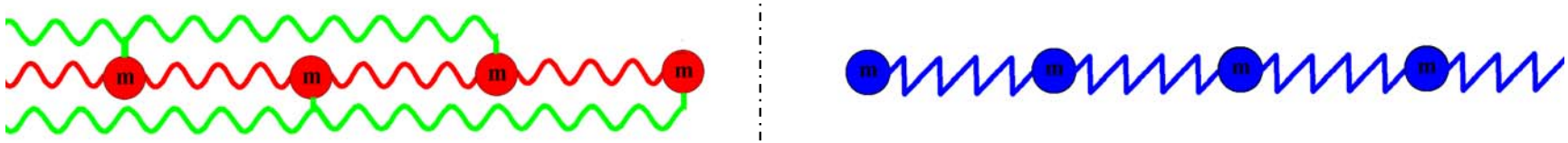


CLASS CONTINUUM .....

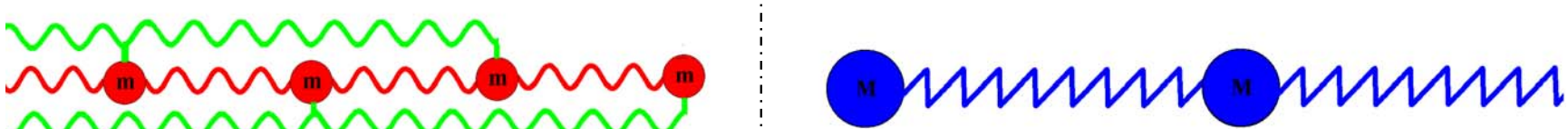
ATOMS NODES

substitutional medium

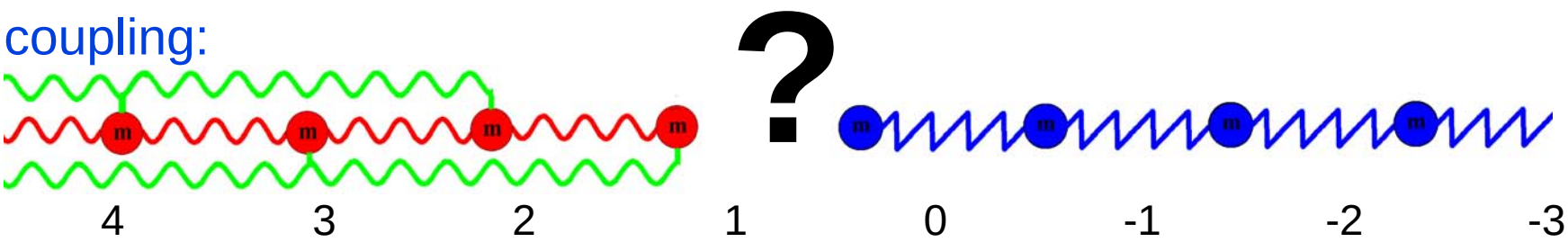
- idea of **FEAt , QC, CLS:** replace nonlocal force field by 1st neighbour forces (from FEM description for nodes), equal atomic and nodal positions



- **SMA:** take heavier nodes on simple cubic lattice



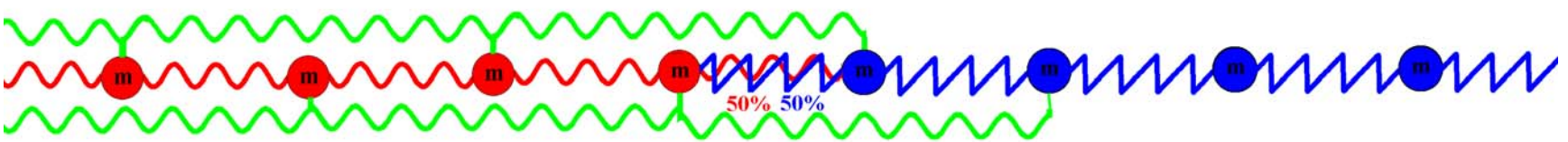
coupling:



pot. energy of atom: $E_i^a = ½ [½ k_1(x_i-x_{i-1})^2 + ½ k_1(x_{i+1}-x_i)^2 + ½ k_2(x_i-x_{i-2})^2 + ½ k_2(x_{i+2}-x_i)^2]$

