Property calculation and interatomic potentials

Lecture 5

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Content overview

I. Fundamentals of particle methods   Lectures 1-12

1.   Atoms, molecules, chemistry   February/March
2.   Statistical mechanics
3.   Molecular dynamics, Monte Carlo
4.   Visualization and data analysis
5.   Mechanical properties – application: how things fail (and how to prevent it)
6.   Multi-scale modeling paradigm
7.   Biological systems (simulation in biophysics) – how proteins work and how to model them

II. Advanced topics in particle methods

1.   Quantum Weirdness: The Theory of Quantum Mechanics   Lectures 13-24
2.   The Many-Body Problem: From Many-Body to Single-Particle March/April/May
3.   Quantum modeling of materials
4.   From Atoms to Solids
5.   Basic properties of materials
6.   Advanced properties of materials
7.   Materials Informatics

Lecture 5: Property calculation and interatomic potentials

Outline:

1. Advanced analysis methods: Radial distribution function (RDF)

2. How to model chemical interactions

    2.1 Pair potentials & examples

Goals of today's lecture:

- Advanced analysis method (making sense of atomistic data)
- Modeling atomic interactions
- Examples for simulations of work hardening (plastic deformation of metals, etc.)

Brief review – Monte Carlo (Metropolis Hastings)

Monte Carlo scheme for integration

- **Step 1**: Pick random point $\overset{\rho}{x}_i$ in Ω
- **Step 2**: Accept/reject point based on criterion (e.g. if inside or outside of circle and if in area not yet counted)
- **Step 3**: If accepted, add $f(\overset{\rho}{x}_i) = 1$ to the total sum

length r=1
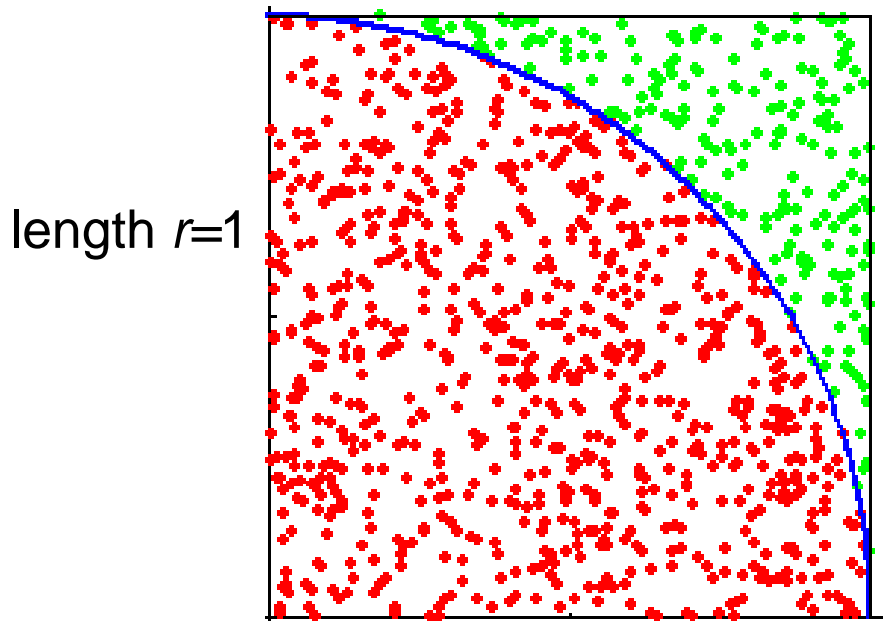
$$A_C = \int_\Omega f(\overset{\rho}{x}) d\Omega \qquad A_C = \frac{\pi}{16}$$

$$A_C = \frac{1}{N_A} \sum_i f(\overset{\rho}{x}_i)$$

N_A: Attempts made

Metropolis-Hastings Algorithm: *NVT*

Have: State A (initial state) + energy function $H(A)$

Step 1:   Generate new state B (random move)

Step 2:   if $H(B)<H(A)$ then $a = 1$ $a =$ true[1]/false[0]
                                                                      for acceptance

        else

                Draw random number $0 < p < 1$

                if $p < \exp\left[-\dfrac{H(B)-H(A)}{k_B T}\right]$ $a = 1$

                else

                        $a = 0$

                endif $a=$variable either 0 or 1
                                                (used to detect acceptance
        endif   of state B when $a=1$)

Step 3:   if $a = 1$ **then accept state B**

        endif

repeat N_A times

$$<A> = \frac{1}{N_A}\sum_{i=1..N_A} A(i)$$

1. Advanced analysis methods: Radial distribution function (RDF)

Goals

- ***Define algorithms that enable us to "make sense" of positions, velocities etc. and time histories to relate with experimentally measurable quantities***

- So far: temperature, MSD (mean square displacement function)

- Here: extend towards other properties

MD modeling of crystals – solid, liquid, gas phase

- Crystals: Regular, ordered structure

- The corresponding particle motions are small-amplitude vibrations about the lattice site, diffusive movements over a local region, and long free flights interrupted by a collision every now and then.

- Liquids: Particles follow Brownian motion (collisions)

- Gas: Very long free paths

J. A. Barker and D. Henderson, Scientific American, 1981
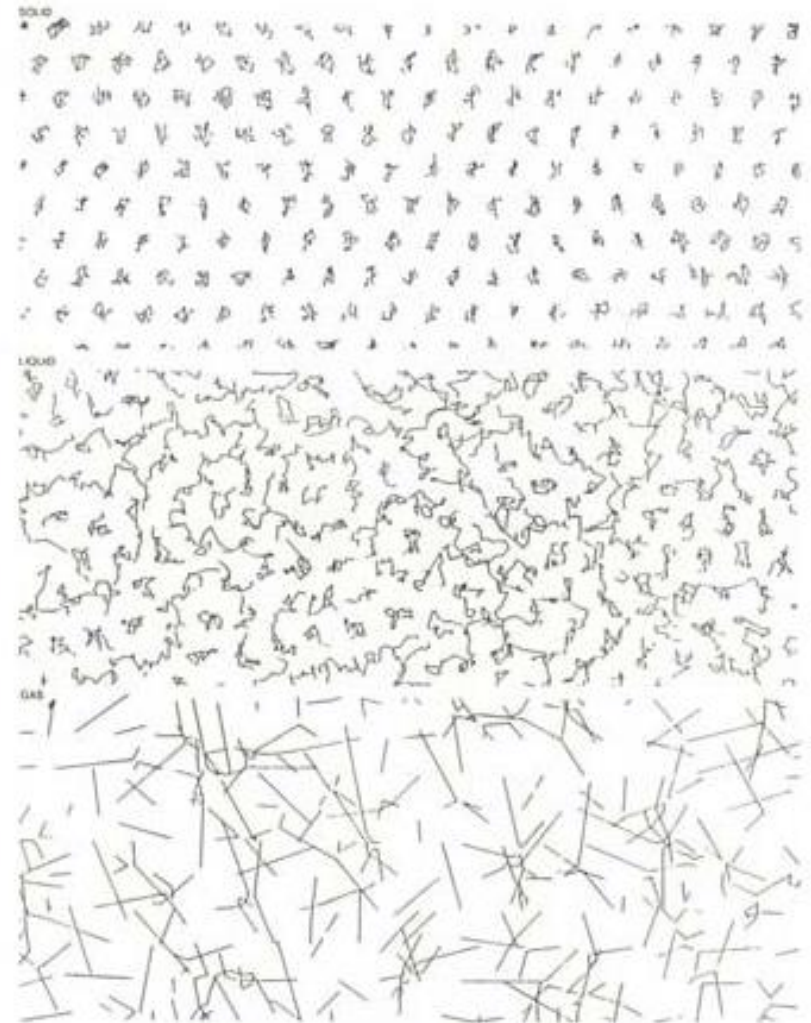
Atomistic trajectory – through MSD
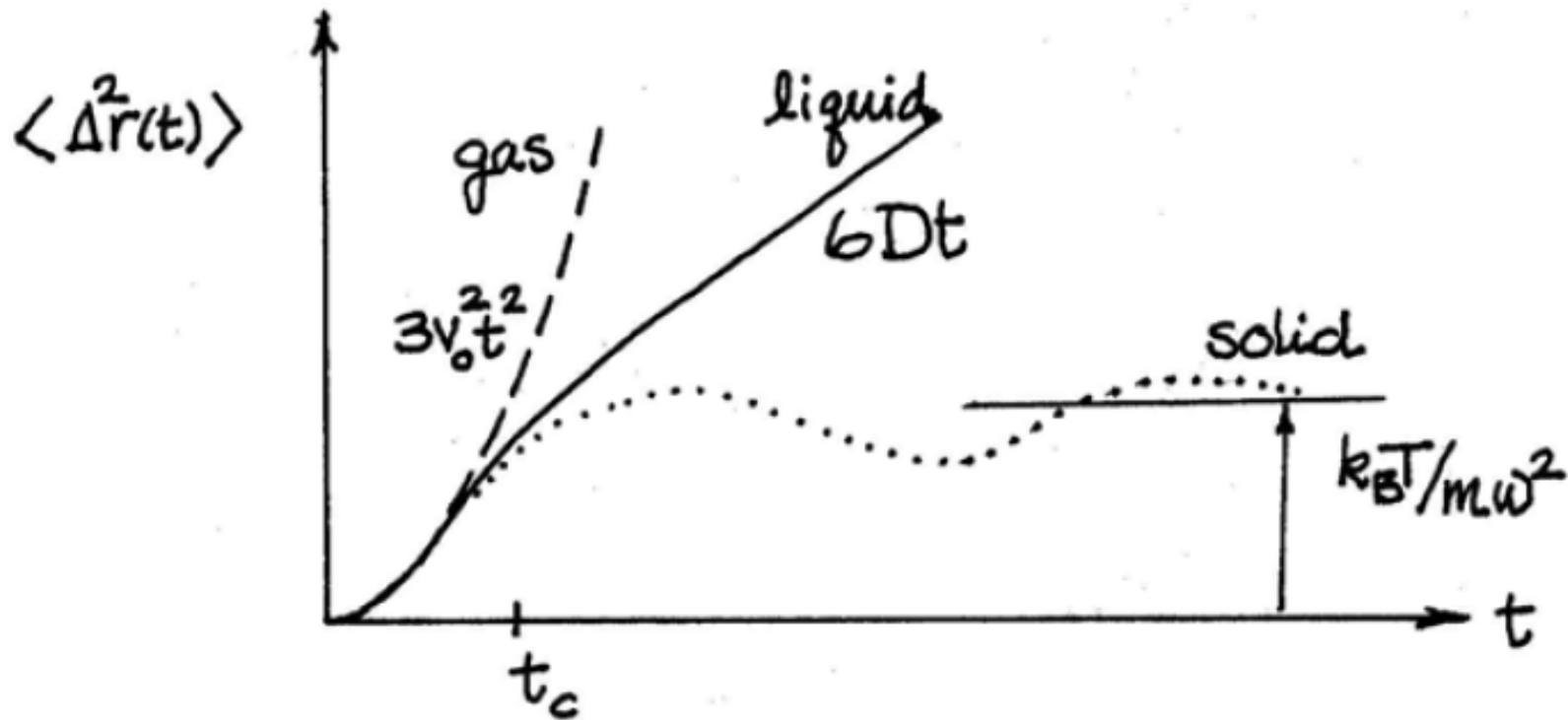
source: S. Yip, lecture notes

Need **positions over time** – **what if not available?**

How to characterize material state (solid, liquid, gas)

- Application: Simulate phase transformation (melting)
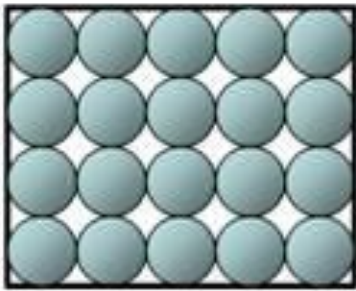
Solid State
Ordered and dense
Has a definite
shape and volume.
Solids are very slightly
compressible.
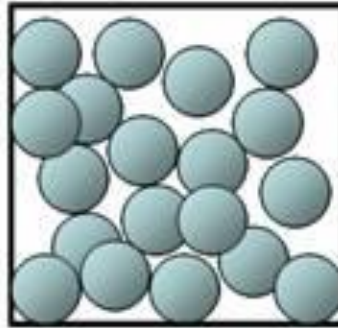
Liquid State
Disordered and usually
slightly less dense.
Has a definite volume
and takes the shape of
the container.
Liquids are slightly
compressible.
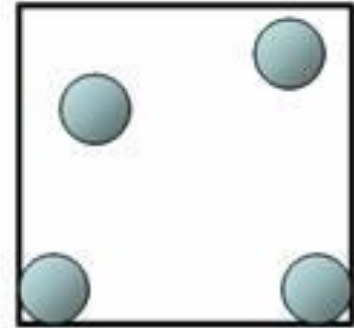
Gas State
Disordered and
much lower density
than crystal or liquid.
Does not have
definite shape and
volume.
Gases are highly
compressible.

How to characterize material state (solid, liquid, gas)
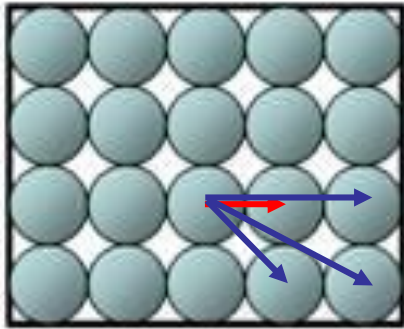
Regular spacing

Neighboring particles found at characteristic distances
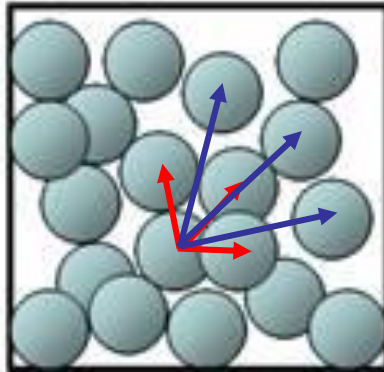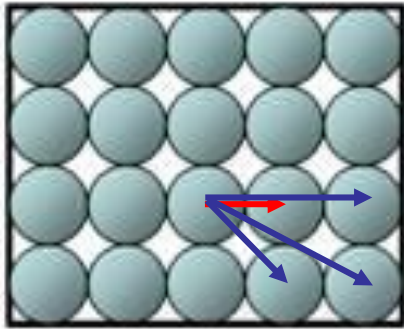
Irregular spacing

Neighboring particles found at approximate distances (smooth variation)
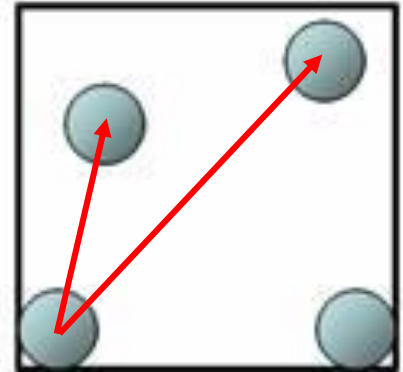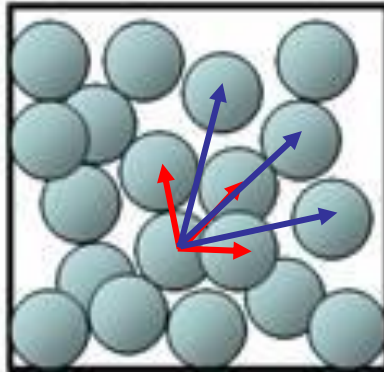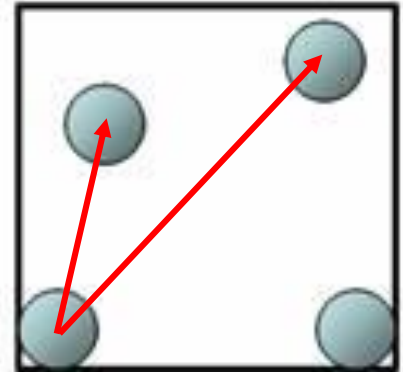
More irregular spacing

More random distances, less defined

How to characterize material state (solid, liquid, gas)

Regular spacing

Neighboring particles found at characteristic distances

Irregular spacing

Neighboring particles found at approximate distances (smooth variation)

More irregular spacing

More random distances, less defined

Concept:

- Measure distance of particles to their neighbors
- Average over large number of particles
- Average over time (MD) or iterations (MC)

Formal approach: Radial distribution function (RDF)

Ratio of density of atoms at distance r (in control area dr) by overall density = relative density of atoms as function of radius

$$g(r) = \rho(r) / \rho$$

Reference atom

r
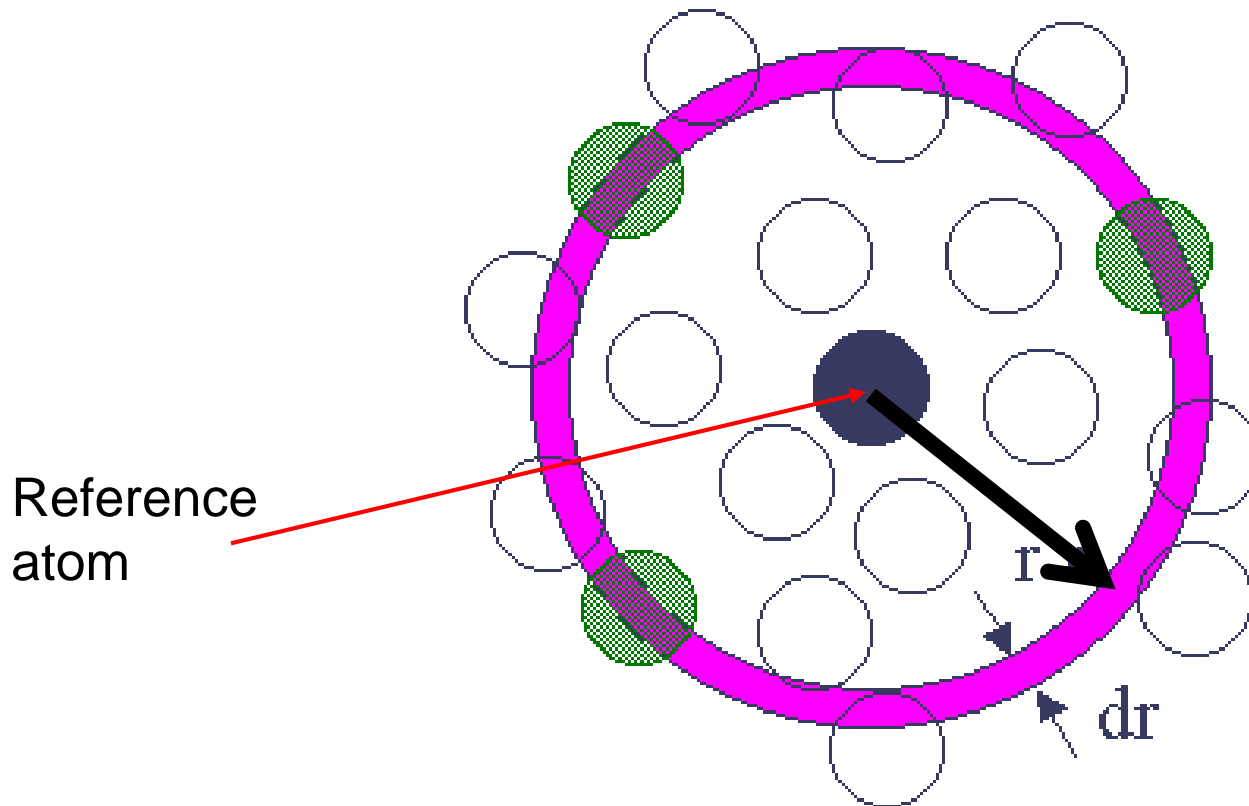
dr

Formal approach: Radial distribution function (RDF)

