Image matching and beyond: tools and techniques

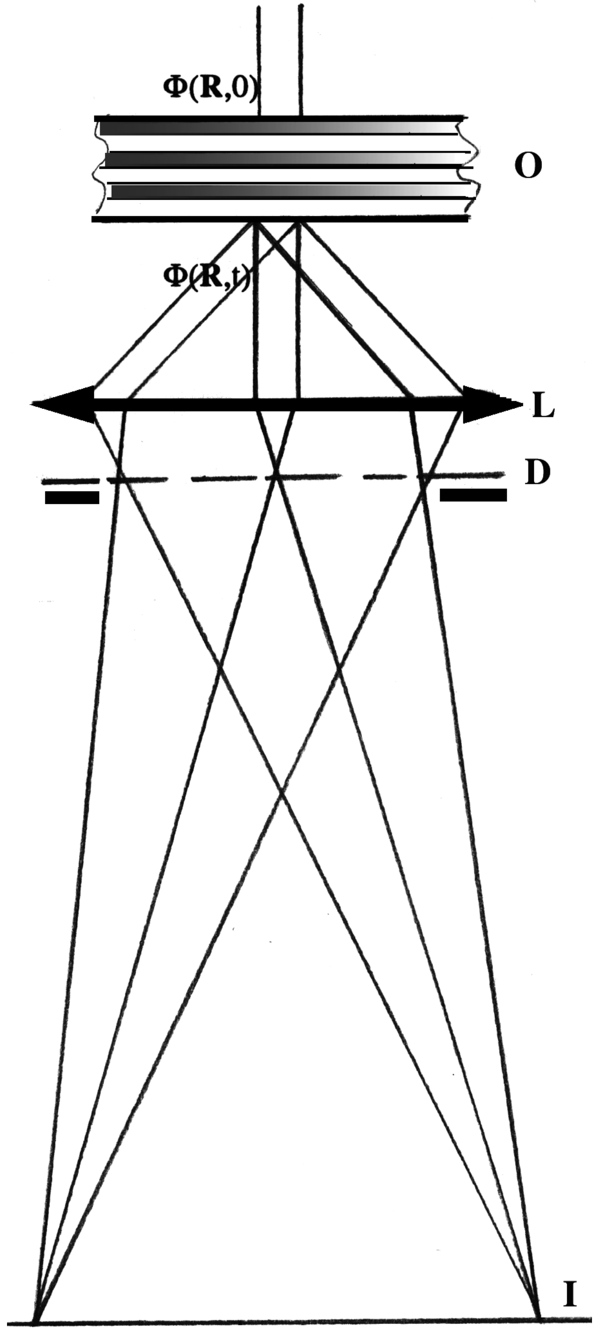
but:

reminiscence
questions
introduction

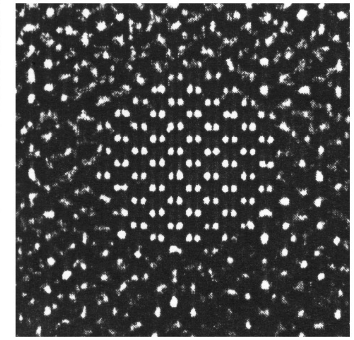
trial-and-error image analysis

1. object modeling
2. wave simulation
3. image process
4. likelihood measure

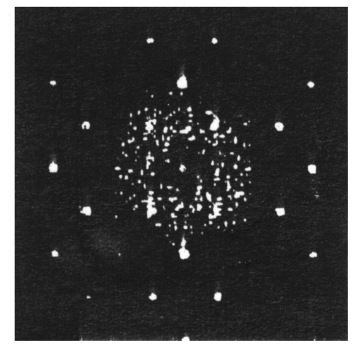
r e p e t i t i o n



Potential

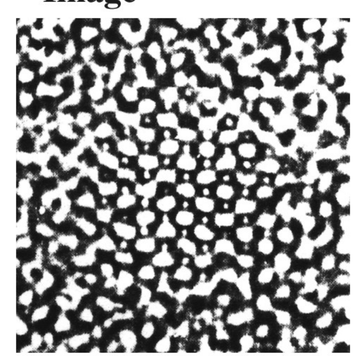


Diffraction



FT FT^{-1}

Image



crystal vs amorphous

elasticity vs defects

dynamical theory (Bloch waves vs plane waves vs multislice) approximations

aberrations

matching & fit criteria (Head: line printer)

ca 1970

Reminiscence - Anniversary

General Theory Cowley, Laue, Howie&Whelan et.al., Wilkens, Takagi, vanDyck, Spence, Rez…....
Hans Bethe, Ann. Phys. 87 (**1928**) 55: Theorie der Beugung von Elektronen an Kristallen

Ernst Lamla, Ann. Phys 32 (**1938**) 178: Zur Theorie der Elektronenbeugung bei Berücksichitgung von mehr als 2 Strahlen und zur Erklärung der Kikuchi-Enveloppen

Simulation & Matching (besides Multi-Slice …...)
P. Humble, Aust.J.Phys 21 (**1968**) 325, Computer generation of electron micrographs of defects in crystals (based on papers of A.K. Head on elasticity theory of dislocations, etc.)

Inverse problem
A.K. Head, Aust.J.Phys 22 (1969) 43: The reconstruction of displacement fields of defects in crystals from electron micrographs (the manuscript received July 24, **1968**)

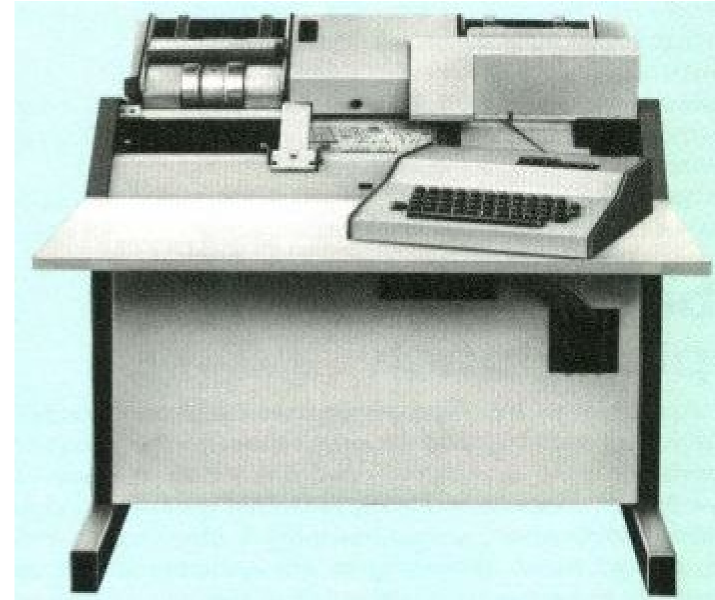
Inelastic scattering Fujimoto, Yoshioka, Kainuma, Moliere, Howie, Kasper, Kohl&Weickenmeier, Wang, Rossouw, Kambe&Lehmpfuhl..….
G. Radi, Z. Physik 212 (**1968**) 146: Unelastische Streuung in der Theorie der Elektronenbeugung