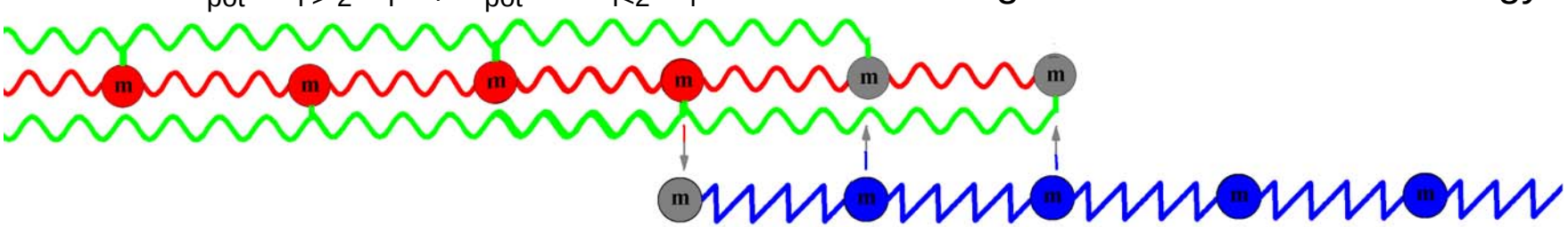
node: $E_i^c = ½ [½ k_c(x_i-x_{i-1})^2 + ½ k_c(x_{i+1}-x_i)^2]$

- **QC, CLS:** $E_{pot}=S_{i>0} E_i^a + S_{i<1} E_i^c$ advantage: Hamiltonfct. → isoenergetic dynamics



disadvantage: unbalanced („ghost“) forces

- **FEAt**: $E^a_{pot}=S_{i>-2} E_i^a$, $E_{pot}^c = S_{i<2} E_i^c$ disadvantage: no Hamiltonfct. → energy loss in MD