The radial distribution function is defined as

Overall density of atoms (volume)

$$g(r) = \rho(r) / \rho$$

Local density

Provides information about the density of atoms at a given radius r; $\rho(r)$ is the local density of atoms

Formal approach: Radial distribution function (RDF)

The radial distribution function is defined as

Overall density of atoms (volume)

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Local density

Provides information about the density of atoms at a given radius r; $\rho(r)$ is the local density of atoms

Discrete: Number of atoms in the interval $r \pm \frac{\Delta r}{2}$

$$g(r) = \frac{< N(r \pm \frac{\Delta r}{2}) >}{\Omega(r \pm \frac{\Delta r}{2})} \frac{1}{\rho}$$

Volume of this shell (dr)

$g(r)2\pi r^2 dr =$ Number of particles that lie in a spherical shell of radius r and thickness dr

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Radial distribution function

$$\Omega(r \pm \tfrac{\Delta r}{2}) \quad \text{considered volume}$$

$$\frac{\Delta r}{2}$$

$$\frac{\Delta r}{2}$$
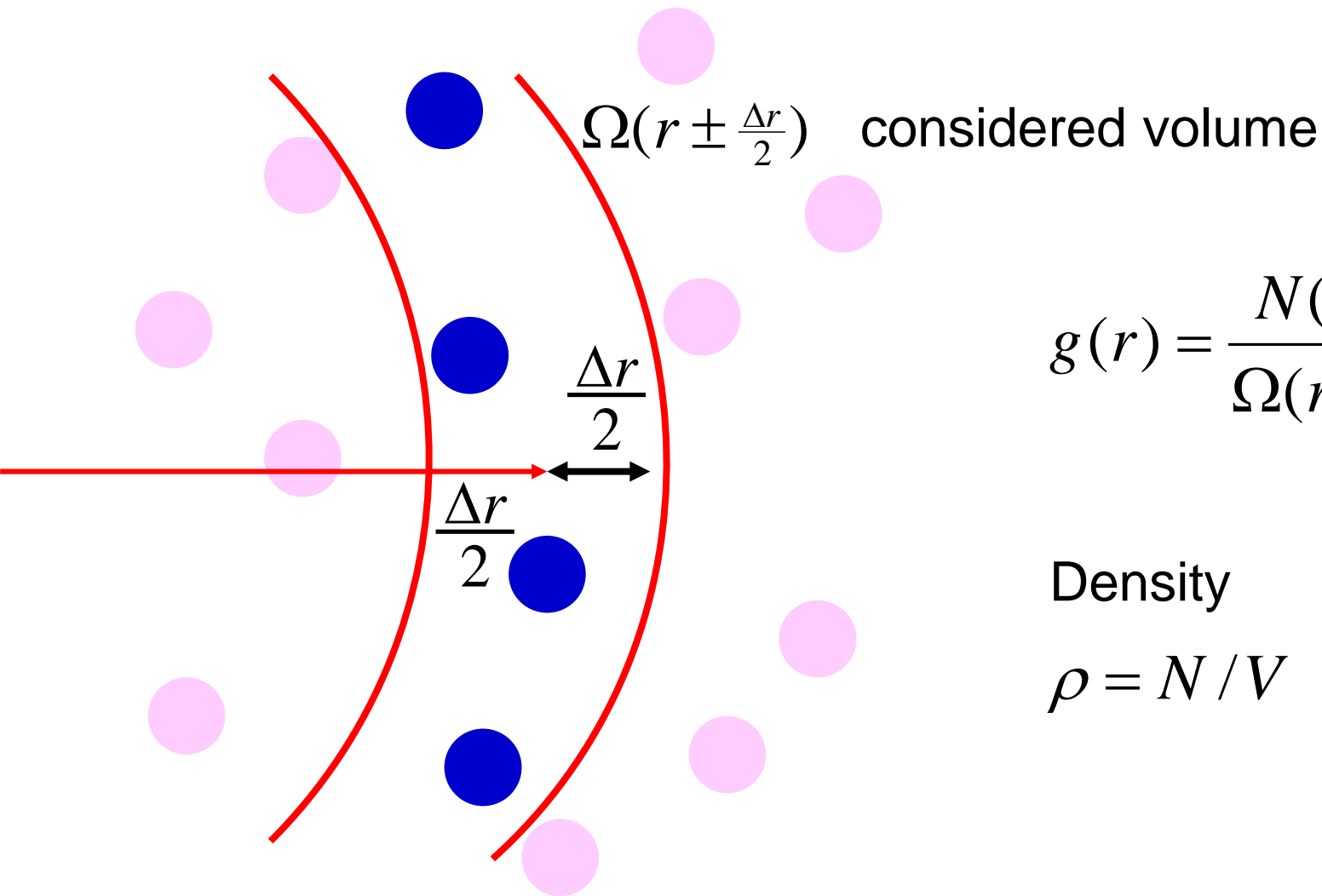
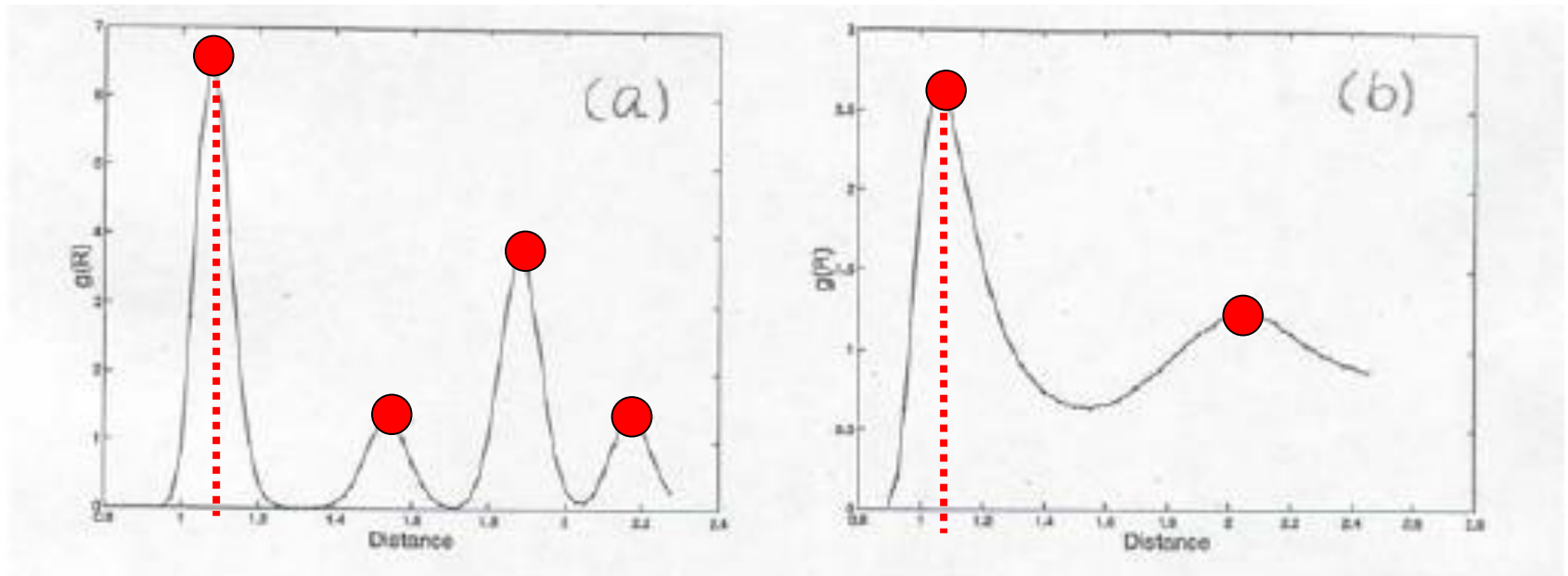$$g(r) = \frac{N(r \pm \tfrac{\Delta r}{2})}{\Omega(r \pm \tfrac{\Delta r}{2})\rho}$$

Density

$$\rho = N/V$$

Note: RDF can be measured experimentally using x-ray or neutron-scattering techniques

Radial distribution function:
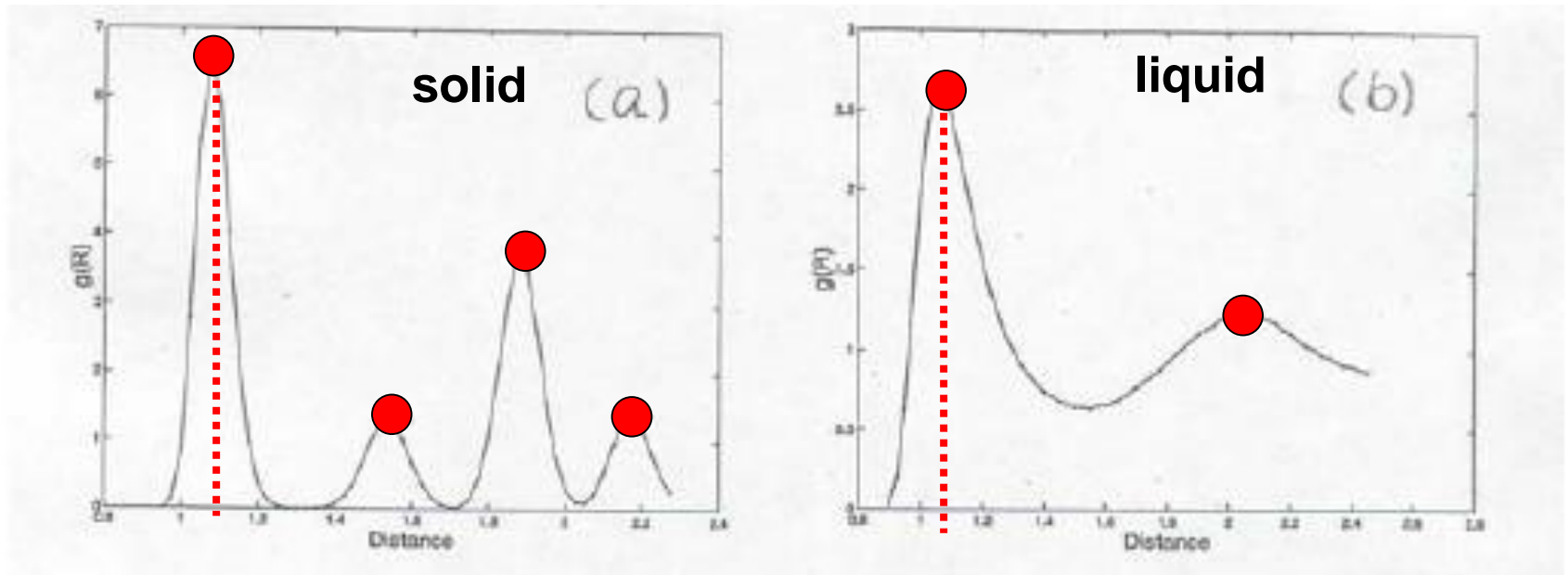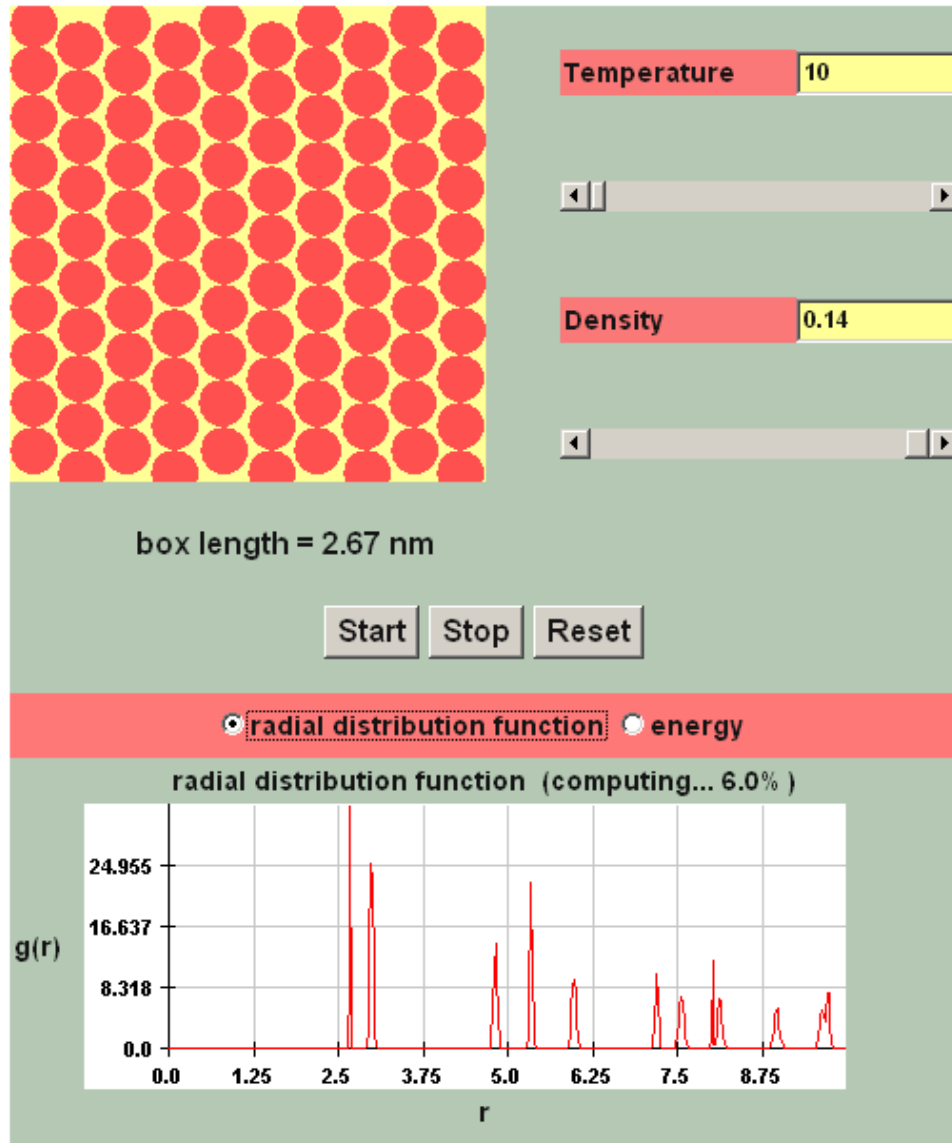# **Which one is solid / liquid?**

Interpretation: A peak indicates a particularly favored separation distance for the neighbors to a given particle
Thus, RDF reveals details about the atomic structure of the system being simulated

Java applet:
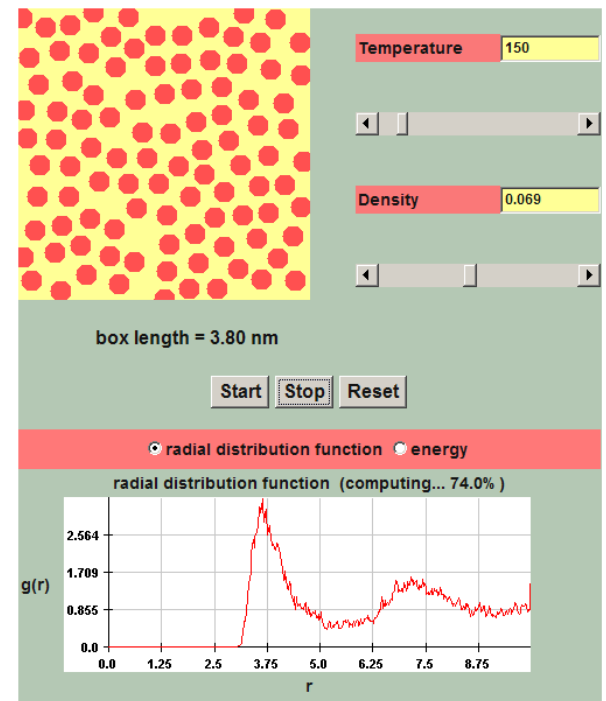http://physchem.ox.ac.uk/~rkt/lectures/liqsolns/liquids.html

Radial distribution function

Interpretation: A peak indicates a particularly favored separation distance for the neighbors to a given particle Thus, RDF reveals details about the atomic structure of the system being simulated

Java applet:
http://physchem.ox.ac.uk/~rkt/lectures/liqsolns/liquids.html

Radial distribution function: JAVA applet

Java applet:

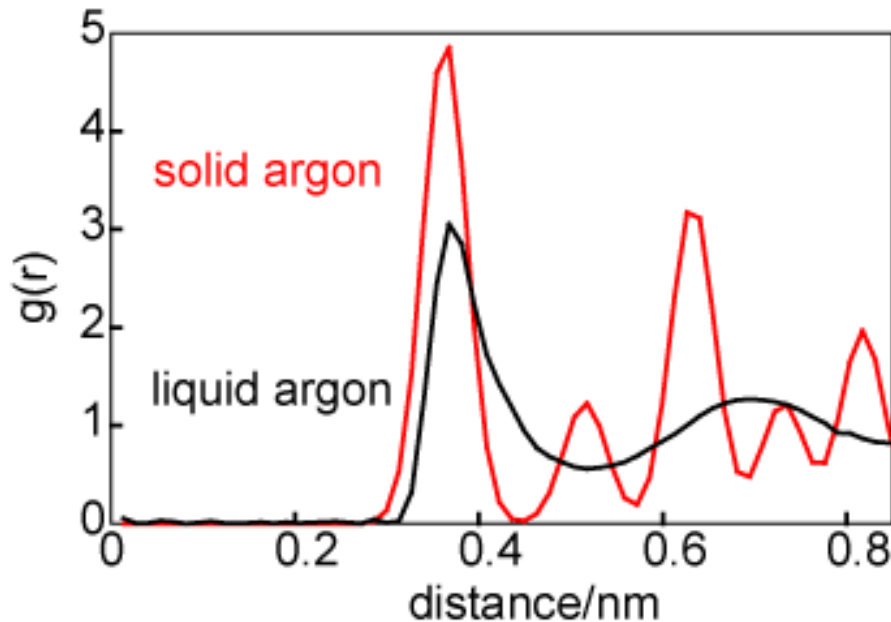http://physchem.ox.ac.uk/~rkt/lectures/liqsolns/liquids.html

Radial distribution function:
Solid versus liquid versus gas
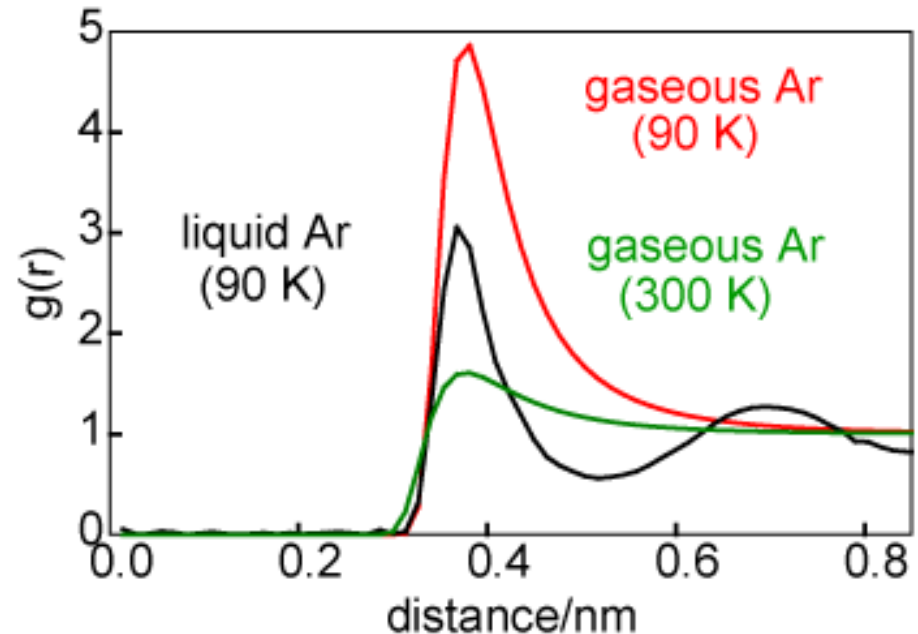
Note: The first peak corresponds to the nearest neighbor shell, the second peak to the second nearest neighbor shell, etc.

In FCC: 12, 6, 24, and 12 in first four shells

Notes: Radial distribution function (RDF)

- Pair correlation function (consider only pairs of atoms)
- Provides structural information
- Can provide information about dynamical change of structure, but not about transport properties (how fast atoms move)

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- Pair correlation function (consider only pairs of atoms)
- Provides structural information
- Can provide information about dynamical change of structure, but not about transport properties (how fast atoms move)

Additional comments:

- Describes how - on average - atoms in a system are radially packed around each other
- Particularly effective way of describing the structure of disordered molecular systems (liquids)
- In liquids there is continual movement of the atoms and a single snapshot of the system shows only the instantaneous disorder it is extremely useful to be able to deal with the average structure
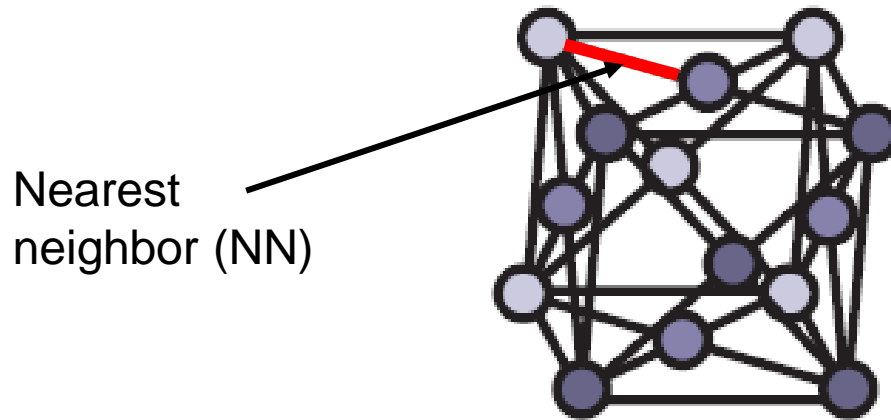
Example RDFs for different materials

RDF and crystal structure
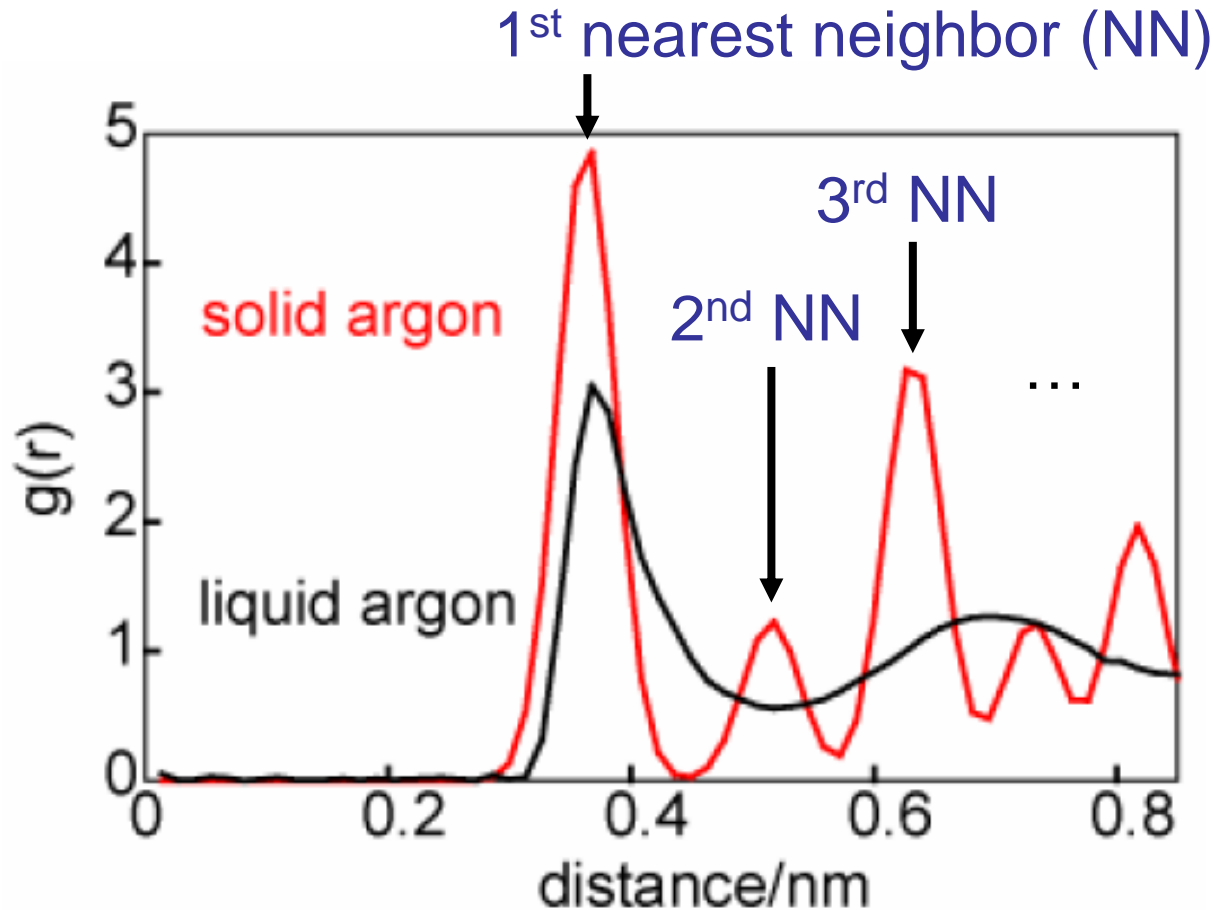
*Peaks in RDF characterize NN distance,
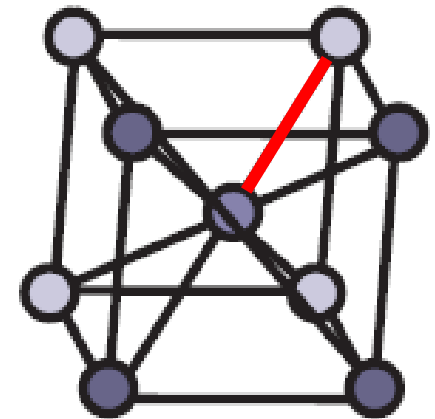can infer from RDF about crystal structure*

http://physchem.ox.ac.uk/~rkt/lectures/liqsolns/liquids.html

Face centered cubic (FCC), body centered cubic (BCC)

Nearest neighbor (NN)

FCC

BCC

Aluminum, NN: 2.863 Å (a_0=4.04 Å)

Copper, NN: 2.556 Å (a_0=3.615 Å))

Chromium, NN: 2.498 Å (a_0=2.91 Å)

Iron, NN: 2.482 Å (a_0=2.86 Å)

http://www.webelements.com/

Hexagonal closed packed (HCP)

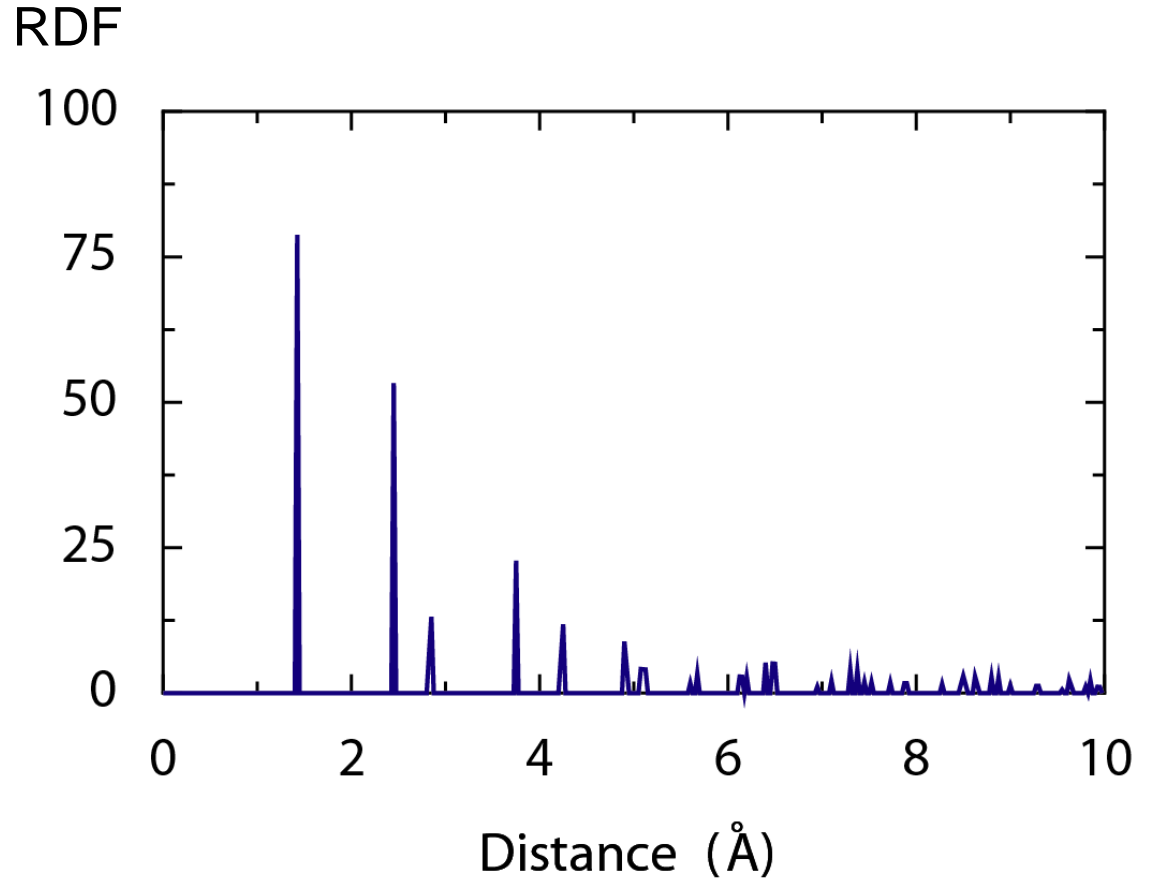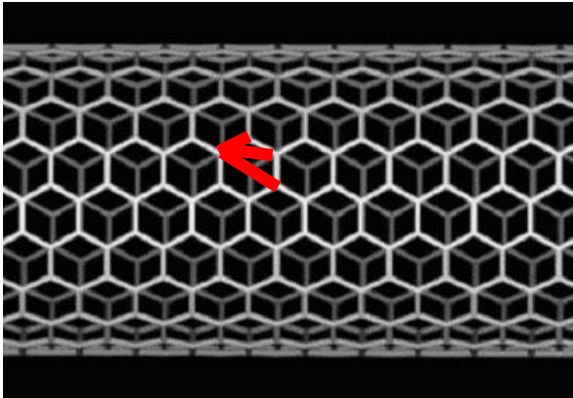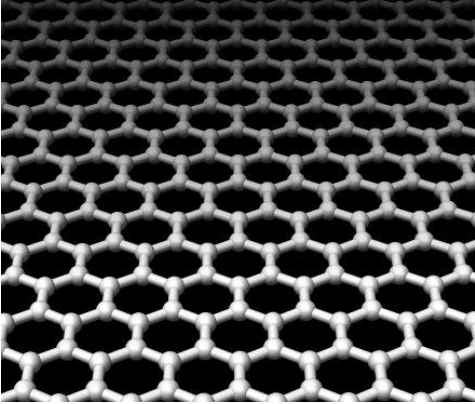Nearest neighbor (NN)
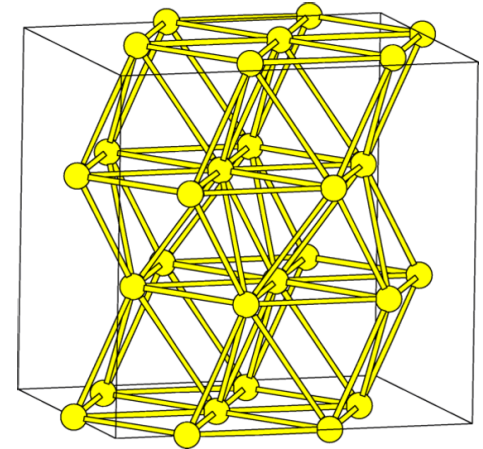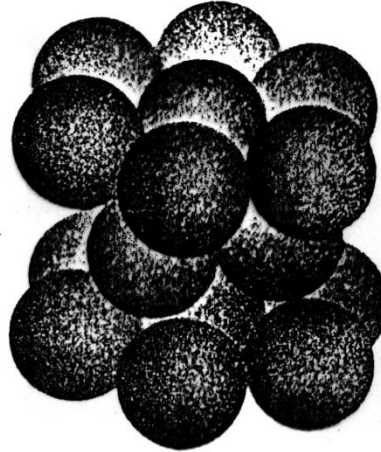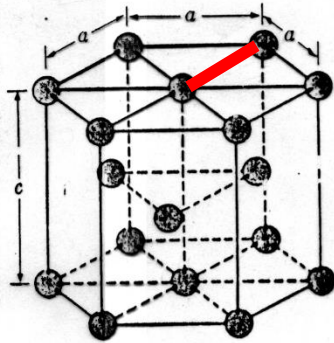
Cobalt
a: 250.71 pm
b: 250.71 pm
c: 406.95 pm
α: 90.000°
β: 90.000°
γ: 120.000°
NN: 2.506 Å

Zinc
a: 266.49 pm
b: 266.49 pm
c: 494.68 pm
α: 90.000°
β: 90.000°
γ: 120.000°
NN: 2.665 Å