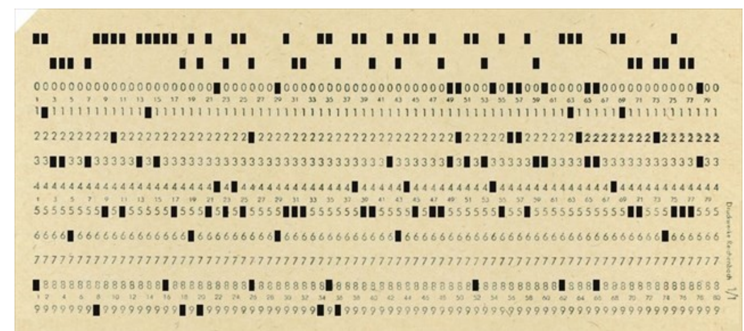
Non-column approximation (3D)
A.Howie, Z.S.Basinski, Phil. Mag. 17 (**1968**) 1039: Approximations of the Dynamical Theory of Diffraction Contrast

K.Scheerschmidt, S.Carl, Kristall und Technik 13 (**1978**) 1131: Anwendung der Riemannschen Integrationsmethode auf Beugungsprobleme in Blochwellendarstellung

N.V.Berry, N.L.Balazs, J.Phys.A:Math.Gen 12 (1979) 625: Evolution of semiclassical quantum states in phases space (manuscript September **1978** finishing 10-years work M.V.Berry, J.Phys.C 4 (1971) 697: Diffraction in crystals at high energies)

DESY Hamburg & Zeuthen
AdW Institute of High Energy Physics



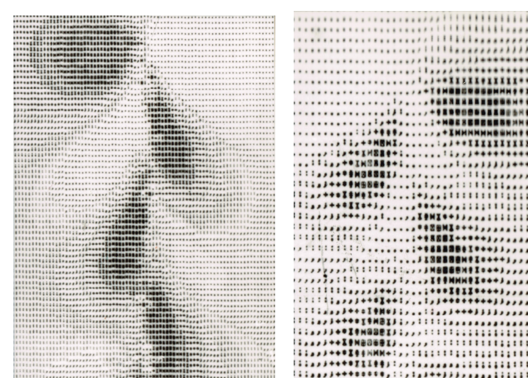


BESM-6 (1967)

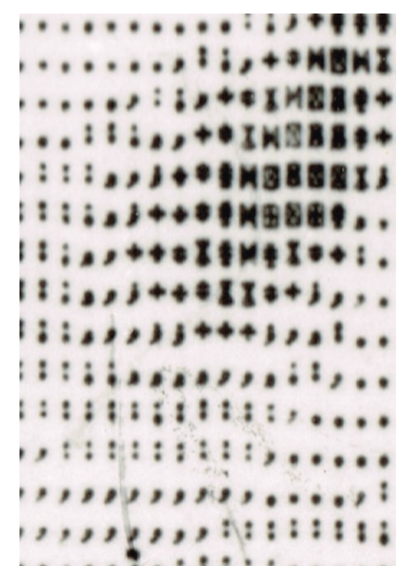
Большая Электронно-Счётная Машина

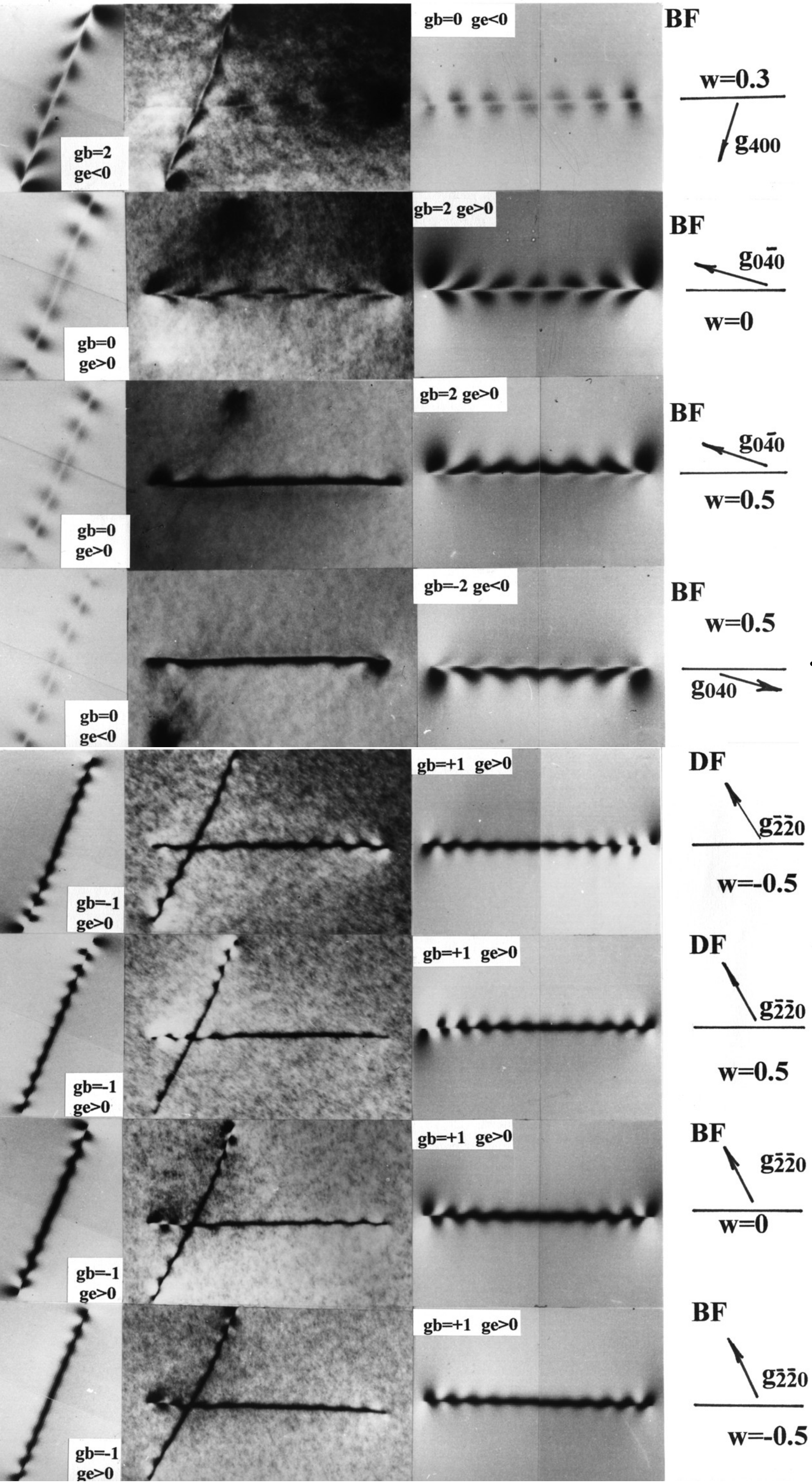
Performance	About 1 MIPS (MFLOPS)
Clock frequency	9 MHz
Element base	60,000 transistors
	170,000 diodes
Word size	48 bits
Address size	15 bits
Addressable memory	192 Kb

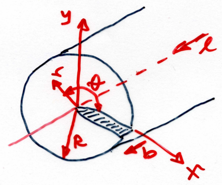
Pipelined CPU, Virtual addressing, Printer output, Magnetic tapes and drum storage, Punch card



Dislocation diffraction contrast:
Edge 10 degr — Screw-Pair 45 degr 0.1Ext.