Advantage: forces balanced

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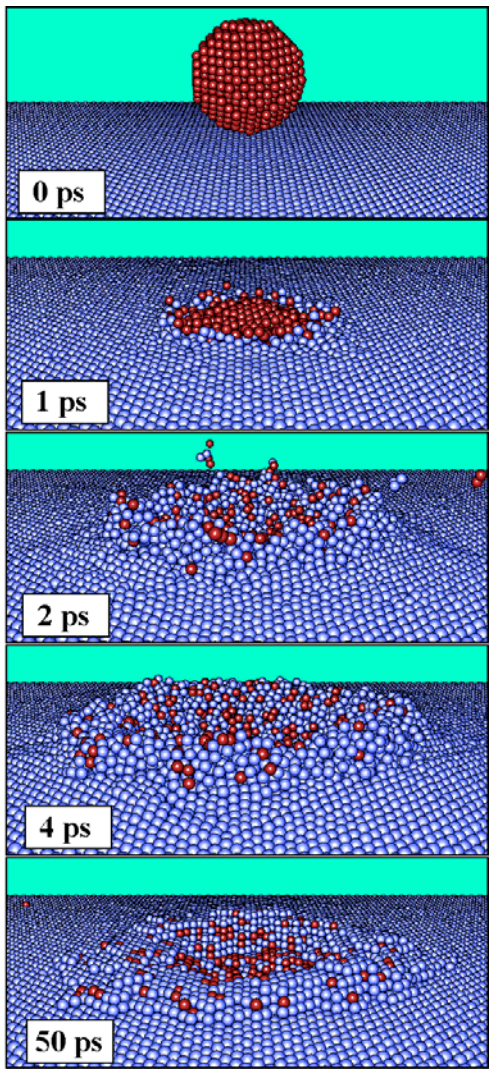
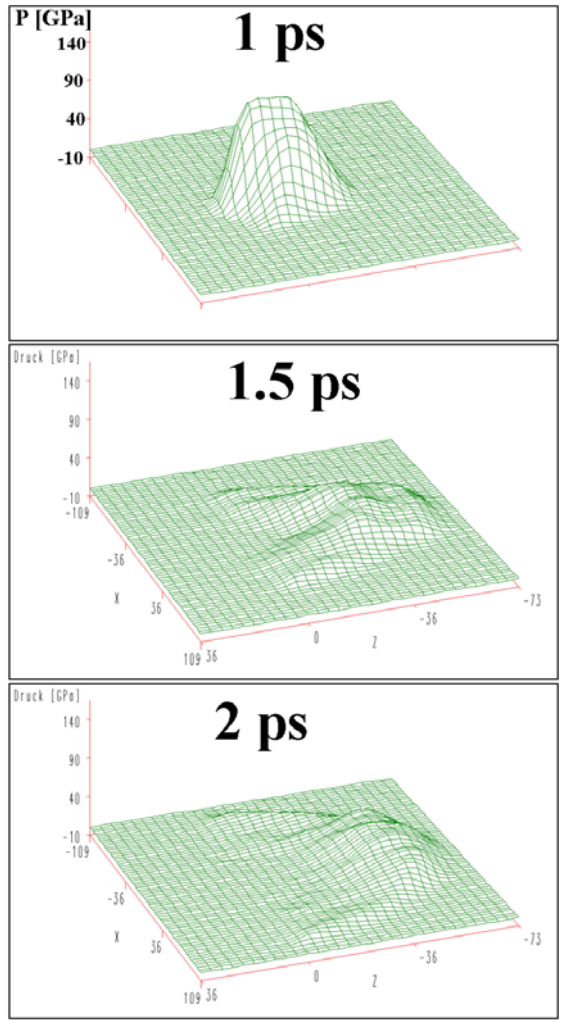
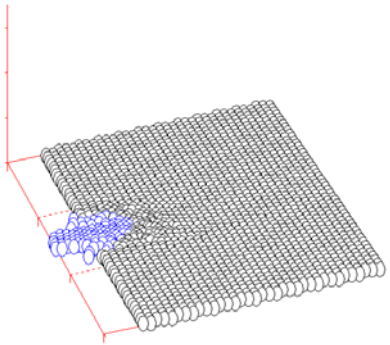
the high-freqency problem







Energetic Cluster Impact (ECI): Moseler et al., NIMB 164, 522 (2000)

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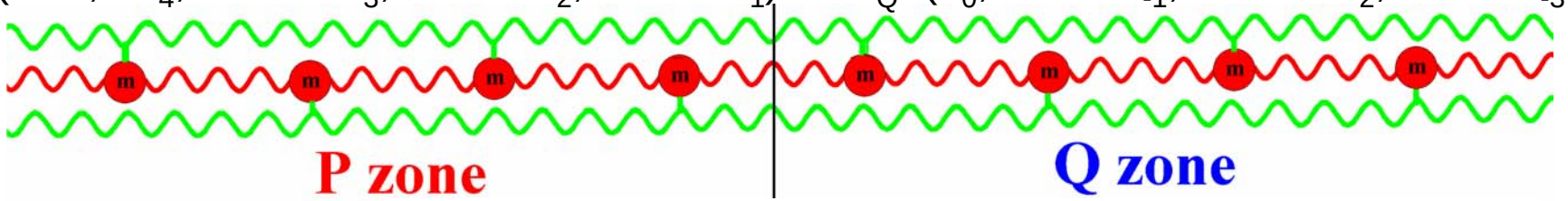
systematic way to derive coupling

- partition displacement:

$\mathbf{u}_P$=(….., u_4, u_3, u_2, u_1) $\mathbf{u}_Q$=(u_0, u_{-1}, u_{-2}, u_{-3}, …….