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Graphene/carbon nanotubes

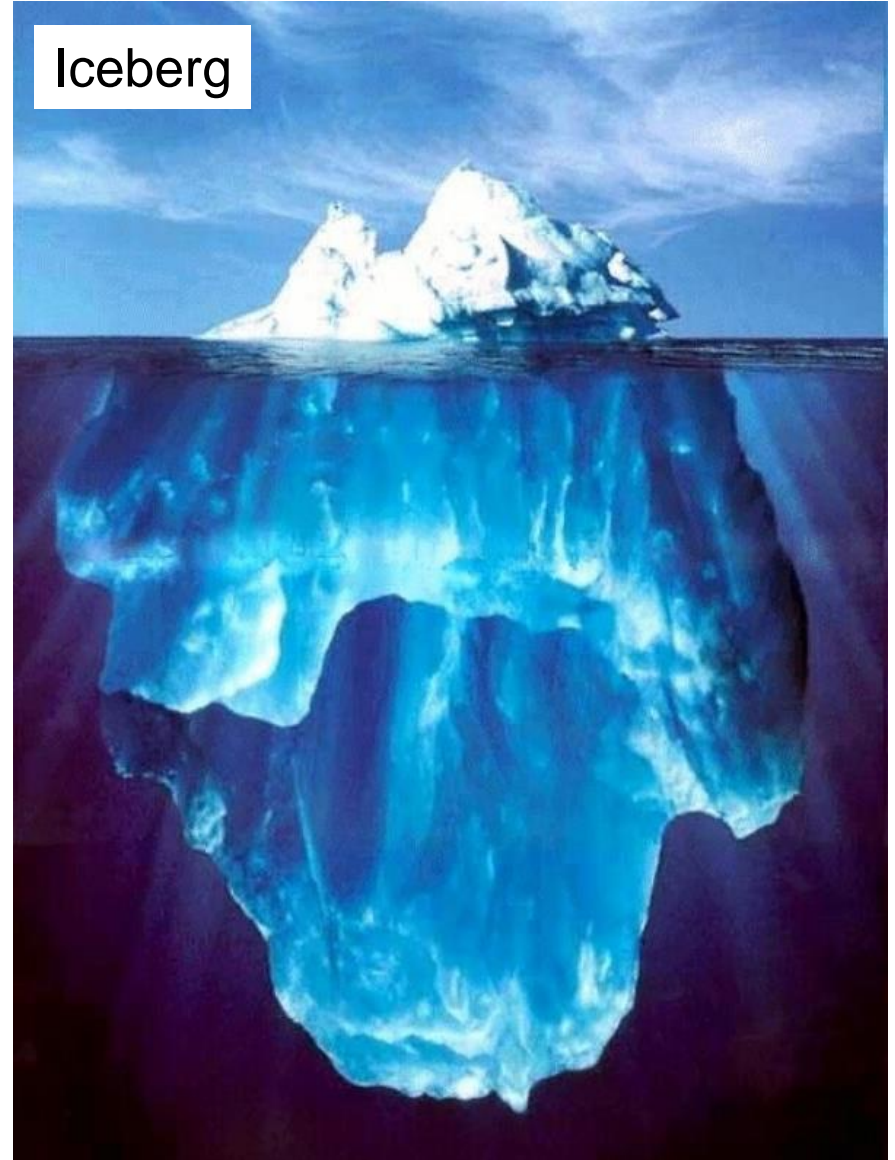**Graphene/carbon nanotubes (rolled up graphene)**
NN: 1.42 Å, second NN 2.46 Å …
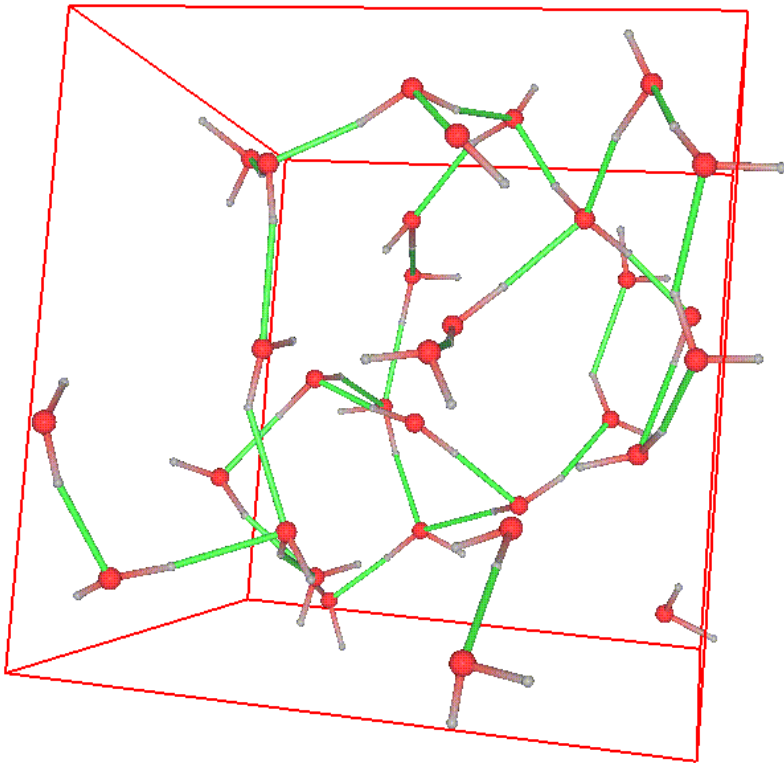
Macroscale view of water

Pamukkale (Turkey)

www.amanda.co.nz

Iceberg

RDF of water (H_2O)

http://www.nyu.edu/classes/tuckerman/stat.mech/lectures/lecture_8/node1.html

RDF of water (H_2O)

O-O distance

H-O distance

RDF of water (H_2O)

O-O distance

H-bonding
(≈2.8 Å)

H-O distance

H-O covalent bonding
(≈1 Å)
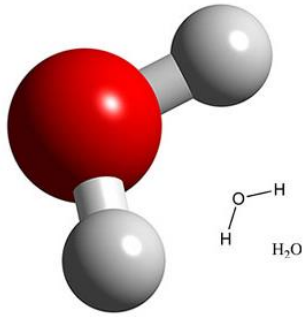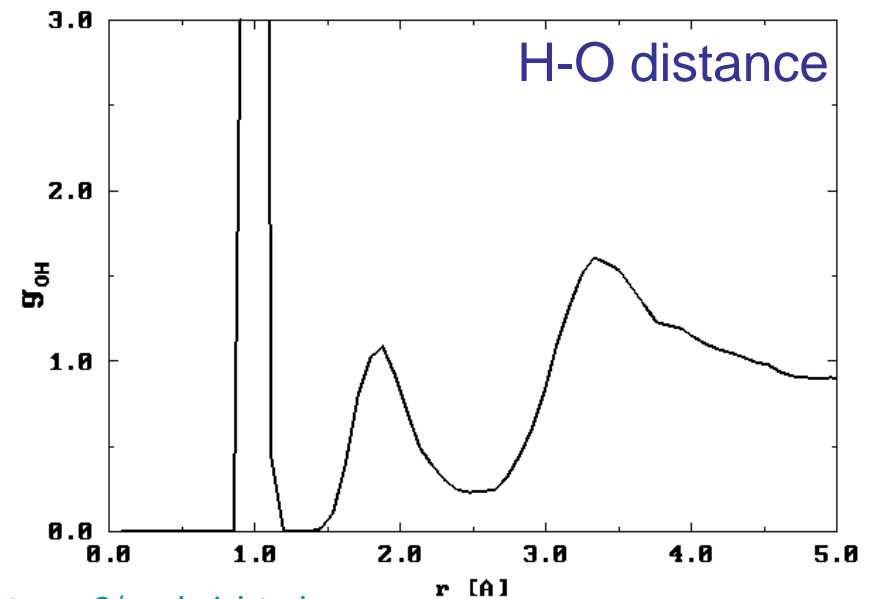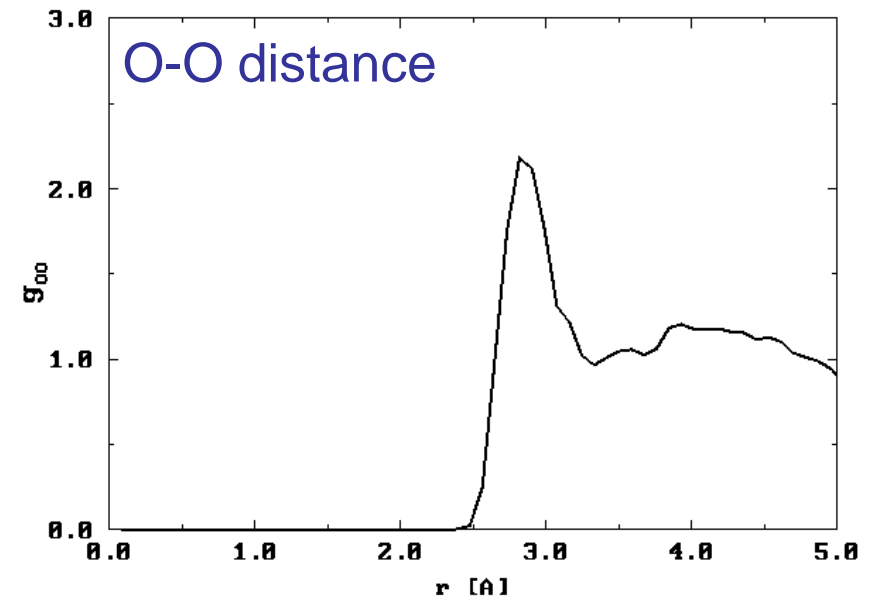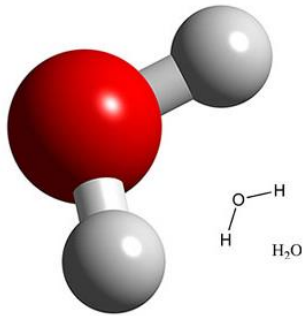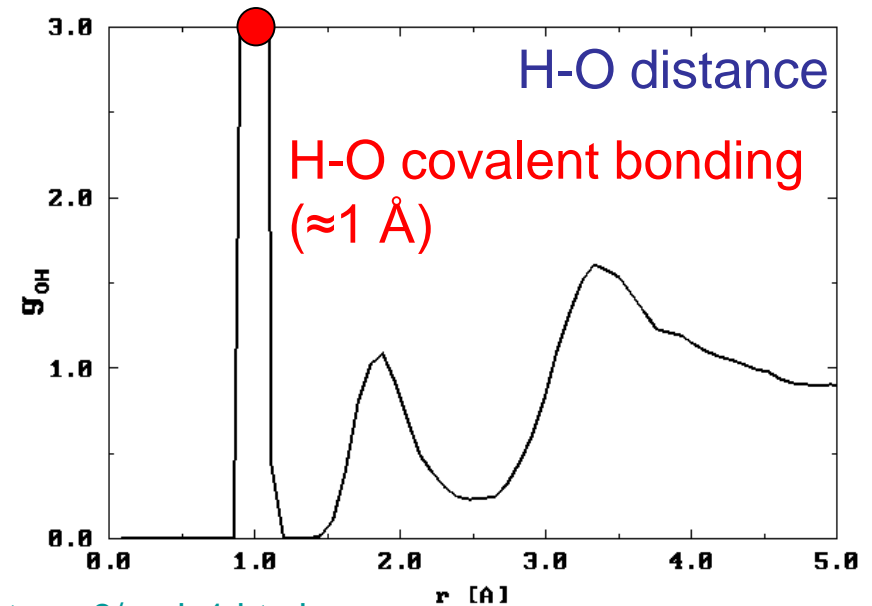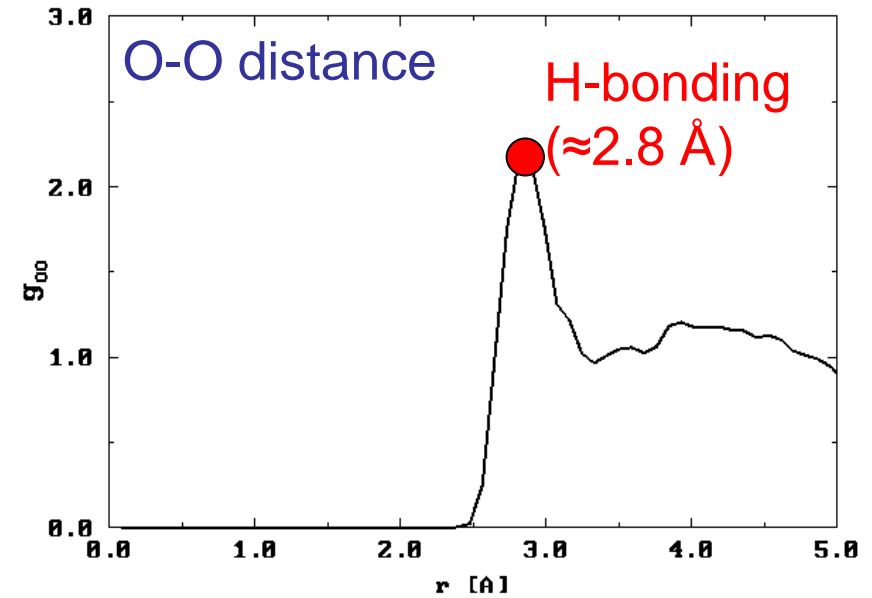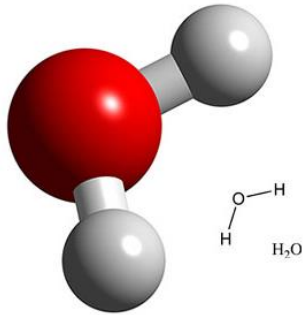
2. How to model chemical interactions

Molecular dynamics: A "bold" idea
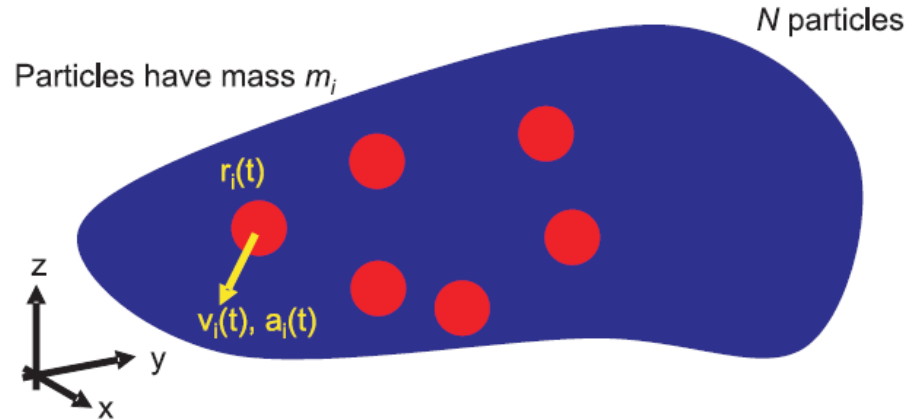
$$r_i(t_0 + \Delta t) = -r_i(t_0 - \Delta t) + 2r_i(t_0)\Delta t + a_i(t_0)\left(\Delta t\right)^2 + ...$$

Positions
at t_0-Δt

Positions
at t_0

Accelerations
at t_0

$$a_i = f_i / m$$

Forces between atoms… how to obtain?

How are forces calculated?

Force magnitude: Derivative of potential energy with respect to atomic distance

$$f = -\frac{\mathrm{d}U(r)}{\mathrm{d}r}$$

To obtain force vector f_i, take projections into the three axial directions

$$f_i = f\,\frac{x_i}{r}$$

$\vec{r}_{ij}$

i

$\vec{f}$

f_2

f_1

x_2

x_1

x_2

x_1
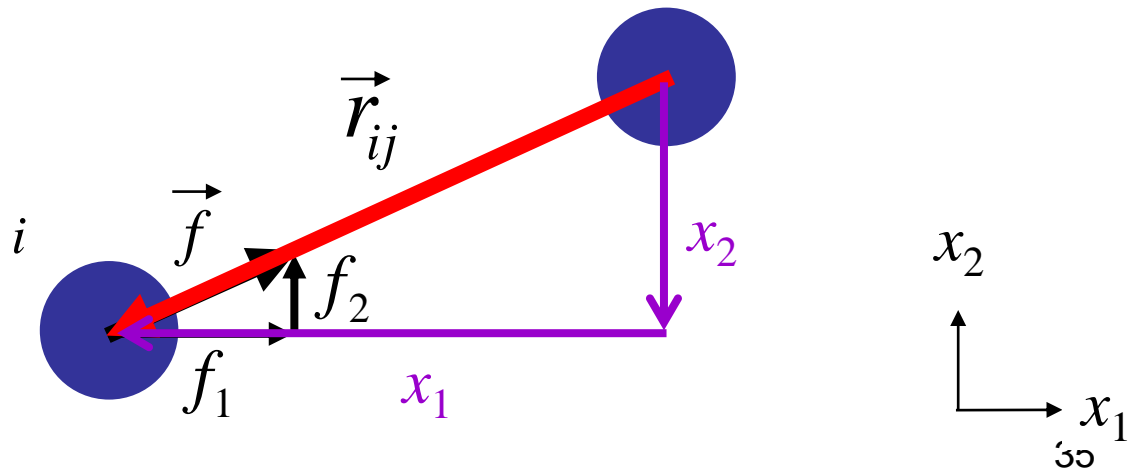
Atomic interactions – quantum perspective