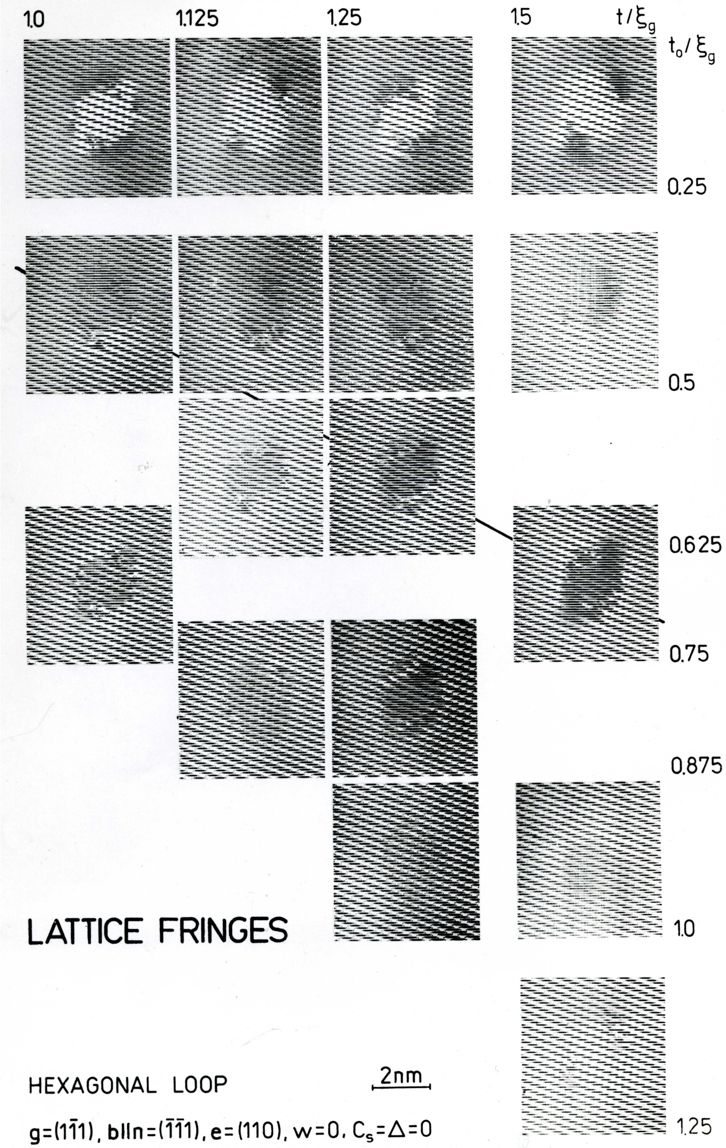
$$\lim_{\substack{\varepsilon \to 0 \\ x>0}} \left[u_z(x,-\varepsilon) - u_z(x,\varepsilon)\right] = b$$

$$u_z(r,\theta) = b\frac{\theta}{2\pi} = \frac{b}{2\pi}\arctan\frac{y}{x}$$

$$u_x = u_y = 0$$

Simulation of Diffraction Contrast & Lattice Fringe Images of Dislocation Structures

- Continuum Elasticity
- Deformable Ion Approximation of the Crystal Potential



Rigid ion approximation

$$V(\vec{r}) = \sum_n v_n\left(\vec{r} - \vec{r}_n - \vec{u}(\vec{r}_n)\right)$$

Deformable ion approximation

$$V(\vec{r}) = V^0\left(\vec{r} - \vec{u}(\vec{r})\right)$$

$$\rightarrow V_g = V_g^0\, e^{-2\pi i \vec{g}\vec{u}(\vec{r})}$$

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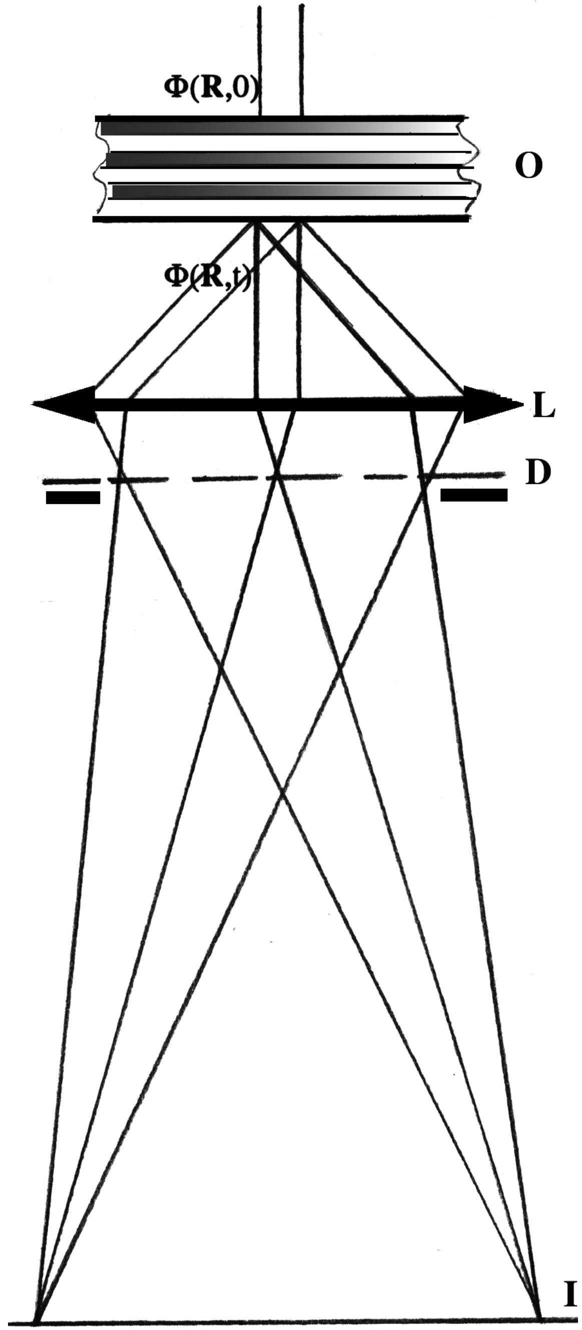
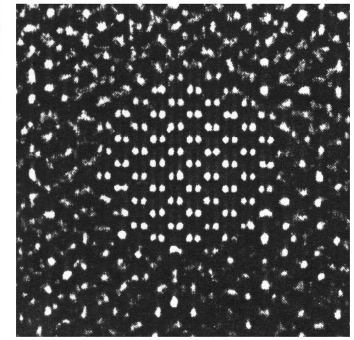
repetition

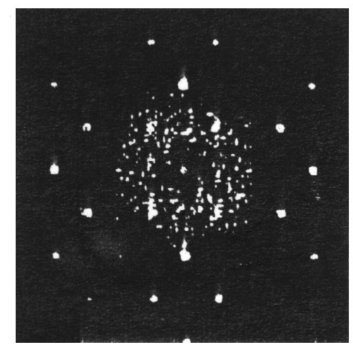


Potential



MD structure modeling,
DFT scattering potentials

Diffraction

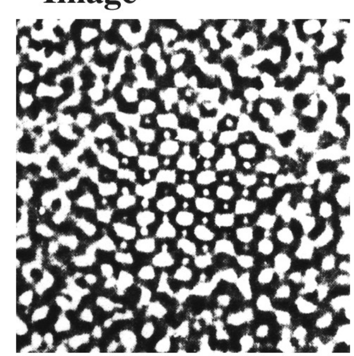


dynamical theory
„weak phase approx. will make us blind“
scattering factors vs electron density
inelastic vs absorption