- equations of motion:

$$-m_P\omega^2\tilde{\mathbf{u}}_P(\omega) = \tilde{\mathbf{f}}_P(\omega) - \Phi_{PP}\tilde{\mathbf{u}}_P(\omega) - \Phi_{PQ}\tilde{\mathbf{u}}_Q(\omega)$$
$$-m_Q\omega^2\tilde{\mathbf{u}}_Q(\omega) = \tilde{\mathbf{f}}_Q(\omega) - \Phi_{QP}\tilde{\mathbf{u}}_P(\omega) - \Phi_{QQ}\tilde{\mathbf{u}}_Q(\omega).$$

- Greens function:

$$m_Q\omega^2\mathbf{G}_{QQ}(\omega) - \Phi_{QQ}\mathbf{G}_{QQ}(\omega) = \mathbf{1}_{QQ}$$

- Formal solution:

$$\tilde{\mathbf{u}}_Q(\omega) = \tilde{\mathbf{G}}_{QQ}(\omega)\left(-\tilde{\mathbf{f}}_Q(\omega) + \Phi_{QP}\tilde{\mathbf{u}}_P(\omega)\right)$$

- Generalized Langevin equation:

$$-m_P\omega^2\tilde{\mathbf{u}}_P(\omega) = \tilde{\mathbf{f}}_P(\omega) - \Phi_{PP}\tilde{\mathbf{u}}_P(\omega) + \tilde{\mathbf{R}}_P(\omega) + \tilde{\mathbf{\Theta}}_{PP}(\omega)\tilde{\mathbf{u}}_P(\omega)$$

Random force term:

$$\tilde{\mathbf{R}}_P(\omega) = \Phi_{PQ}\tilde{\mathbf{G}}_{QQ}(\omega)\tilde{\mathbf{f}}_Q(\omega)$$

Friction Kernel:

$$\tilde{\mathbf{\Theta}}_{PP}(\omega) = -\Phi_{PQ}\tilde{\mathbf{G}}_{QQ}(\omega)\Phi_{QP}$$

substitutional medium approach

Moseler et al., PRB 56, 15439 (1997)

new Q medium: $$-m_Q^*\omega^2\tilde{\mathbf{u}}_Q^*(\omega) = -\Phi_{QP}^*\tilde{\mathbf{u}}_P(\omega) - \Phi_{QQ}^*\tilde{\mathbf{u}}_Q^*(\omega)$$

coupled to old P zone:

$$-m_P\omega^2\tilde{\mathbf{u}}_P(\omega) = \tilde{\mathbf{f}}_P(\omega) - \Phi_{PP}\tilde{\mathbf{u}}_P(\omega) + \tilde{\mathbf{\Theta}}_{PP}^*(\omega)\tilde{\mathbf{u}}_P(\omega)$$

$$\tilde{\mathbf{\Theta}}_{PP}^*(\omega) = -\Phi_{PQ}^*\tilde{\mathbf{G}}_{QQ}^*(\omega)\Phi_{QP}^*$$

dynamic of $\mathbf{u}_P$ after substitution should be the same:

$$\begin{aligned} -m_P\omega^2\tilde{\mathbf{u}}_P(\omega) &= \tilde{\mathbf{f}}_P(\omega) - \Phi_{PP}\tilde{\mathbf{u}}_P(\omega) + \tilde{\mathbf{\Theta}}_{PP}^*(\omega)\tilde{\mathbf{u}}_P(\omega) \\ &+ \tilde{\mathbf{R}}_P(\omega) + \tilde{\mathbf{\Delta}}_{PP}(\omega)\tilde{\mathbf{u}}_P(\omega) \end{aligned}$$

$$\tilde{\mathbf{\Delta}}_{PP}(\omega) = \tilde{\mathbf{\Theta}}_{PP}(\omega) - \tilde{\mathbf{\Theta}}_{PP}^*(\omega)$$

if SM has the same long wave length (ω=0) behaviour:

$$\tilde{\mathbf{\Delta}}_{PP}(\omega) = \tilde{\mathbf{\Delta}}_{PP}(-i0) + \omega\tilde{\mathbf{\Delta}}'_{PP}(-i0) + \frac{1}{2}\omega^2\tilde{\mathbf{\Delta}}''_{PP}(-i0) + \frac{1}{6}\omega^3\tilde{\mathbf{\Delta}}'''_{PP}(-i0) + \dots$$