How electrons from different atoms interact defines nature of chemical bond

Density distribution of electrons around a H-H molecule

H   H   H$_2$
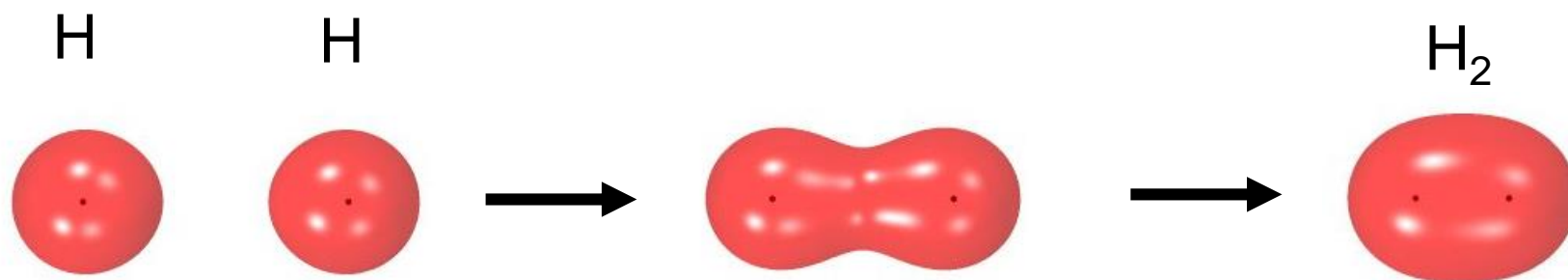
Much more about it in part II

http://winter.group.shef.ac.uk/orbitron/MOs/H2/1s1s-sigma/index.html

Concept: Interatomic potential
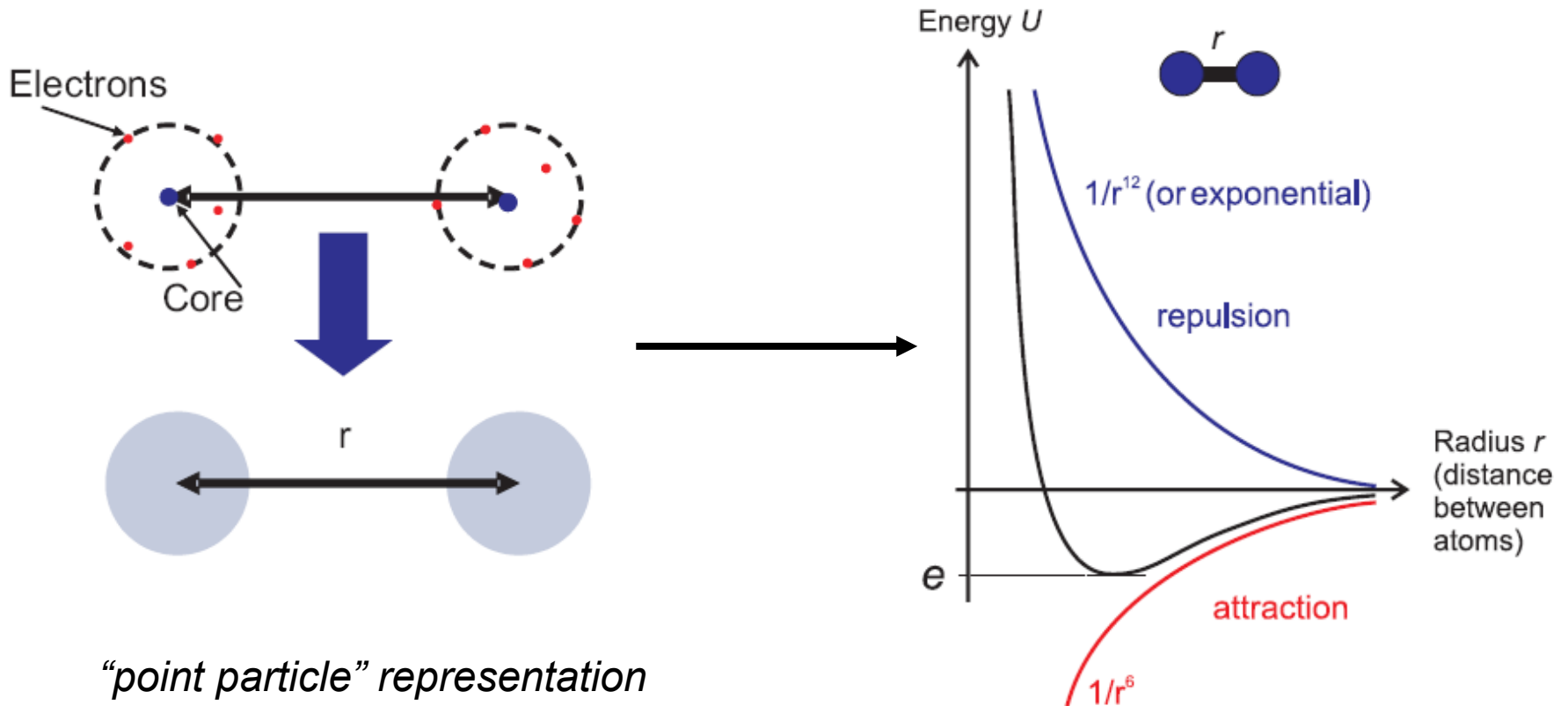
"point particle" representation

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

Interatomic bond - model
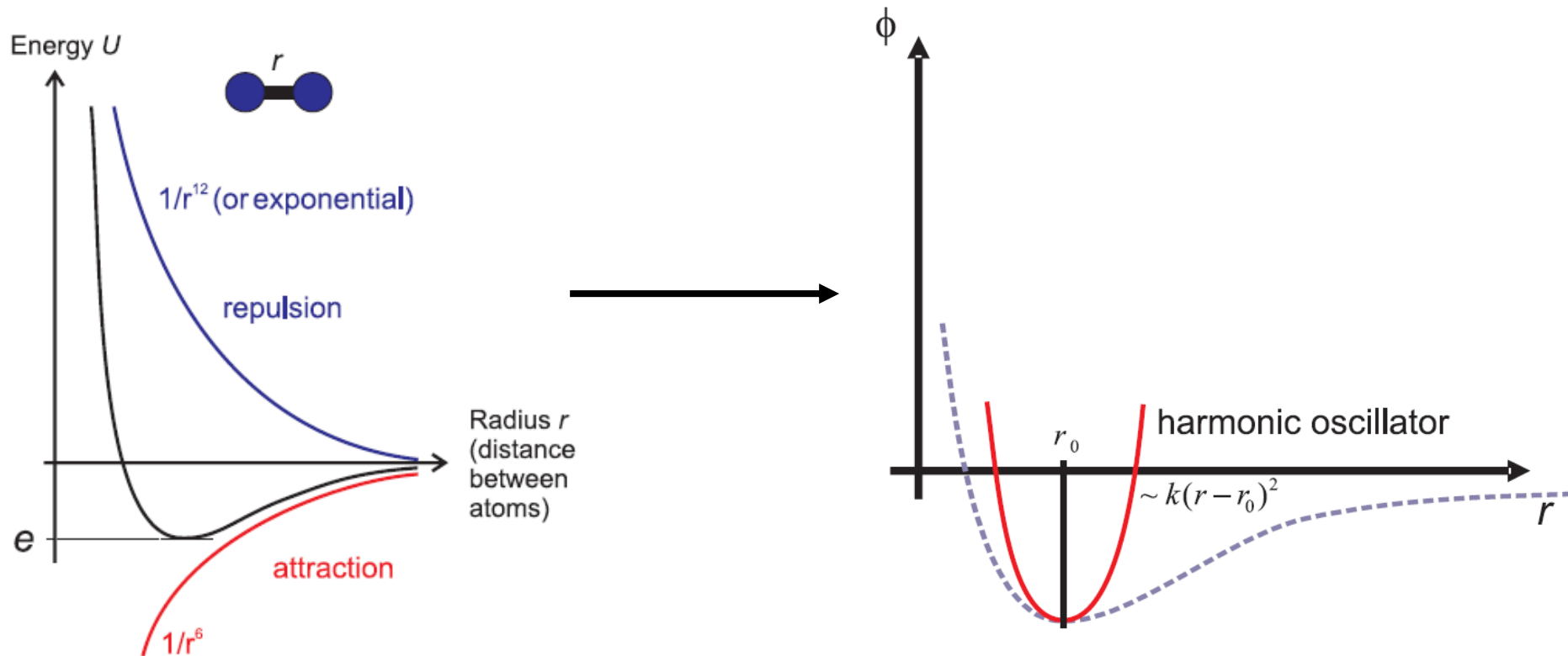
Energy U

$1/r^{12}$ (or exponential)

repulsion

Radius r (distance between atoms)

e

attraction

$1/r^6$

ϕ

harmonic oscillator

r_0

$\sim k(r-r_0)^2$

r

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

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4.1 Different types of chemical bonds

Atomic interactions – different types of chemical bonds

- **Primary bonds ("strong")**
    - Ionic (ceramics, quartz, feldspar - **rocks**)
    - Covalent (**silicon**)
    - Metallic (copper, nickel, **gold**, silver)
      (high melting point, 1000-5,000K)

- **Secondary bonds ("weak")**
    - Van der Waals (**wax**, low melting point)
    - Hydrogen bonds (proteins, **spider silk**)
      (melting point 100-500K)

- Ionic: Non-directional (point charges interacting)
- Covalent: Directional (bond angles, torsions matter)
- Metallic: Non-directional (electron gas concept)

Difference of material properties originates from different atomic interactions

Types of bonding (illustrations)

charge +/-

Ionic bonding

electron density (localized!)

Covalent bonding

Hydrogen bonding

H_2O

donor/acceptor

Metallic bonding

After: Pavel Korzhavyi, *Royal Institute of Technology (KTH)*
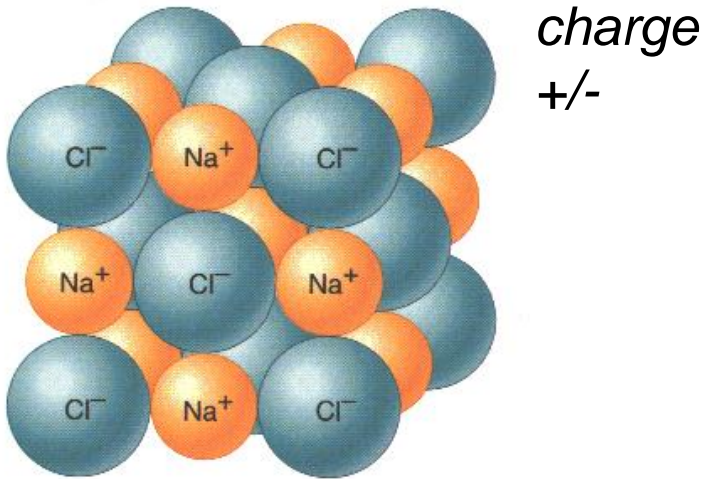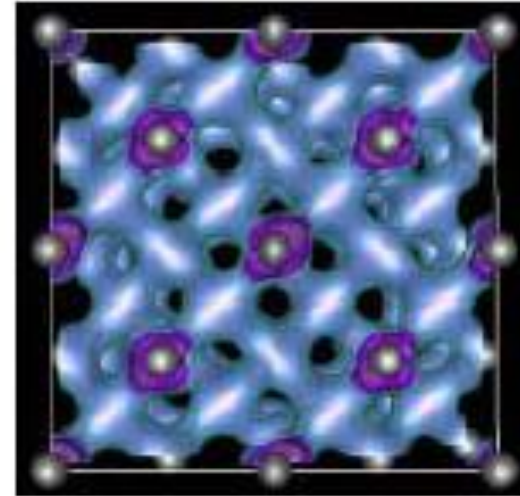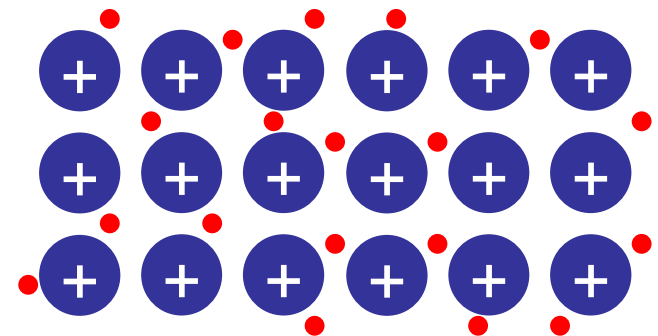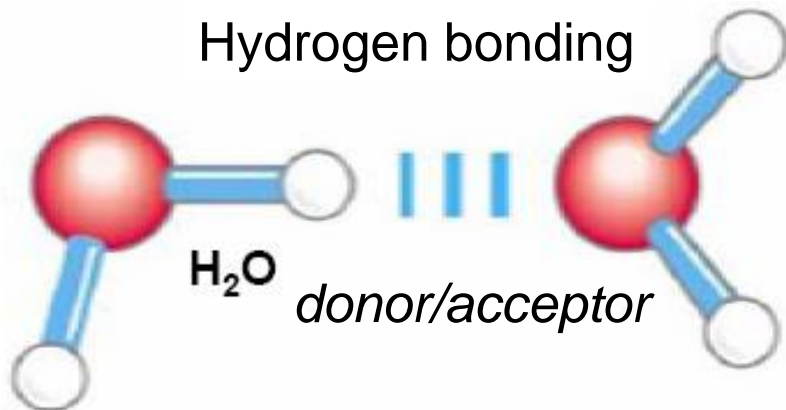
Wax

Soft, deformable, does not break under deformation

Rocks

Quite brittle (breaks e.g. during earthquake)

Gold

Very "soft" metal, deformable, high density

Silicon

Very brittle – shatters into many pieces if dropped

Spider web

Very extensible, deformation, yet very strong (similar to steel)

Brittle or ductile?

brittle

ductile
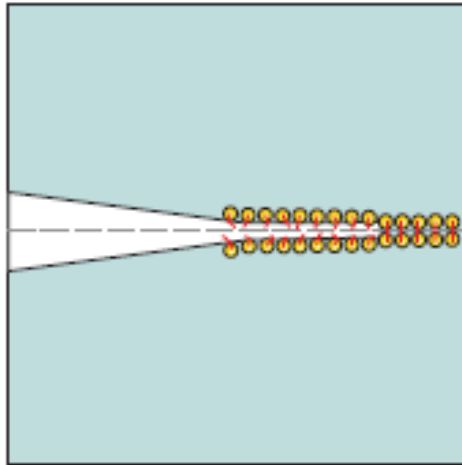
Glass,
Polymers,
Ice…
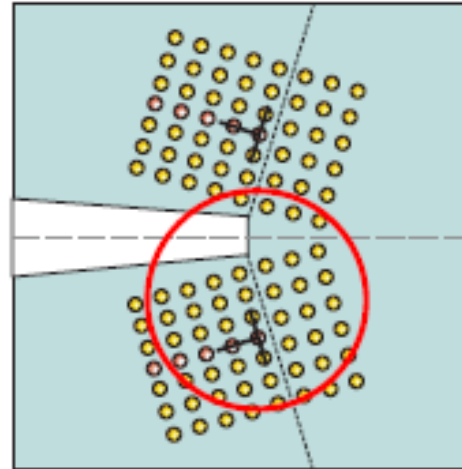
Copper,
Gold,
…

shear load

Outline

- Goal: model chemical bonds with the objective to enable force calculation (basic MD algorithm) or energy calculation (TODAY, MC)

- **Two-step approach**:

  1. Define energy landscape, *i.e.* defines how distance between particles controls the energy stored in the bond
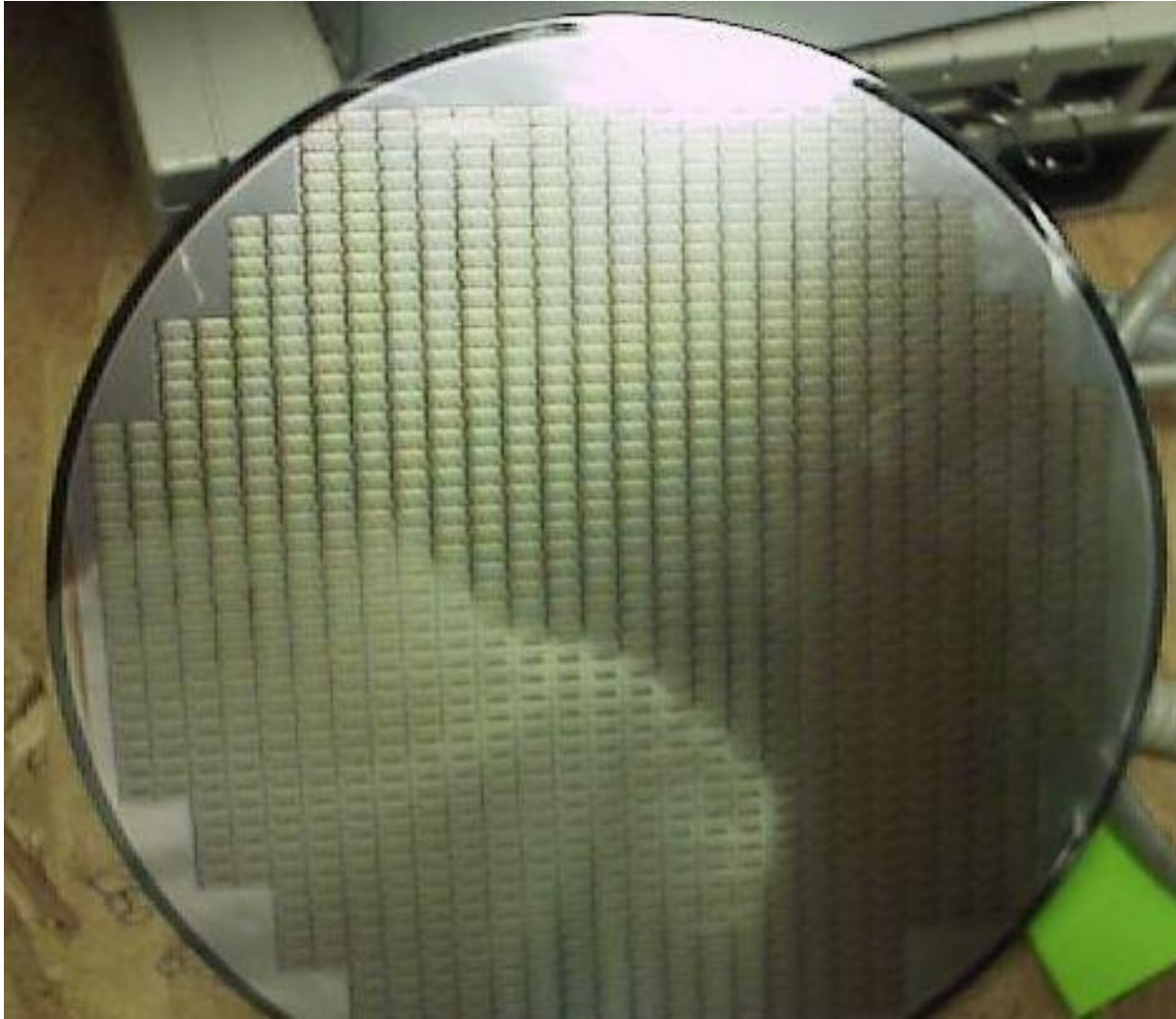
  2. Then take derivatives to obtain forces, to be used in the MD algorithm

"Modeling and simulation" paradigm:

- First, develop mathematical expressions (modeling)
- Second, use model in numerical solution (simulation, =MD)

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Models for atomic interactions

- Define interatomic potentials that describe the energy of a set of atoms as a function of their coordinates r:

$$r = \left\{ \vec{r}_j \right\} \quad j = 1..N$$

$$U_{total} = U_{total}(r)$$

Depends on position of all other atoms

$$\boxed{\vec{F}_i = -\nabla_{\vec{r}_i} U_{total}(r)} \quad i = 1..N$$
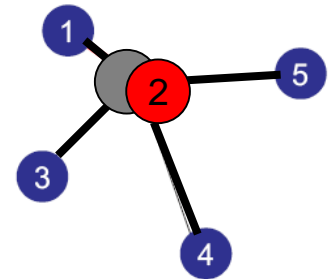
$$\nabla_{\vec{r}_i} = \left(\frac{\partial}{\partial r_{1,i}}, \frac{\partial}{\partial r_{2,i}}, \frac{\partial}{\partial r_{3,i}} \right)$$

Change of potential energy due to change of position of particle i ("gradient")