FT ↕ FT^{-1}

measurements:
aberrations, thickness, orientation, tilt, bending, adsorbates, composition, defects, surface structure

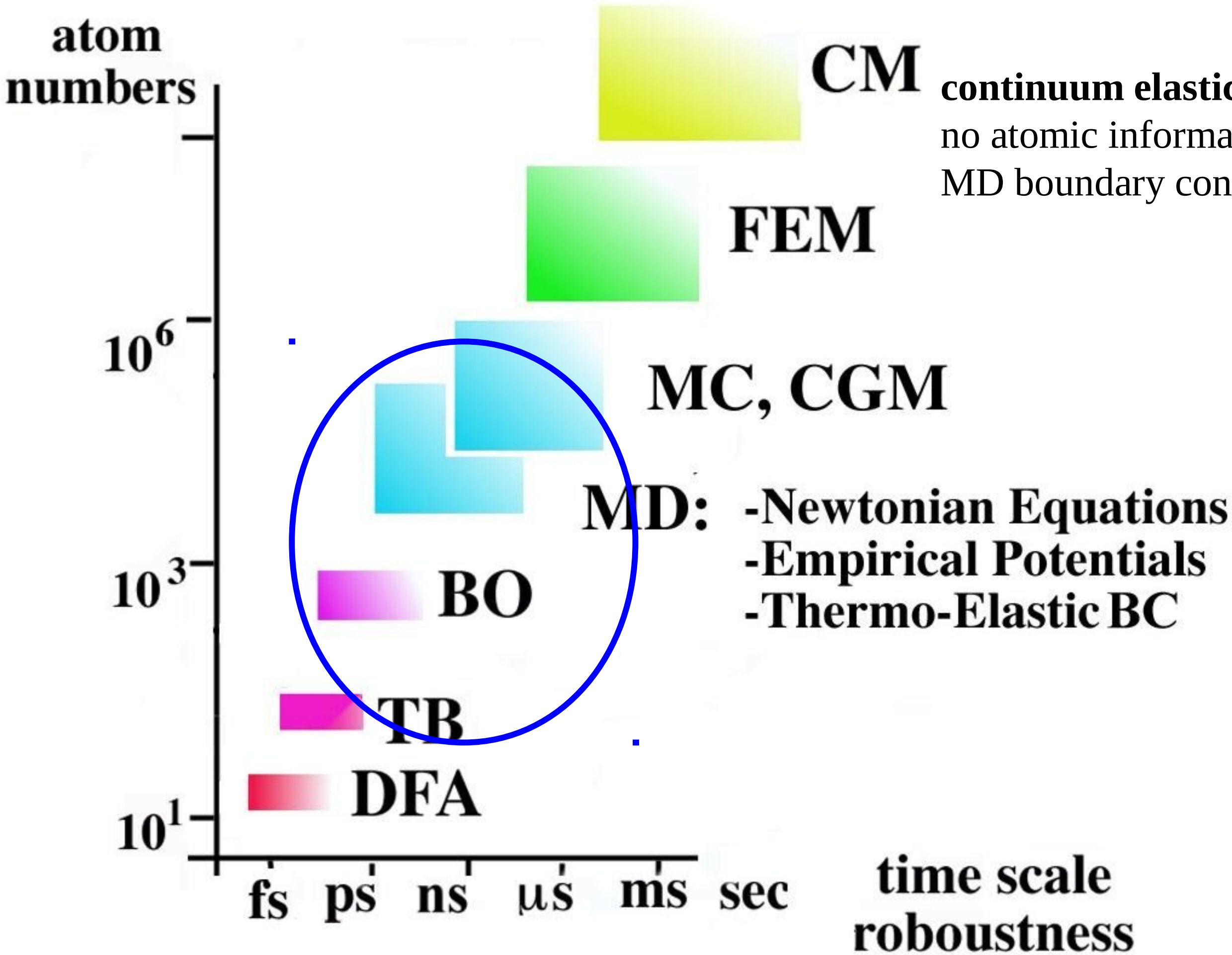
Image



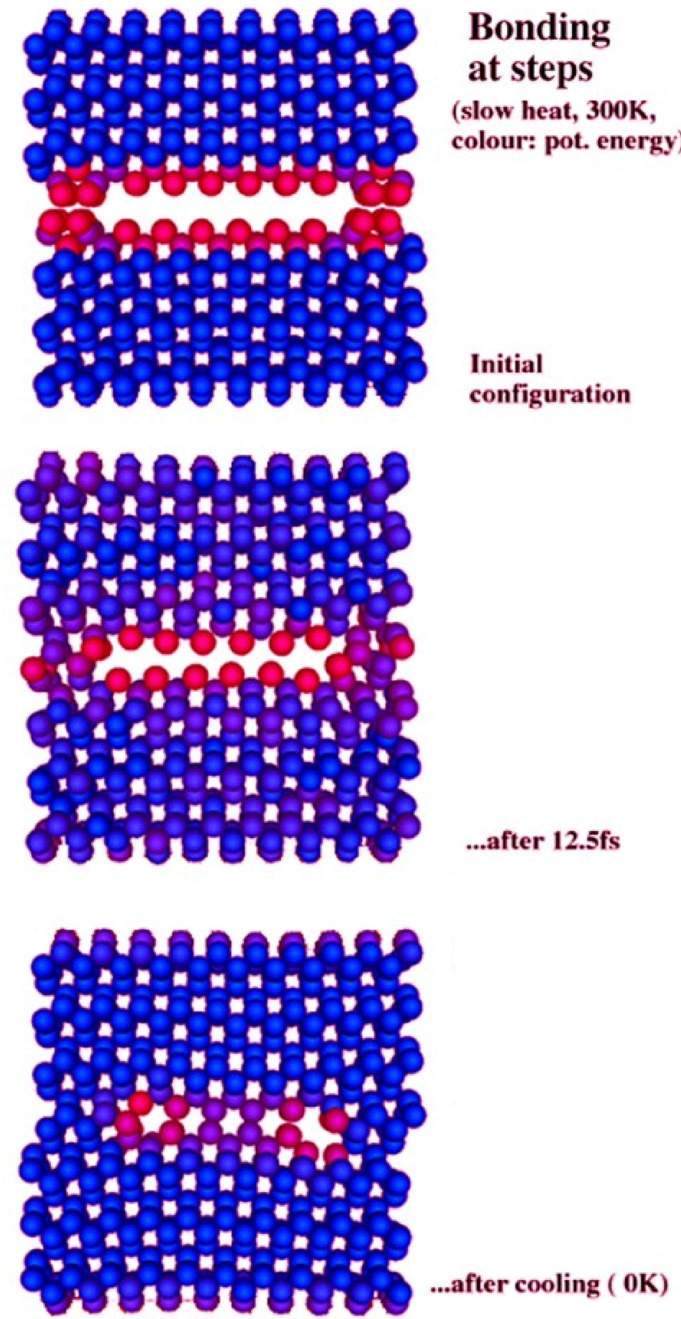
matching & fit criteria
Stobbs factor

ca 1990

empirical MD: macroscopic relevance