New equation of motion for P boundary atoms:

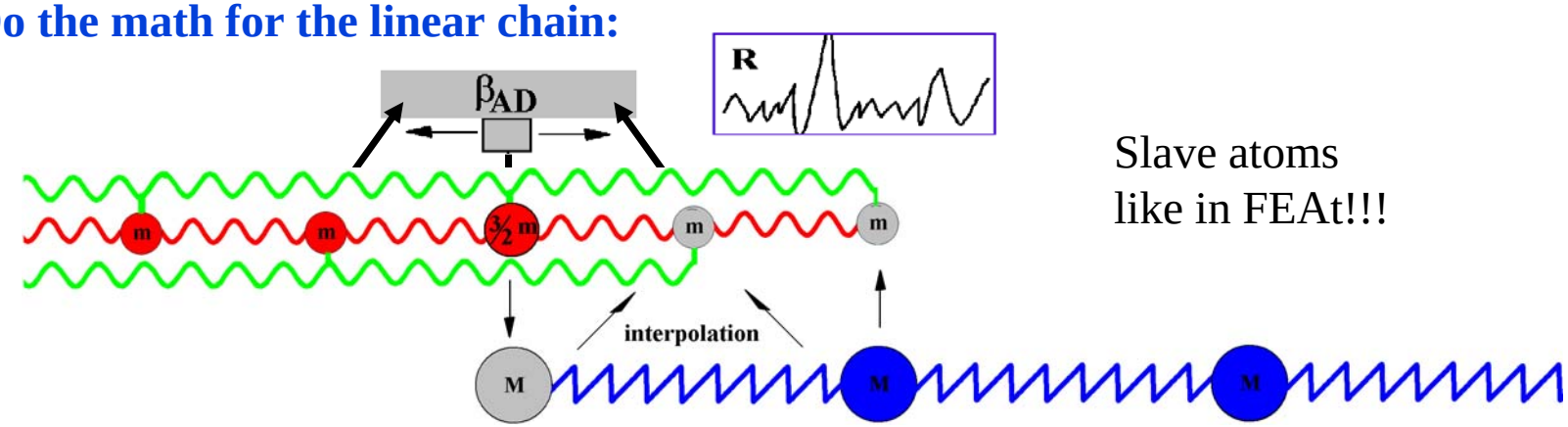
$$\begin{aligned}\mathbf{M}^*_{PP}\ddot{\mathbf{u}}_P(t) &= \mathbf{f}_P(t) - \Phi^*_{PP}\mathbf{u}_P(t) - \Phi^*_{PQ}\mathbf{u}^*_Q(t)\\ &- \mathbf{M}^*_{PP}\beta_{PP}\dot{\mathbf{u}}_P(t) - \mathbf{M}^*_{PP}\beta_{PQ}\dot{\mathbf{u}}^*_Q(t)\end{aligned}$$

$$\mathbf{M}^*_{PP} = \mathbf{M}_{PP} - \frac{1}{6}\tilde{\Delta}'''_{PP}(-i0)\mathbf{M}^{-1}_{PP}\tilde{\Delta}'_{PP}(-i0)$$

$$\mathbf{M}_{PP}=m_P\mathbf{1}_{PP}+\tilde{\Delta}''_{PP}(-i0)/2$$

$$\begin{aligned}\beta_{PP} &= i{\mathbf{M}^*_{PP}}^{-1}\left(\tilde{\Delta}'_{PP}(-i0) + \tfrac{1}{6}\tilde{\Delta}'''_{PP}(-i0)\mathbf{M}^{-1}_{PP}\Phi^*_{PP}\right)\\ \beta_{PQ} &= i{\mathbf{M}^*_{PP}}^{-1}\frac{1}{6}\tilde{\Delta}'''_{PP}(-i0)\mathbf{M}^{-1}_{PP}\Phi^*_{PQ}\end{aligned}$$