2.1 Pair potentials

Pair potentials: energy calculation

Simple approximation: Total energy is sum over the energy of all pairs of atoms in the system

$r_{ij} =$ distance between particles i and j

$\phi(r_{ij})$ Pair wise interaction potential energy for each bond
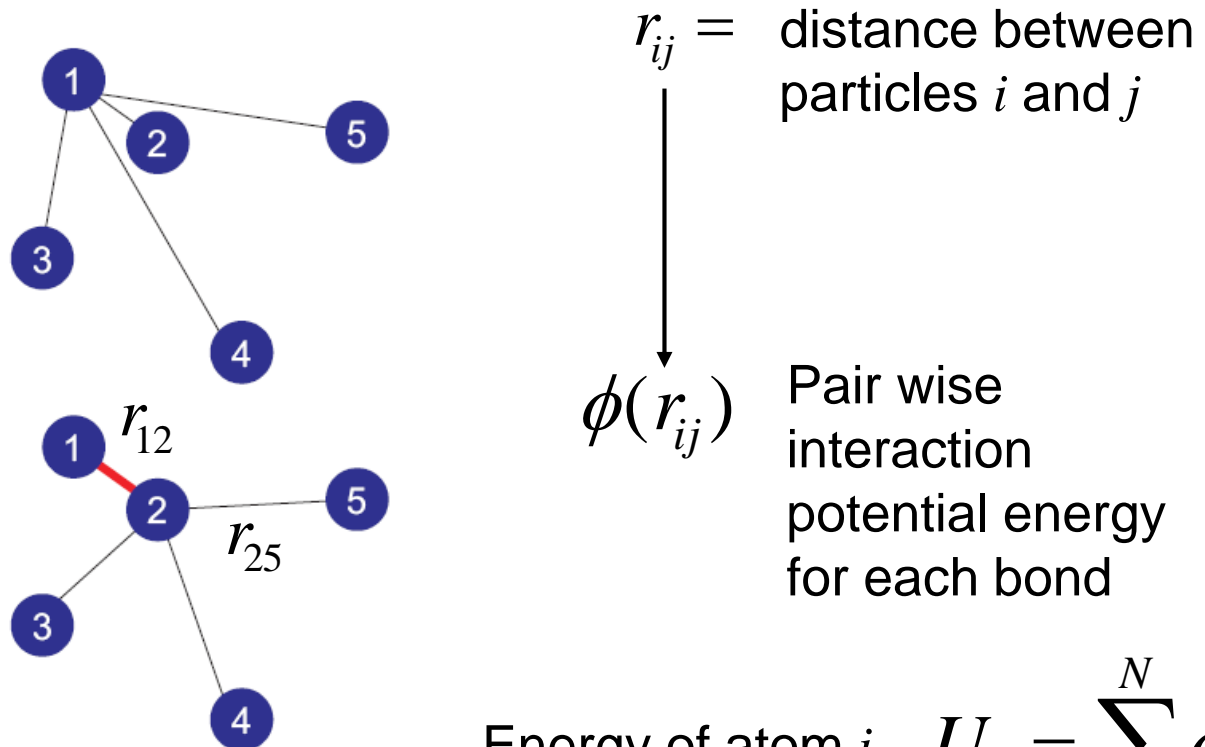
Energy of atom i $\quad U_i = \sum_{j=1}^{N} \phi(r_{ij})$

Overview - pair potentials: total energy calculation

Simple approximation: Total energy is sum over the energy of all pairs of atoms in the system

Pair wise interaction potential

$$\phi(r_{ij})$$

Pair wise summation of bond energies

Energy of atom i
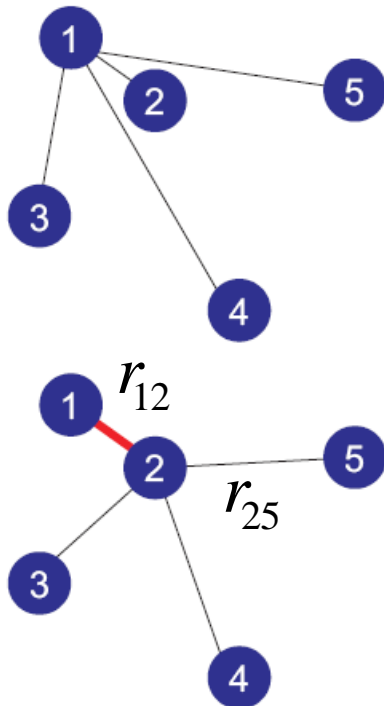
$$U_i = \sum_{j=1}^{N} \phi(r_{ij})$$

avoid double counting

$$U_{total} = \frac{1}{2} \sum_{i=1, i \neq j}^{N} \sum_{j=1}^{N} \phi(r_{ij})$$

$r_{ij} =$ distance between particles i and j

Example: calculation of total energy
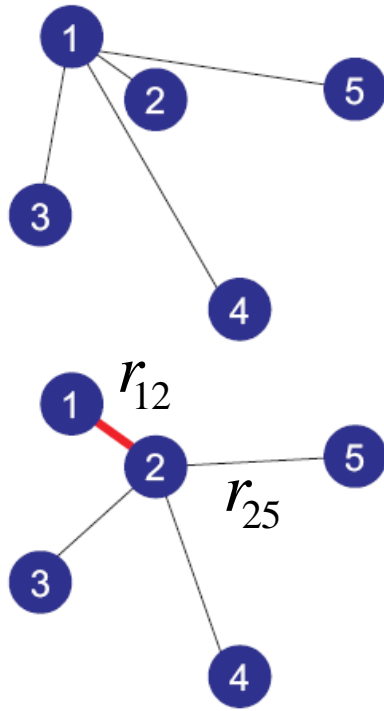
two "loops" over pairs of all particles

$$U_{total} = \tfrac{1}{2} \sum_{i=1,i\neq j}^{N} \sum_{j=1}^{N} \phi(r_{ij})$$

with $\quad \phi_{ij} = \phi(r_{ij})$

$$U_{total} = \frac{1}{2}\left(\phi_{12} + \phi_{13} + \phi_{14} + \phi_{1N}\ldots + \phi_{21} + \phi_{23} + \ldots + \phi_{2N} + \ldots + \phi_{N-1,N}\right)$$

Interatomic pair potentials: examples

$$\phi(r_{ij}) = D\exp\big(-2\alpha(r_{ij} - r_0)\big) - 2D\exp\big(-\alpha(r_{ij} - r_0)\big)$$ Morse potential

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

Lennard-Jones 12:6
potential
(excellent model for noble
Gases, Ar, Ne, Xe..)

$$\phi(r_{ij}) = A\exp\left(-\frac{r_{ij}}{\sigma}\right) - C\left(\frac{\sigma}{r_{ij}}\right)^{6}$$ Buckingham potential

$$\phi(r_{ij}) = a_0 + \frac{1}{2}k(r_{ij} - r_0)^2$$ Harmonic approximation
(no bond breaking)

What is the difference between these models?

Shape of potential (e.g. behavior at short or long distances, around equilibrium)

Number of parameters (to fit)

Ability to describe bond breaking
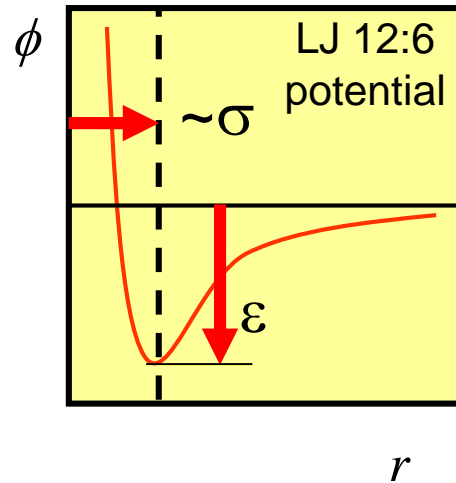
Lennard-Jones potential

Parameters ε, σ

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

Lennard-Jones 12:6

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

Lennard-Jones potential: schematic & parameter meaning

ε : well depth (energy stored per bond)

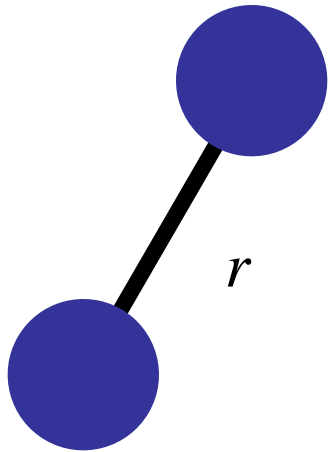σ : proportional to point where force vanishes (equilibrium distance between atoms)

Lennard-Jones 12:6

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

How to identify parameters in a Lennard-Jones potential

(=force field training, force field fitting, parameter coupling, etc.)

Parameter identification for potentials

- Typically done based on more accurate (e.g. **quantum mechanical**) results (or experimental measurements, if available)
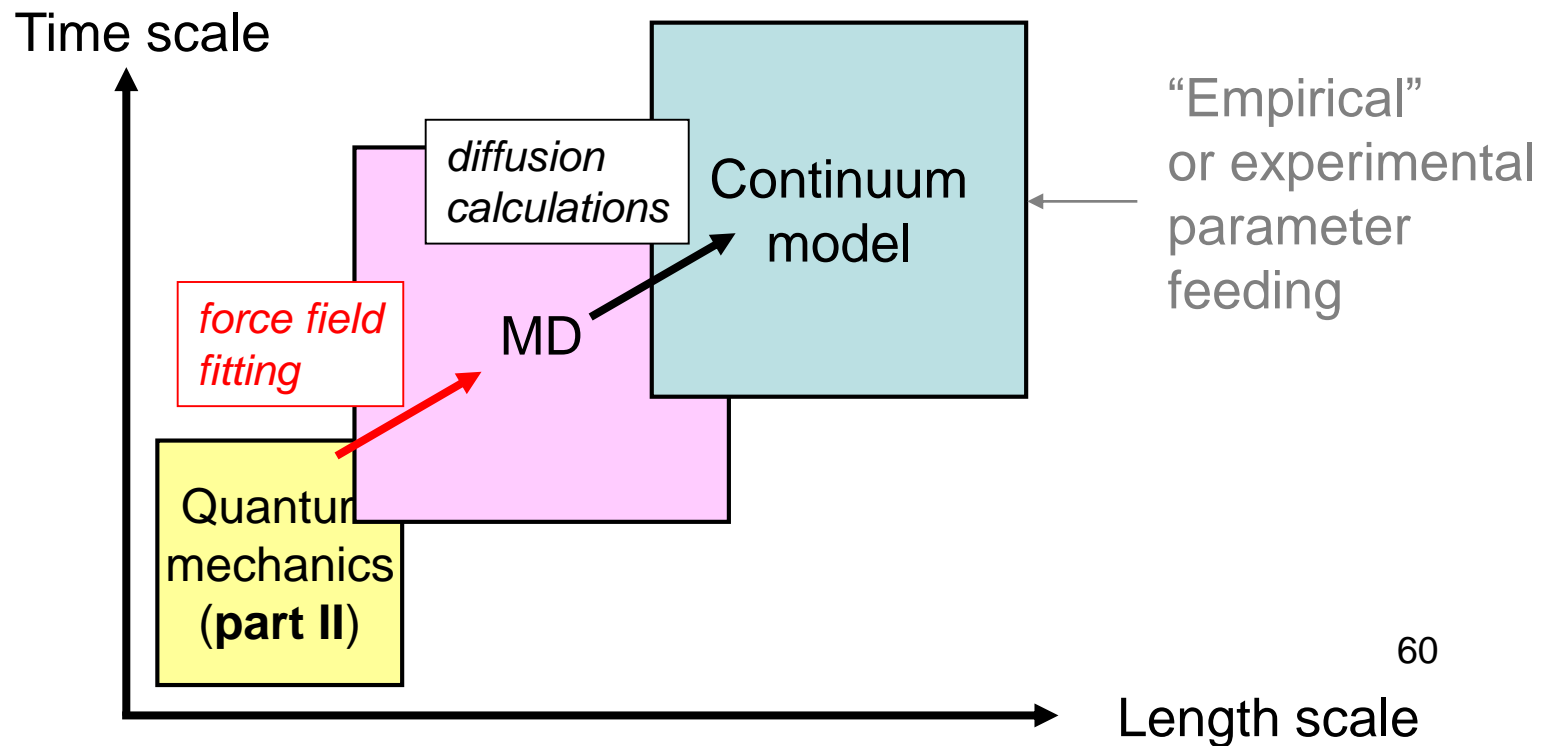
- Properties used include:

  Lattice constant, cohesive bond energy, elastic modulus (bulk, shear, …), equations of state, phonon frequencies (bond vibrations), forces, stability/energy of different crystal structures, surface energy, RDF, etc.

  Potential should closely reproduce these reference values

- **Challenges**: mixed systems, different types of bonds, reactions

Multi-scale paradigm

- Show earlier: molecular dynamics provides a powerful approach to relate the diffusion constant that appears in continuum models to atomistic trajectories

- Force field fitting to identify parameters for potentials (based on quantum mechanical results) is yet another "step" in this multi-scale paradigm

60

Derivative of LJ potential ~ force

$$F = -\frac{\mathrm{d}\,\phi(r)}{\mathrm{d}\,r} = -\phi'$$

$\phi(r)$

$|F_{\mathrm{max},LJ}|$

r_0
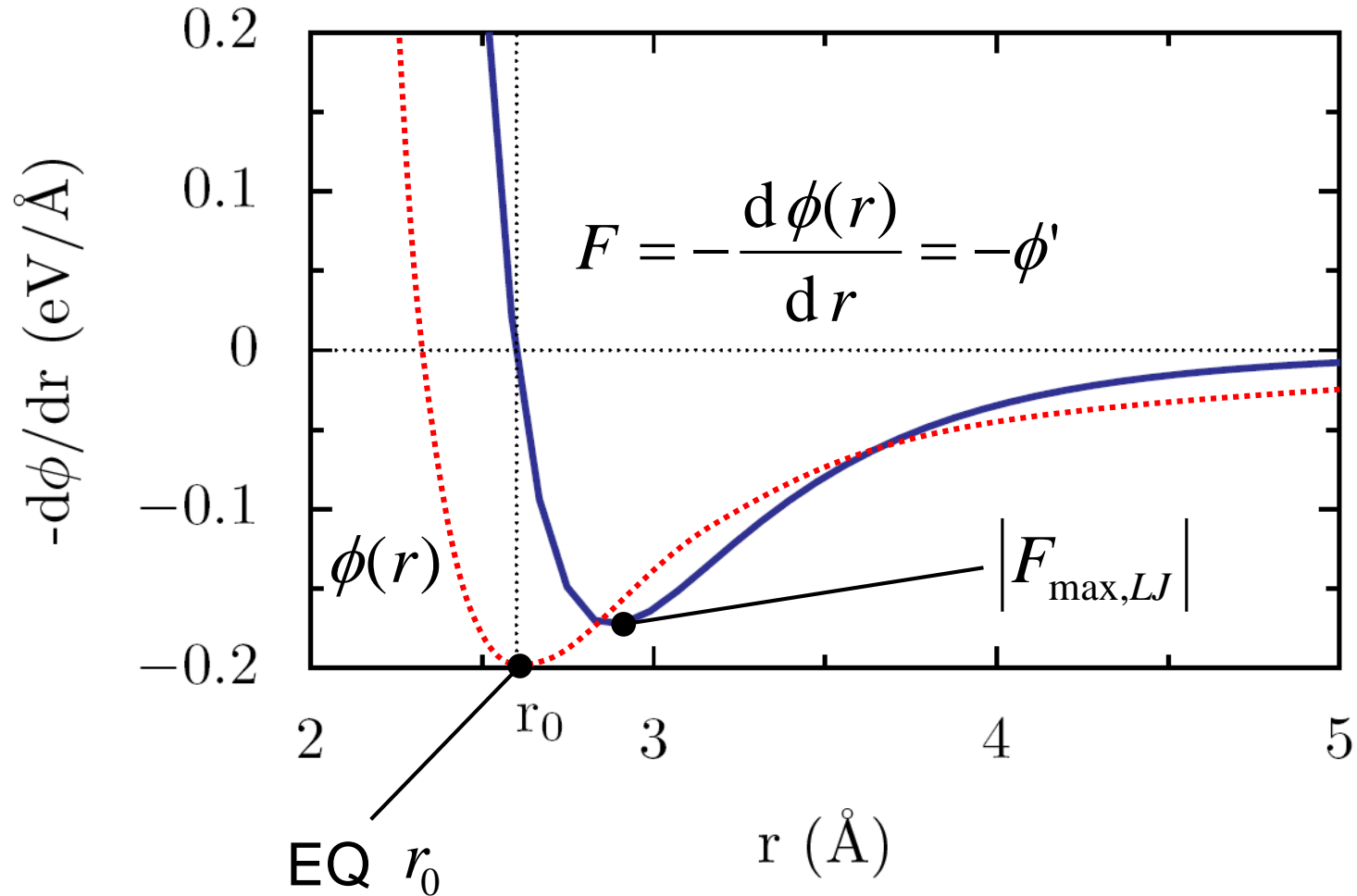
EQ r_0
relates to equilibrium spacing crystal