continuum elasticity:
no atomic information -
MD boundary condition

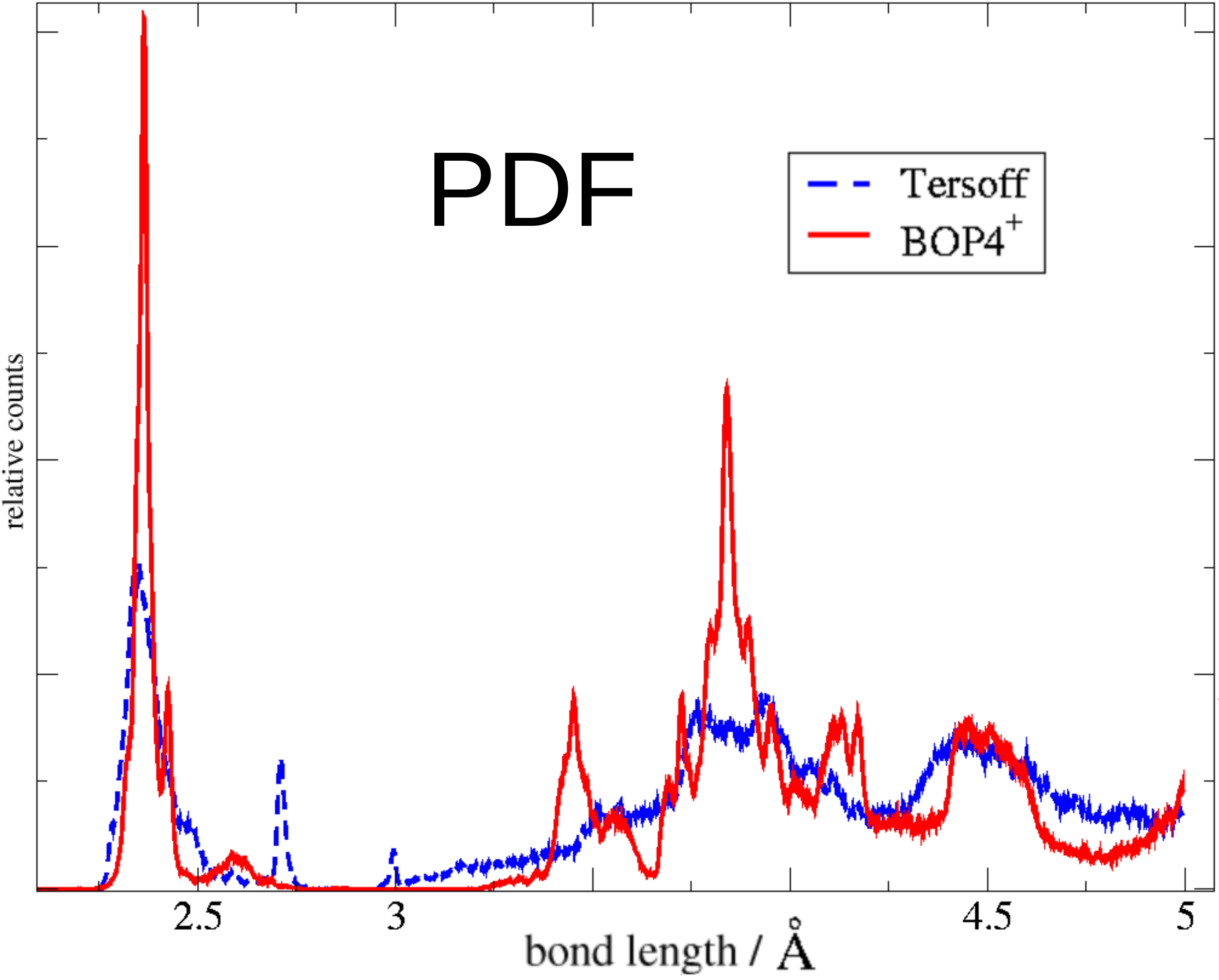


ab initio ~ 100 atoms
parameter free all electron
or pseudopotentials

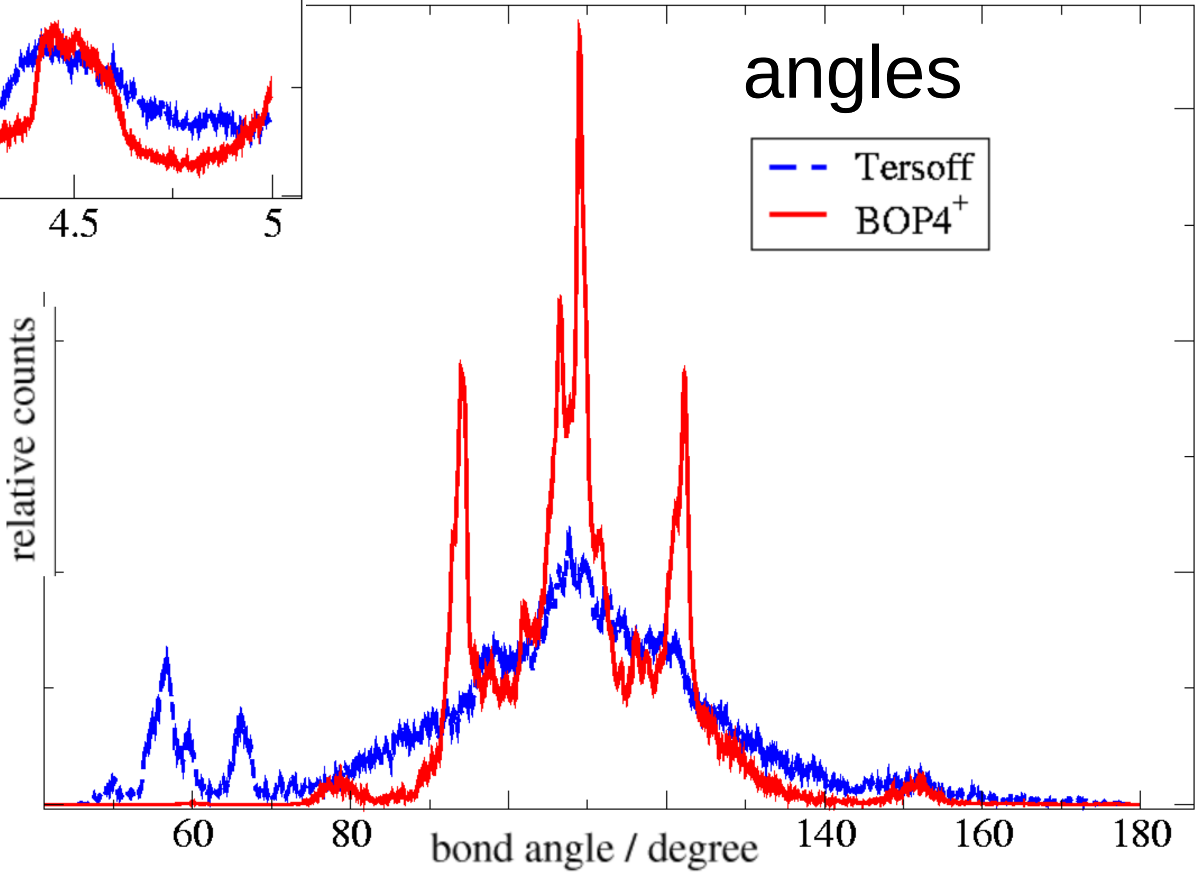
tight-binding ~ 1000 atoms
wavefunction =Σ atomic orbitals,
TB-Hamilton ssσ, spσ, ppσ, ppπ, ...