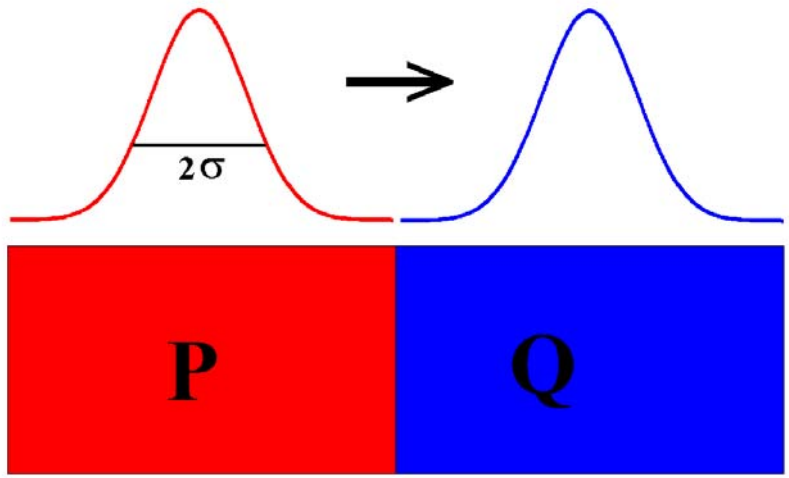
Do the math for the linear chain:



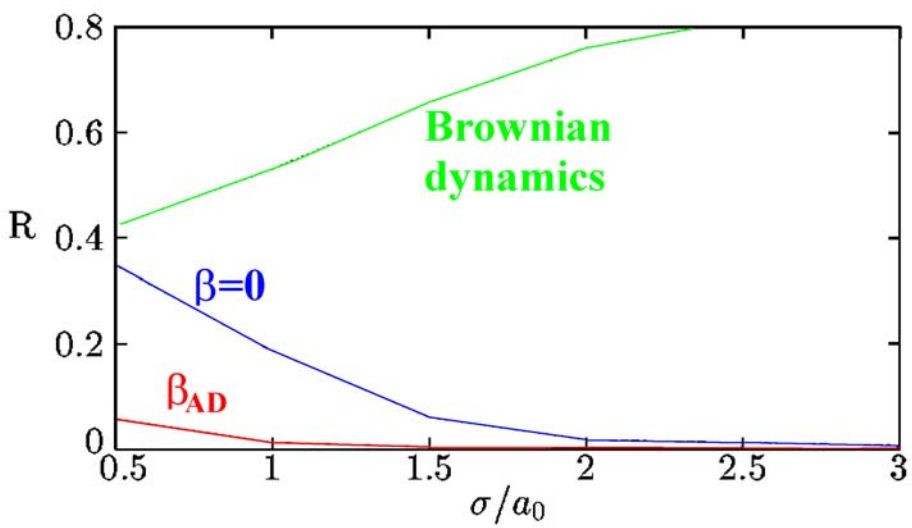
Slave atoms
like in FEAt!!!

Test:

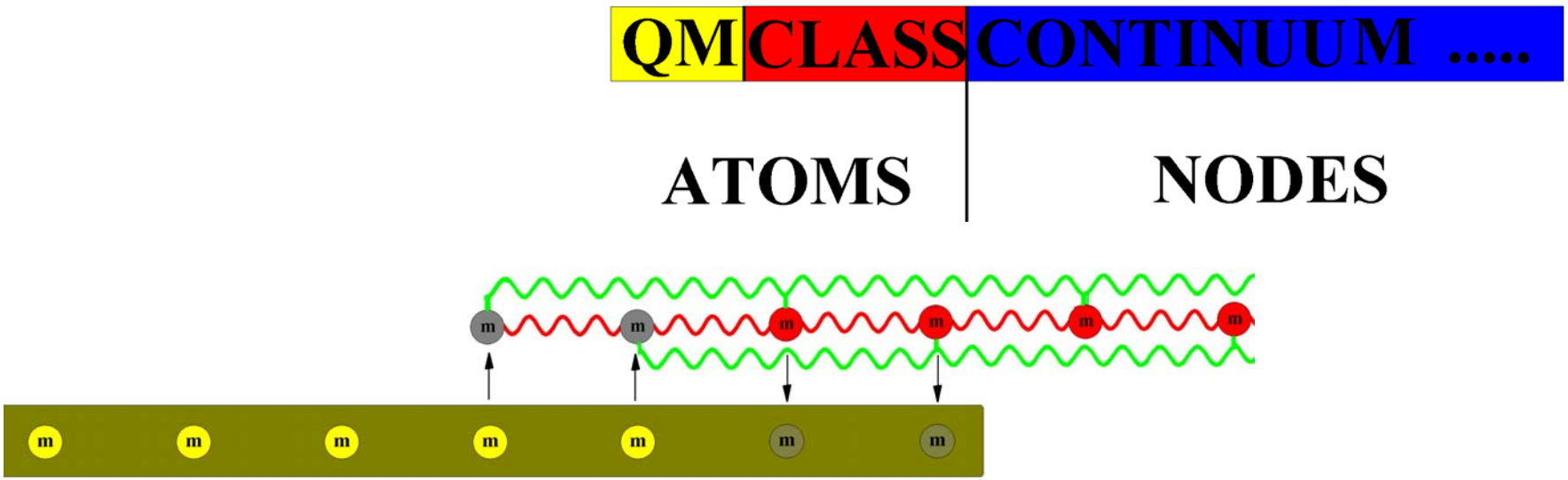
Gaussian wave packet in EAM-Cu:



Reflection:



coupling QM to classical



- embedded cluster calculation
- avoid electronic finite size effects

- covalent materials: H termination
- ionic materials: Madelung potential from classical zone
- metals: **bond order potentials**

Horsfield, Bratkovsky, Pettifor, Aoki, Phys. Rev. B 53, 1656 (1996);
Mrovec, Nguyen-Manh, Pettifor, Vitek, Phys. Rev. B 69, 0941XX (2004);

B: Choice of the potenials

QM: A bond order potential for tungsten

parametrized tight-binding for the d-electrons

$$E_{coh} = E_{bond} + E_{rep}$$

→ captures directional character of covalent bonds

→ reliable description of configurations far from equilibrium

real-space O(N) method

→ can be used for a large number of atoms

→ NO BC for electrons required } excellent for embedding

Bond part

$$E_{bond} = \sum_{i\alpha \neq j\beta} \Theta_{j\beta,i\alpha} \; H_{i\alpha,j\beta}$$

bond orders

$$\Theta_{i\alpha,j\beta} = \frac{1}{2}\left(N^{+}_{i\alpha,j\beta} - N^{-}_{i\alpha,j\beta}\right) = \sum_{n\ occ} 2C^{(n)}_{i\alpha} C^{(n)}_{j\beta}$$

solved **not by diagonalization**

calculated via Green's function formalism

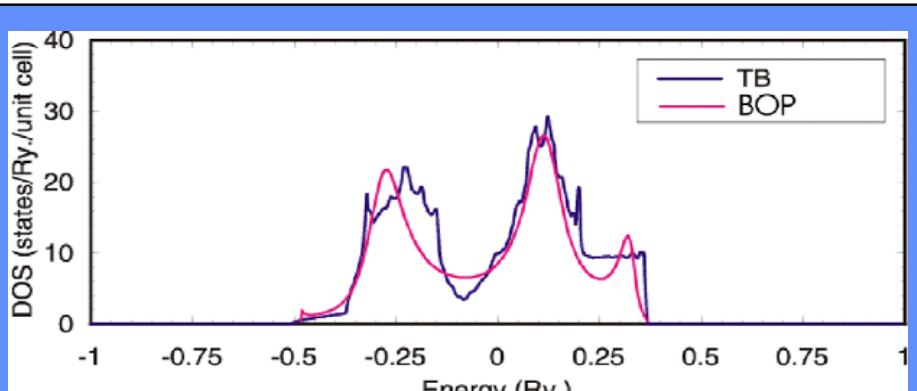
$$\Theta_{i\alpha,j\beta} = -\frac{2}{\pi} \lim_{\eta\to 0} \mathrm{Im} \left\{ \int_{-\infty}^{E_F} G_{i\alpha,j\beta}(E + i\eta)\, dE \right\}$$