Properties of LJ potential as function of parameters ε, σ

Equilibrium distance between atoms r_0 and maximum force

$$\sigma\sqrt[6]{2} = r_0 \qquad\qquad F_{\max,LJ} = \frac{2.394\varepsilon}{\sigma}$$
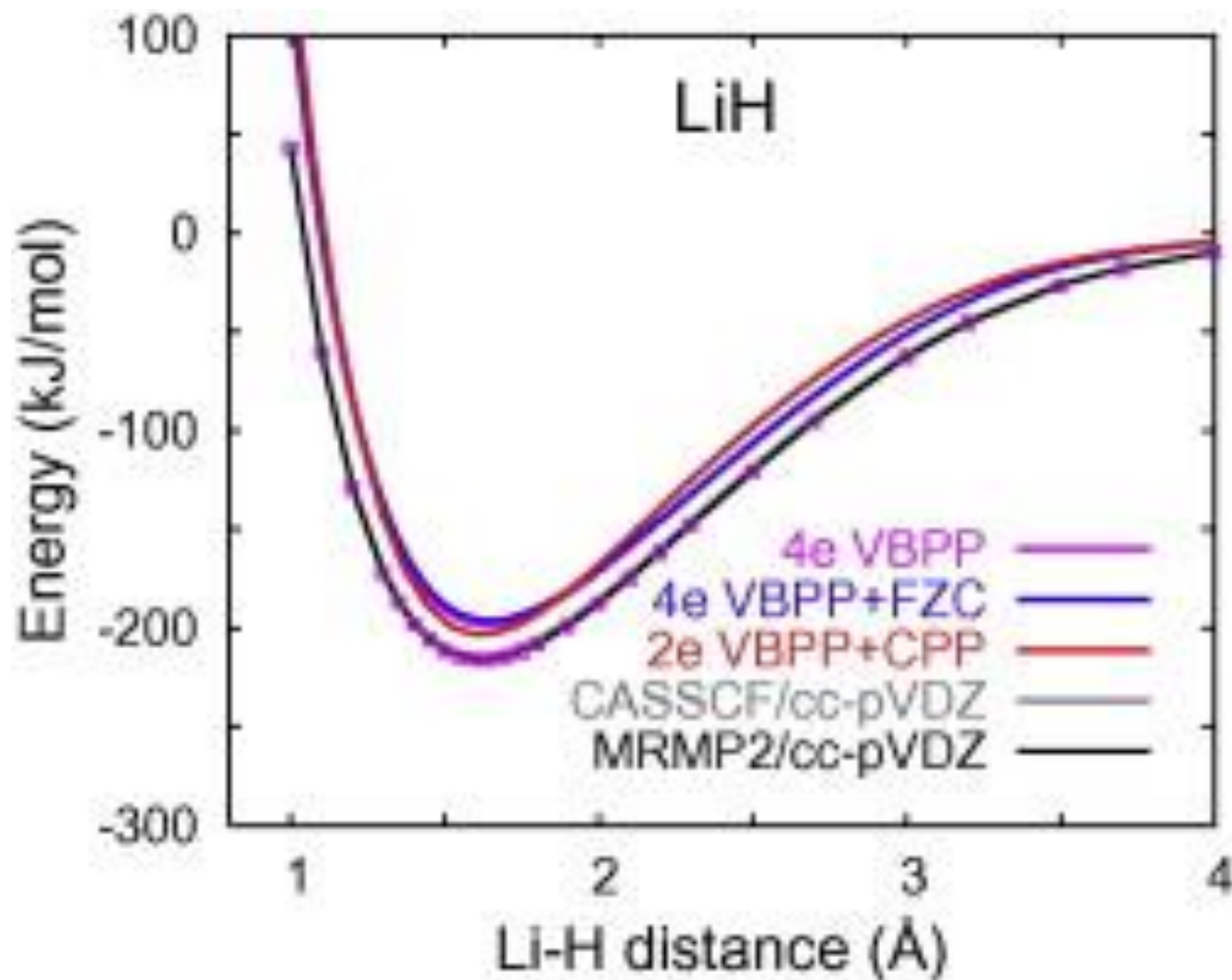
first derivative zero (force)

second derivative zero (=loss of convexity, spring constant=0)

Copper, NN: 2.556 Å (a_0=3.615 Å))

r_0

$r_0 =$ distance of nearest neighbors in a lattice

FCC
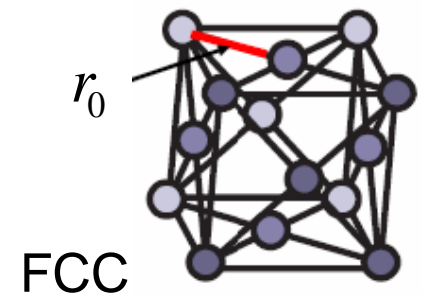
Example quantum result Li-H distance

Ando et al., 2011

How to use a pair potential, e.g. LJ

Force calculation – pair potential

Forces on particles can be calculated by taking derivatives from the potential function & by considering all pairs of atoms

Start with **force magnitude (STEP 1):** Negative derivative of potential energy with respect to atomic distance

$$F = -\frac{\mathrm{d}\phi(r)}{\mathrm{d}r}\bigg|_{r=r_{ij}} = -\frac{\mathrm{d}\phi(r_{ij})}{\mathrm{d}r_{ij}} = -\phi'(r_{ij})$$

Calculate **force vector (STEP 2):**

$$\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$$

Component i of vector $\vec{r}_{ij}$

$$f_i = F\frac{x_i}{r_{ij}} \qquad \vec{f} = f_i \vec{e}_i$$

$$r_{ij} = \left|\vec{r}_{ij}\right|$$

Atomic-Scale Mechanism of Crack-Tip Plasticity: Dislocation Nucleation and Crack-Tip Shielding

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[2]*Divisione Materiali Avanzati, ENEA, Centro Ricerche Casaccia, 00100 Roma A.D., Italy*
[3]*Department of Nuclear Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*
(Received 14 April 1997)

By isolating the process of dislocation emission from a crack tip under an applied tensile stress, we extract from a molecular dynamics simulation the atomic-level displacement and stress fields on the activated slip plane before and after the nucleation event. The stress-displacement relations so obtained provide a direct link with recent continuum descriptions of brittle versus ductile behavior in crack propagation. Crack-tip shielding by the emitted dislocations is demonstrated, as is the role of surface steps in dislocation nucleation and crack-tip blunting.   [S0031-9007(97)03869-6]

PACS numbers: 61.72.Lk, 61.72.Nn, 62.20.Fe, 62.20.Mk

The brittle versus ductile behavior of materials is still an open problem of both fundamental and technological relevance. While brittle fracture is well understood in terms of the Griffith criterion [1], ductile fracture involves dislocation emission from a crack tip, a complex process of nucleation of a dislocation from the crack surface and its subsequent motion away from the crack [2,3]. Criteria for predicting brittle or ductile behavior [4,5] are usually based on the concept of the energy-release rate (actually an energy per unit area) for cleavage decohesion, G_{cleav}, and dislocation nucleation, G_{disl} (which is usually

descriptions, as well as provide a test of their validity. Furthermore, our simulations provide insights into the atomic-level mechanisms of dislocation nucleation, crack-tip blunting, and subsequent shielding.

In the following simulations we use a simple Lennard-Jones (LJ) interatomic potential with parameters $\varepsilon = 0.167$ eV and $\sigma = 2.314$ Å, $a_0 = 1.56\sigma$ being the zero-temperature fcc lattice parameter. This model potential, successfully employed in previous simulations of fcc metals [14,15], is cut off smoothly between the fourth- and fifth-nearest neighbors at $1.49a_0$.

Paper posted on Stellar

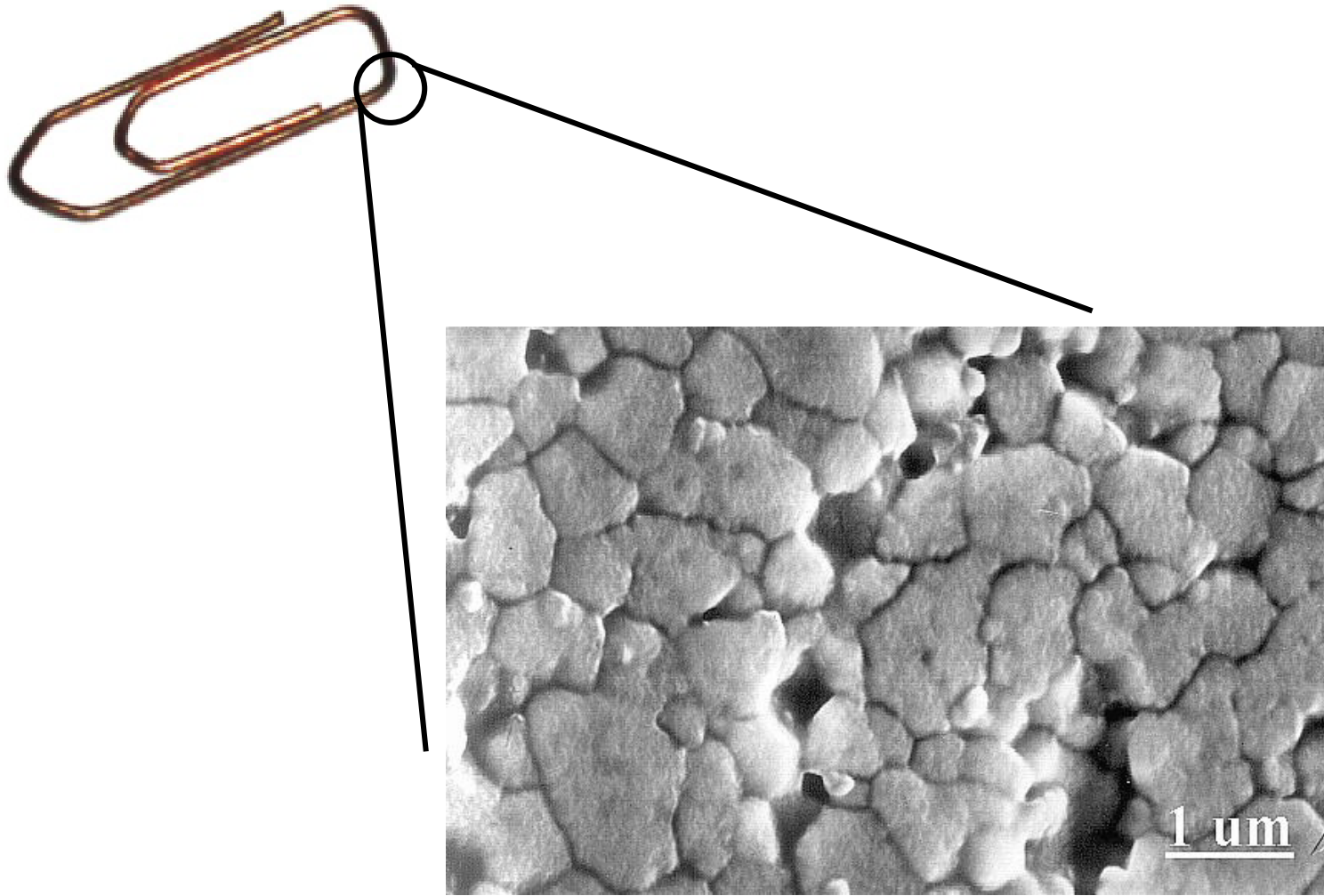# Lennard-Jones potential – example for copper
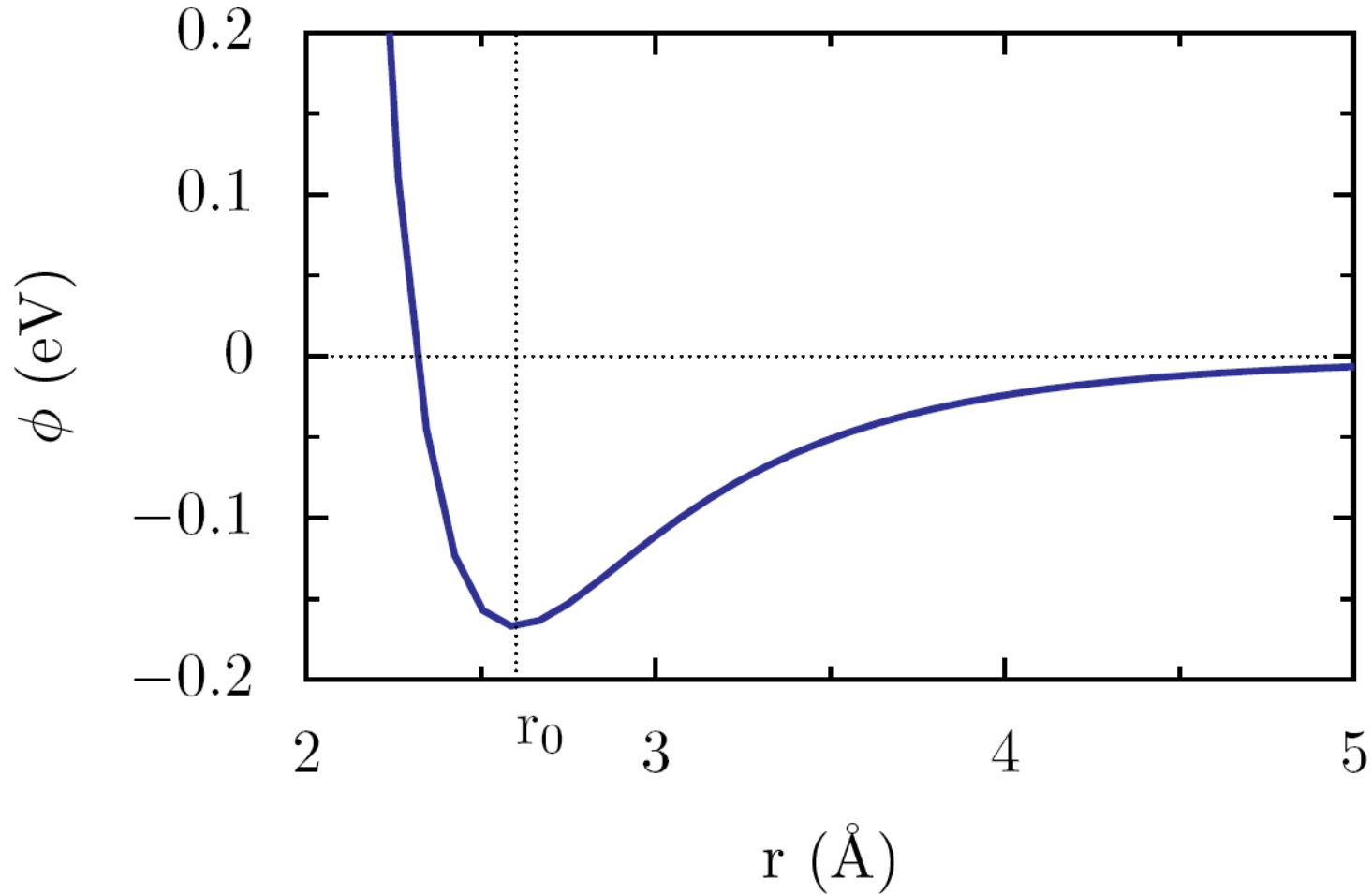
LJ potential – parameters for copper (Cleri *et al.*, 1997)

What can we do with this potential?
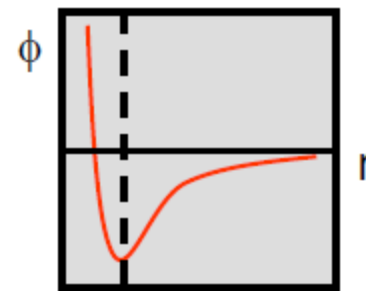
Bending a copper wire until it breaks

A closer look
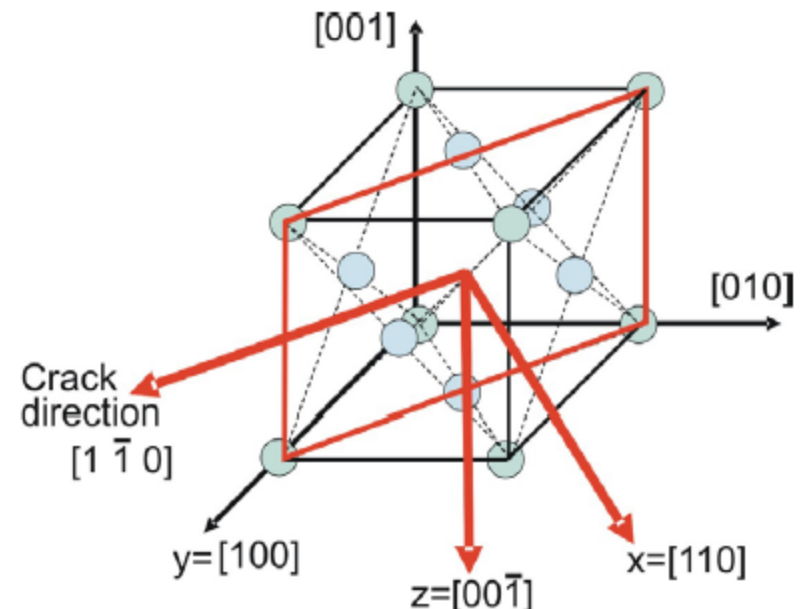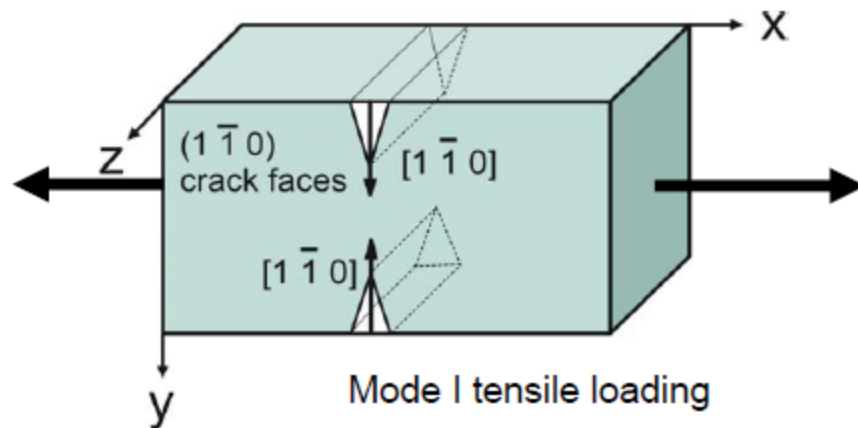
http://www2.ijs.si/~goran/sd96/e6sem1y.gif

Case study: plasticity in a micrometer crystal of copper

Simulation details

- 1,000,000,000 atoms (0.3 micrometer side length)

- 12:6 Lennard-Jones ductile material, for copper

- Visualization using energy filtering method (only show high energy atoms)

Generic features of atomic bonding: „repulsion vs. attraction"

ϕ

r

(1 $\overline{1}$ 0) crack faces   [1 $\overline{1}$ 0]

[1 $\overline{1}$ 0]

Mode I tensile loading

[001]

[010]

Crack direction [1 $\overline{1}$ 0]

y = [100]

z = [00$\overline{1}$]

x = [110]

RESEARCH PAPER

Markus J. Buehler · Alexander Hartmaier
Mark A. Duchaineau · Farid F. Abraham · Huajian Gao

The dynamical complexity of work-hardening: a large-scale molecular dynamics simulation

Abstract We analyze a large-scale molecular dynamics simulation of work hardening in a model system of a ductile solid. With tensile loading, we observe emission of thousands of dislocations from two sharp cracks. The dislocations interact in a complex way, revealing three fundamental mechanisms of work-hardening in this ductile material. These are (1) dislocation cutting processes, jog formation and generation of trails of point defects; (2) activation of secondary slip systems by Frank-Read and cross-slip mechanisms; and (3) formation of sessile dislocations such as Lomer-Cottrell locks. We report the discovery of a new class of point defects referred to as trail of partial point defects, which could play an important role in situations when partial dislocations dominate plasticity. Another important result of the present work is the rediscovery of the Fleischer-mechanism of cross-slip of partial dislocations that was theoretically proposed more than 50 years ago, and is now, for the first time, confirmed by atomistic simulation. On the typical time scale of molecu-

of a many-particle system during failure using ultra-large scale computing.