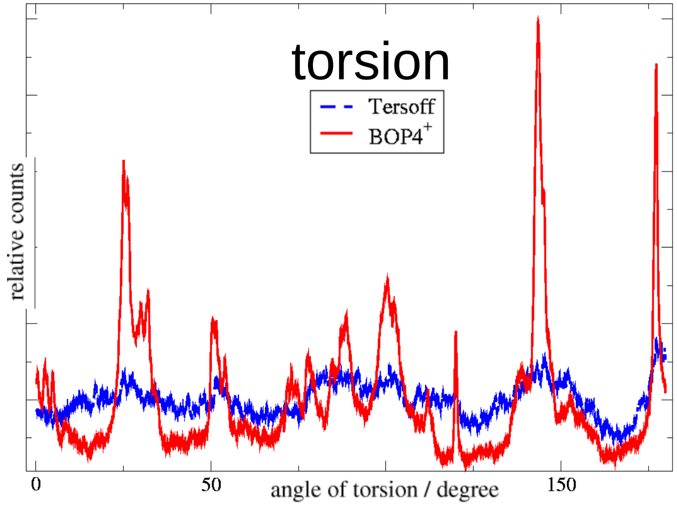
Bond Order Potential

$$U^{i,j}_{bond} = 2\sum_{\alpha,\beta} H_{i\alpha,j\beta}\Theta_{j\beta,i\alpha}$$

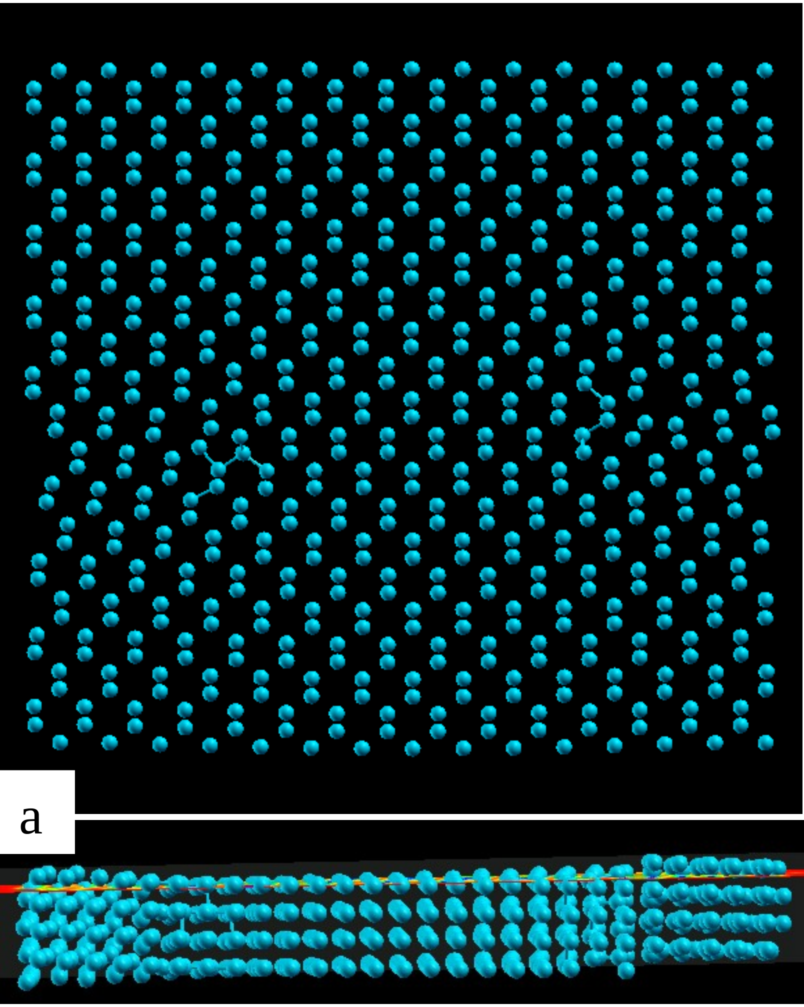


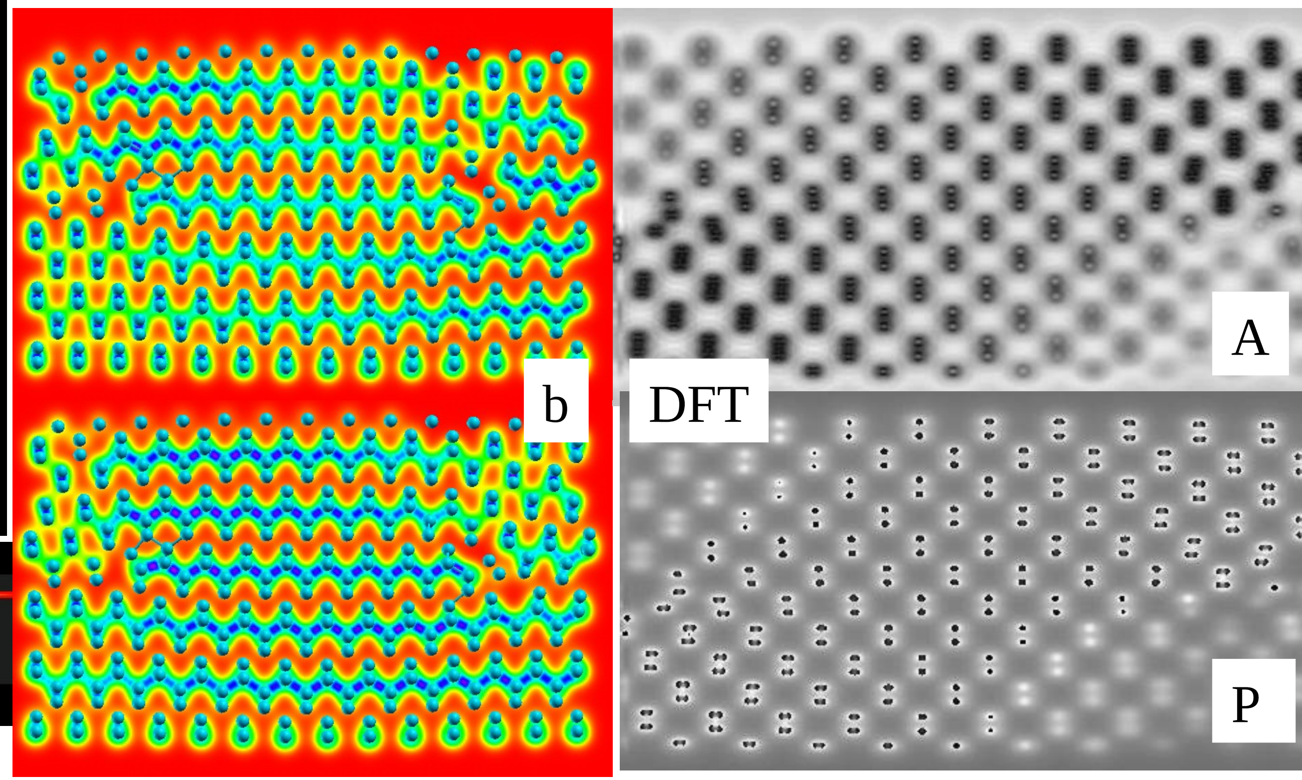
Distribution of pair distances, angles and torsions at the 1.4^o twist bonded Si-001 interface comparing Tersoff and BOP4+ potentials after annealing at 900K