using Lanczos algorithm (recursion method)

$$\widehat{H}|U_n\rangle = a_n|U_n\rangle + b_n|U_{n-1}\rangle + b_{n+1}|U_{n+1}\rangle$$

$$G_{i\alpha,i\alpha}(Z) = \cfrac{1}{Z - a_0 + \cfrac{(b_1)^2}{Z - a_1 - \cfrac{(b_2)^2}{Z - a_2 - \cfrac{(b_3)^2}{\ddots}}}}$$

→



bond integrals

radial parts are functions of interatomic distance

angular dependencies given by Slater&Koster

types of bond integrals depend on materials studied

parametrized according to *ab initio* data

Repulsive part

$$E_{rep} = E_{env} + E_{pair}$$

environment-dependent term E_{env}

- captures the s-p orbital overlap repulsion
- introduced to fit the correct Cauchy pressure

pair potential E_{pair}

- represents the electrostatic interaction between atoms and double counting correction

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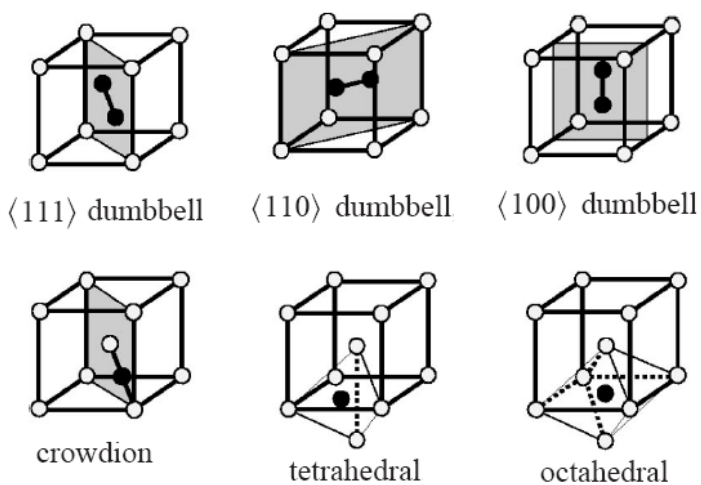
classical atomistic potentials: Second-Moment-Approximation (Finnis-Sinclair) or EAM (Johnson-Oh)

Interstitials in tungsten
Formation energies in eV predicted by various methods



	EAM	***FS***	***BOP***	***MBPP***
<110>	10.55	9.71	9.41	9.87
<111>	11.87	9.02	10.99	10.18
C	12.00	8.99	11.00	
<100>	13.79	9.88	11.91	
O	13.27	10.06	11.99	

Other semi-empirical potentials:

bcc-materials: directional bonding

a) modified embedded atom (Baskes 1991)

or

b) emprirical bond order potentials (Abell-Tersoff-Brenner-Type)

See e.g. Pt-potential of Albe, Nordlund, Averback PRB 65,195124 (2002)

efficiency:

timing:		
	BOP	100000 μs/atom/step
	EAM	30 μs/atom/step
	CM	2 μs/node/step

(tested with Pentium-4 2Ghz)

→ systems sizes: 1 ns MD on 512 CPUs for one day

BOP:	~2000 atoms
EAM:	~10^7 atoms
CM:	~10^8 nodes

conclusion:

hybrid schemes will be important
for future large scale MD simulations of
energetic events in solids

balance between
quantum accuracy ←→
sufficient systems size and statistics

more work has to be done on
QM-order-N-schemes

development of reliable empirical BOPs