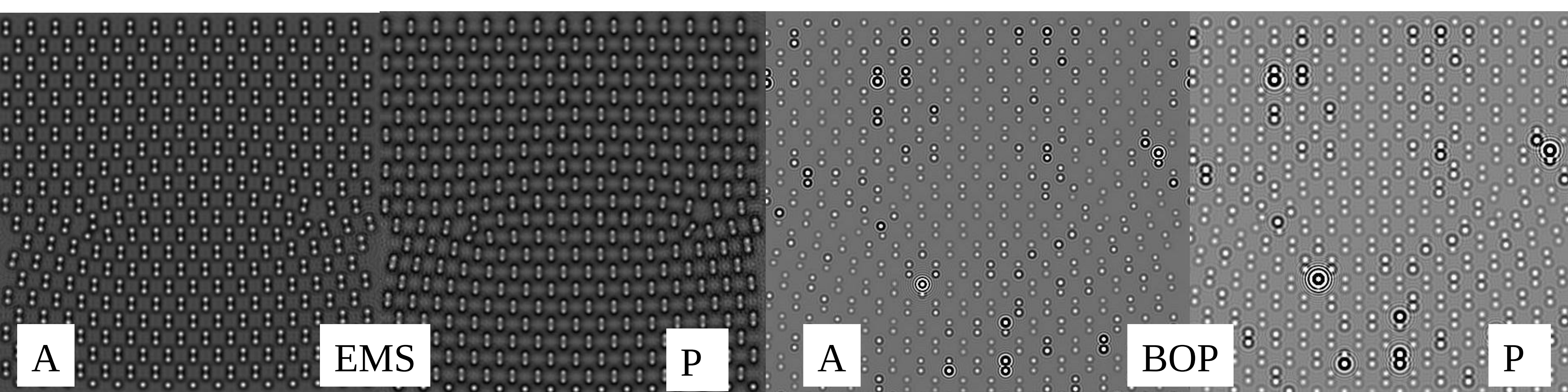


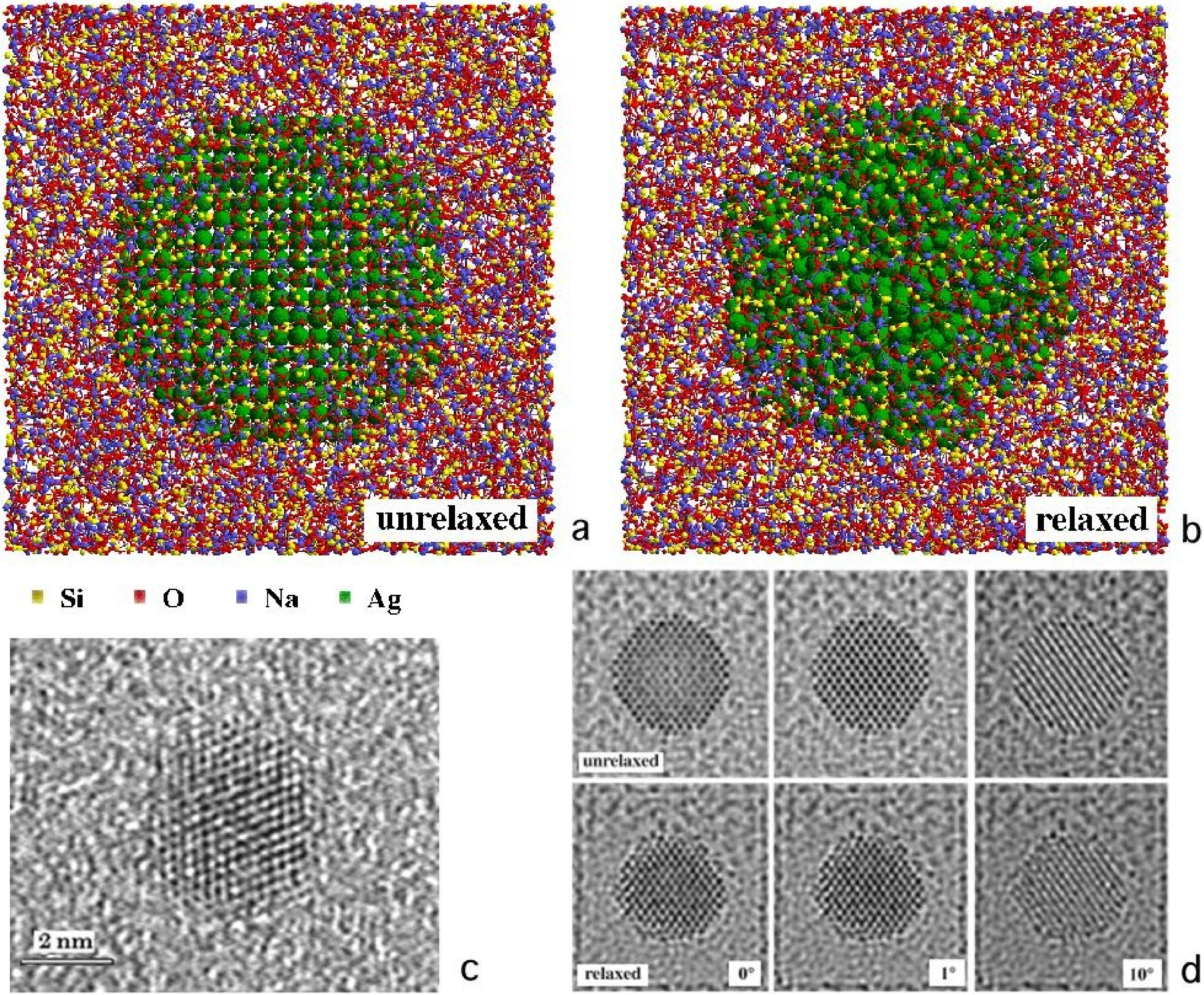


Dislocation dipole in 110-Si: BOP optimized structure (a), charge density (b), and simulated exit waves (amplitude A, phase P) for DFT, standard EMS potentials, and sampled BOP of 16 subslices (200kV, thickness=18.4nm).








unrelaxed
a
relaxed
b
Si
O
Na
Ag
2 nm
c
unrelaxed
relaxed
0°
1°
10°
d

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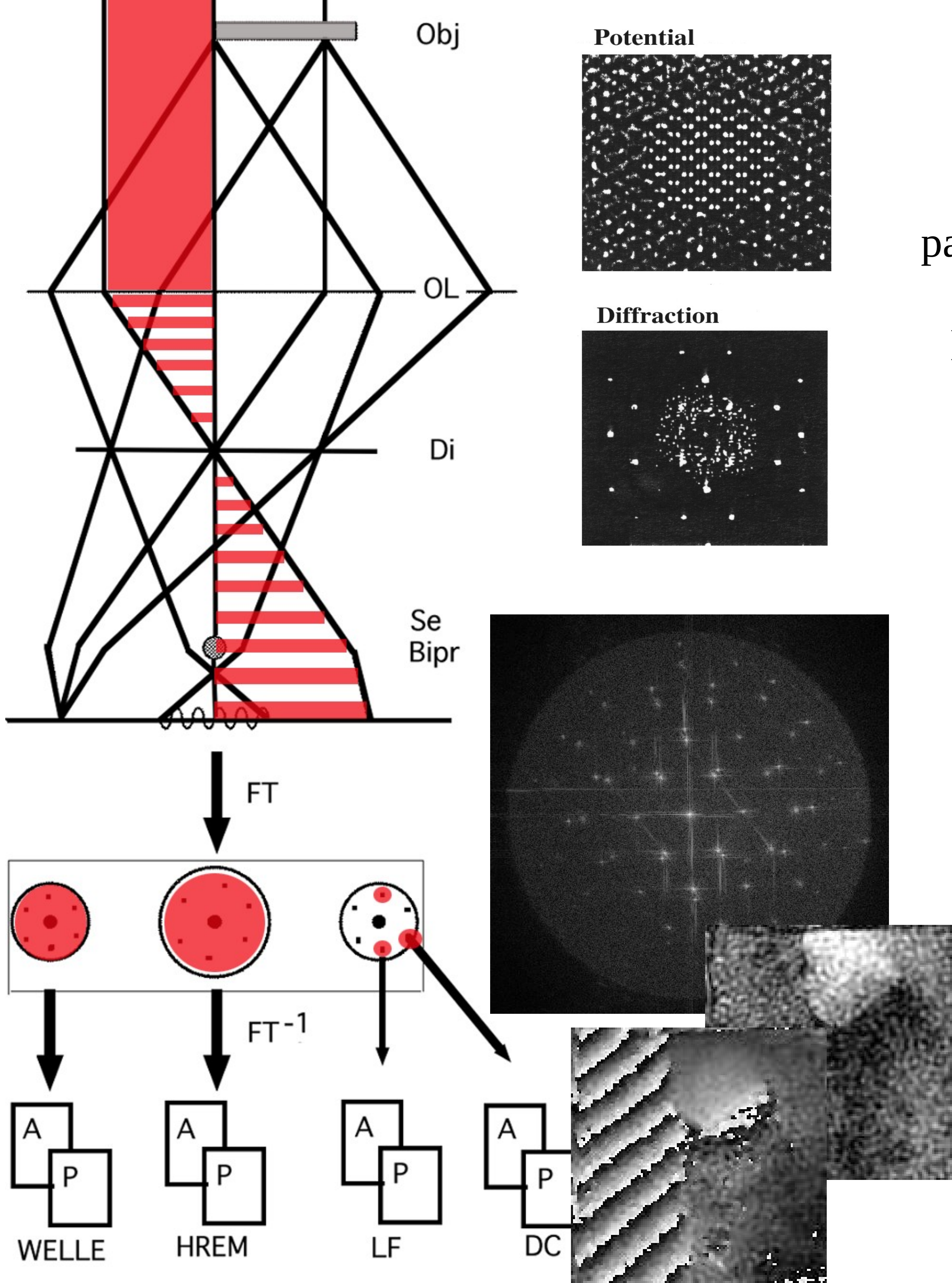


direct object reconstruction

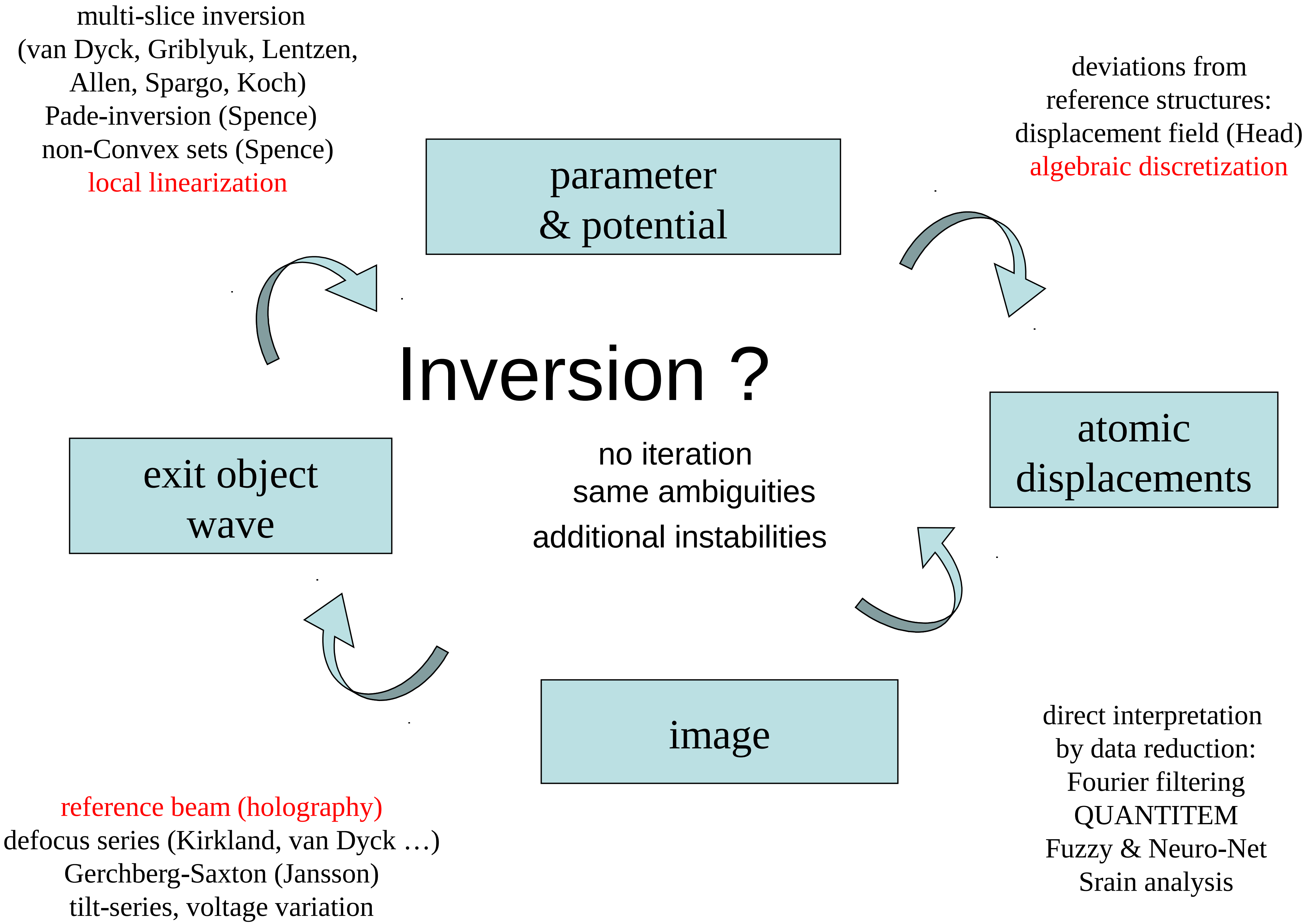
parameter & potential reconstruction
local measurements
3D info
regularization

?

wave reconstruction

?

amplitude & phase image


multi-slice inversion
(van Dyck, Griblyuk, Lentzen,
Allen, Spargo, Koch)
Pade-inversion (Spence)
non-Convex sets (Spence)
local linearization
parameter
& potential
deviations from
reference structures:
displacement field (Head)
algebraic discretization
Inversion ?
no iteration
same ambiguities
additional instabilities
exit object
wave
atomic
displacements
image
reference beam (holography)
defocus series (Kirkland, van Dyck …)
Gerchberg-Saxton (Jansson)
tilt-series, voltage variation
direct interpretation
by data reduction:
Fourier filtering
QUANTITEM
Fuzzy & Neuro-Net
Srain analysis