1 Introduction

The plastic or non-reversible deformation of materials occurs immediately after a regime of recoverable elastic deformations and is governed by the nucleation and motion of defects in the crystal lattice [1–3]. In experiment, researchers often rely on indirect techniques to investigate the creation and interaction of defects. In theory, predictions are primarily based on continuum theory with phenomenological assumptions. While the continuum description has been very successful in the past, some of the key features of plasticity can

paper posted on Stellar

A simulation with 1,000,000,000 particles
Lennard-Jones - copper
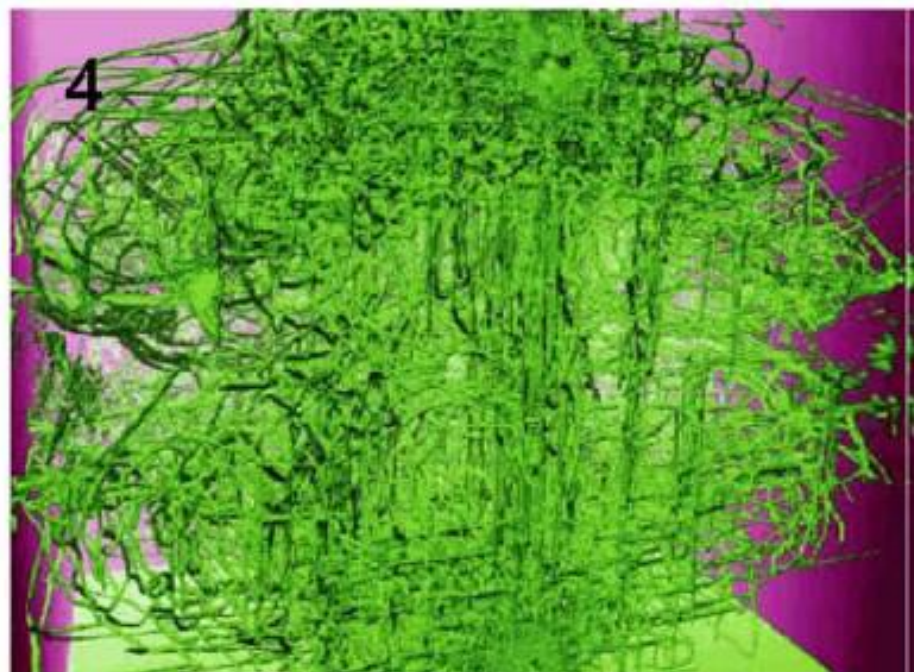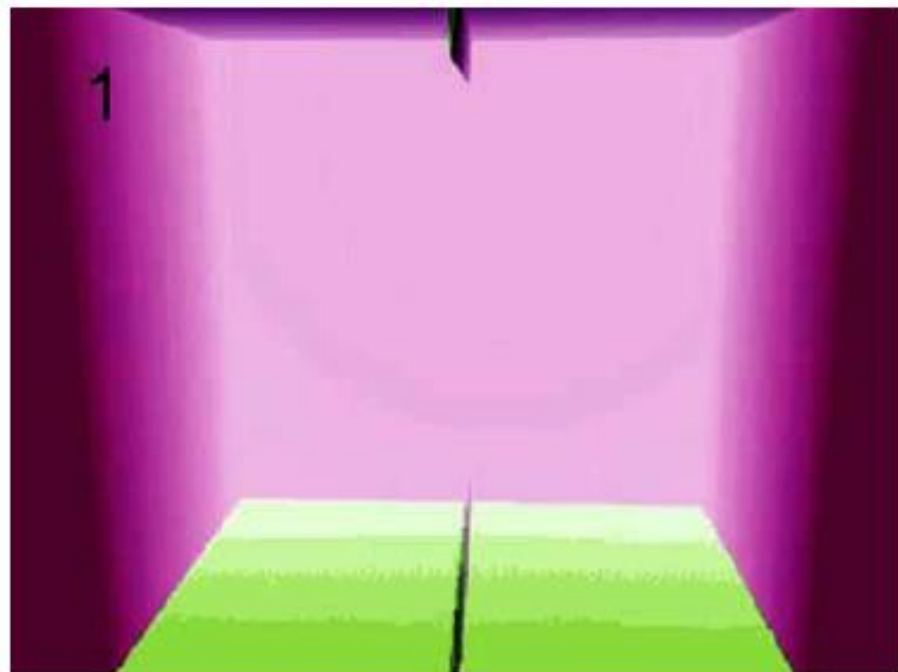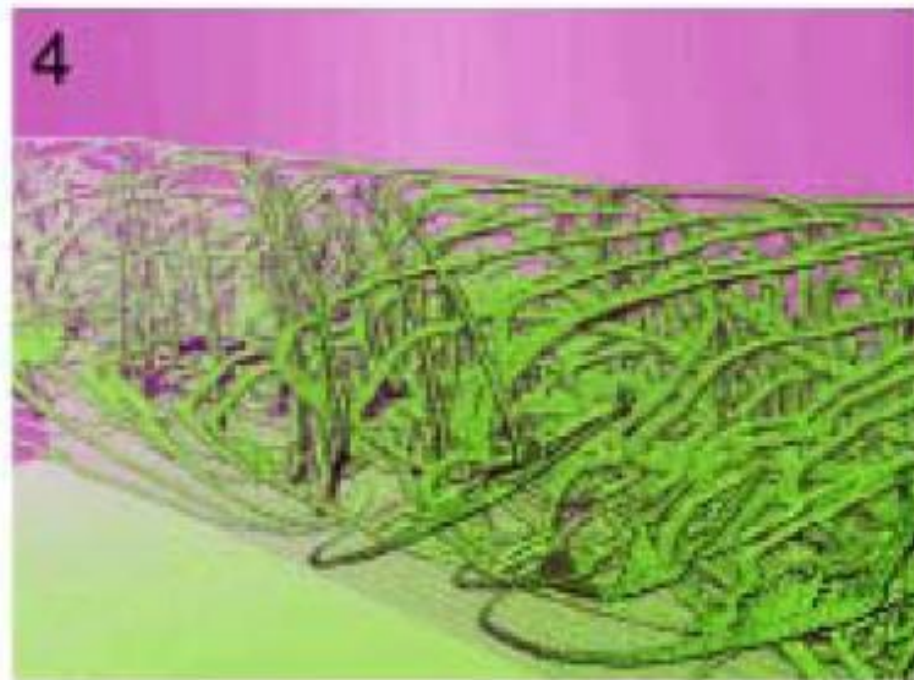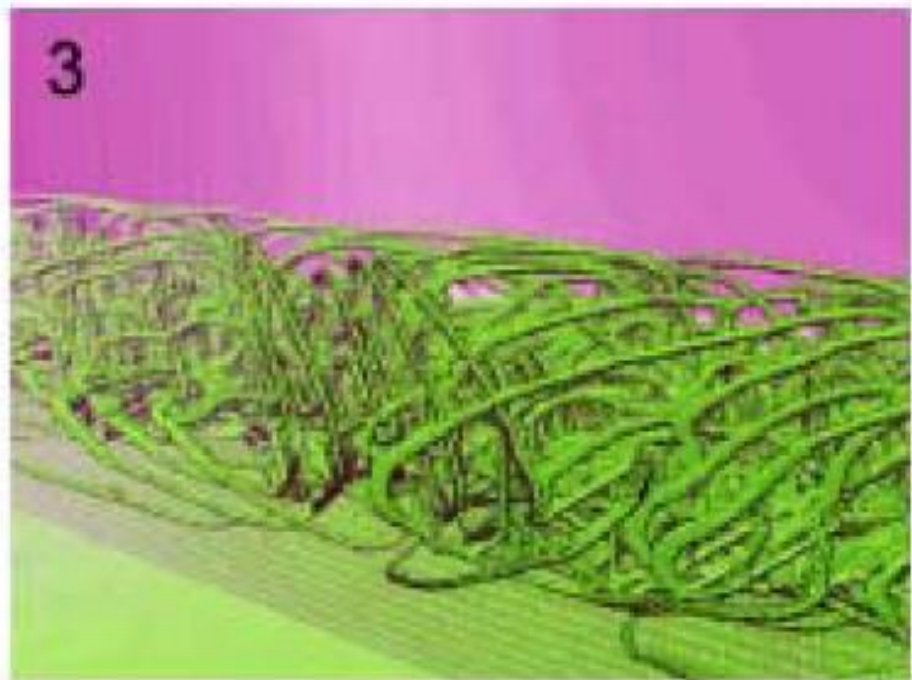
F.F. Abraham, *et al.*, 2000
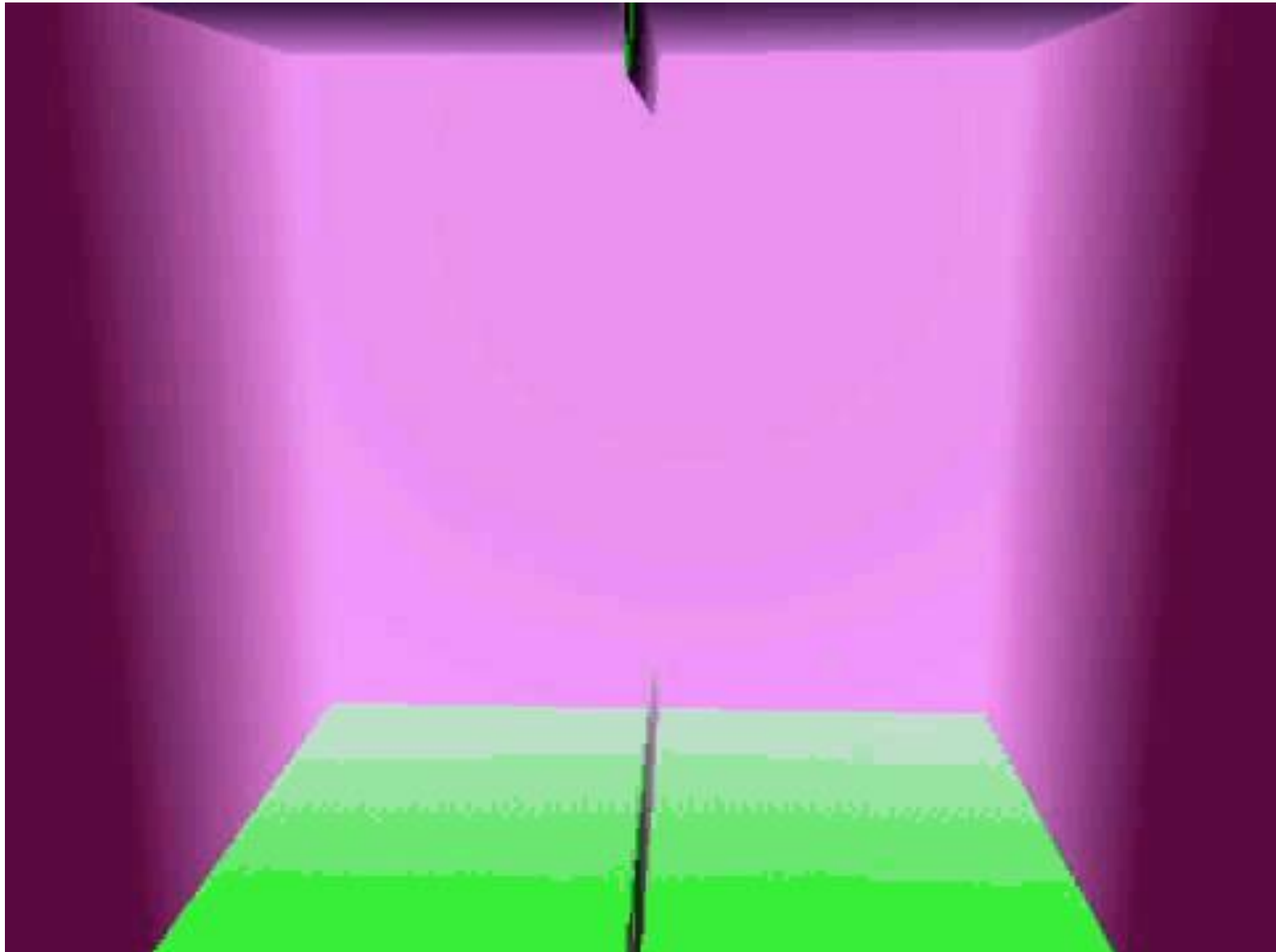
Strengthening mechanisms

???
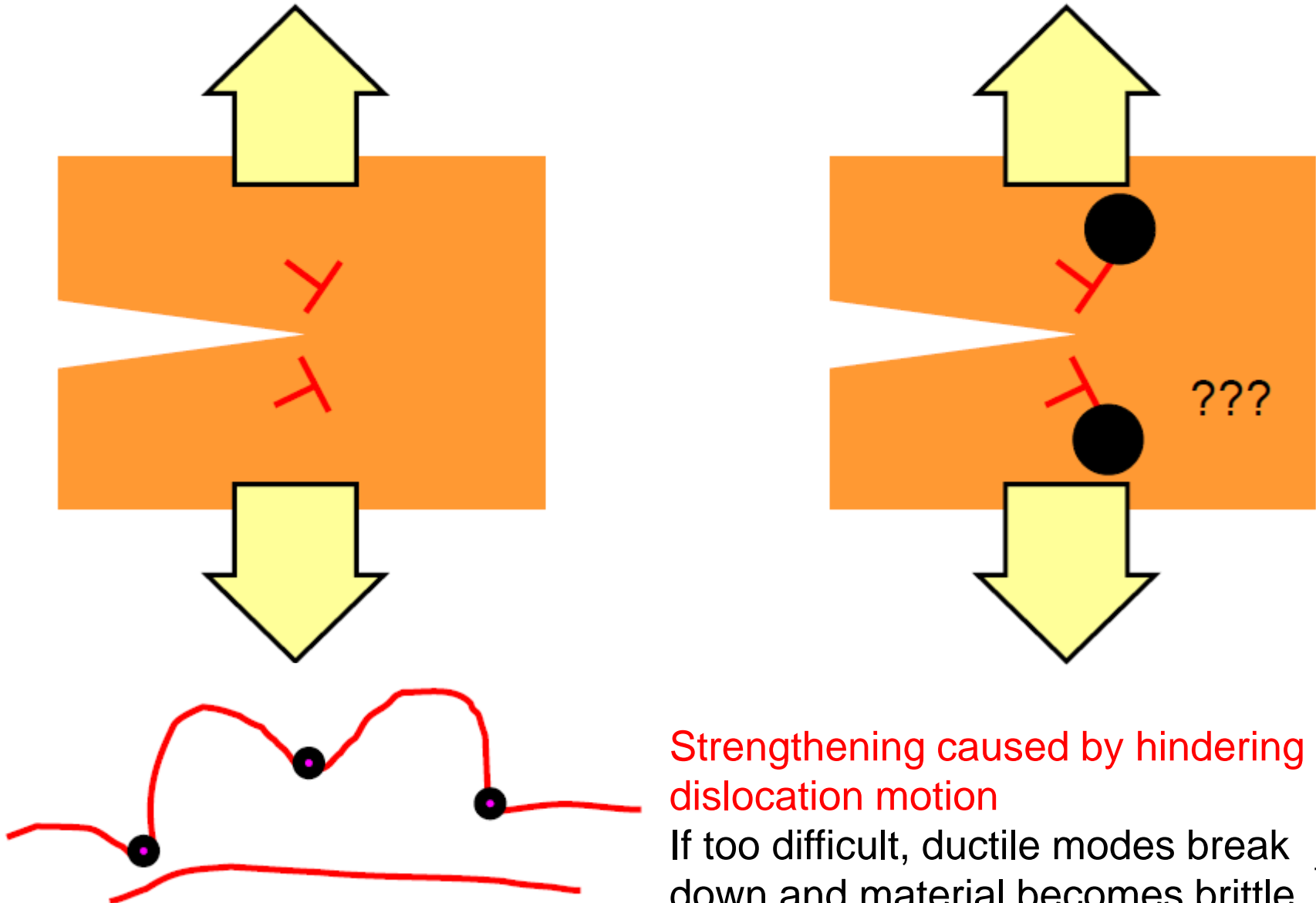
Strengthening caused by hindering dislocation motion

If too difficult, ductile modes break down and material becomes brittle

Putting it all together…

MD updating scheme: Complete

(1) Updating method (integration scheme)

$$r_i(t_0 + \Delta t) = -\underbrace{r_i(t_0 - \Delta t)}_{} + \underbrace{2r_i(t_0)\Delta t}_{} + \underbrace{a_i(t_0)(\Delta t)^2}_{} + \ldots$$

Positions at t_0-Δt   Positions at t_0 Accelerations at t_0

(2) Obtain accelerations from forces

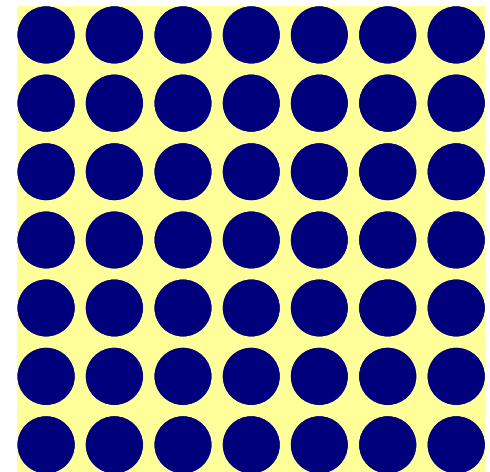$$f_i = ma_i \qquad a_i = f_i / m$$

(4) Crystal (initial conditions)
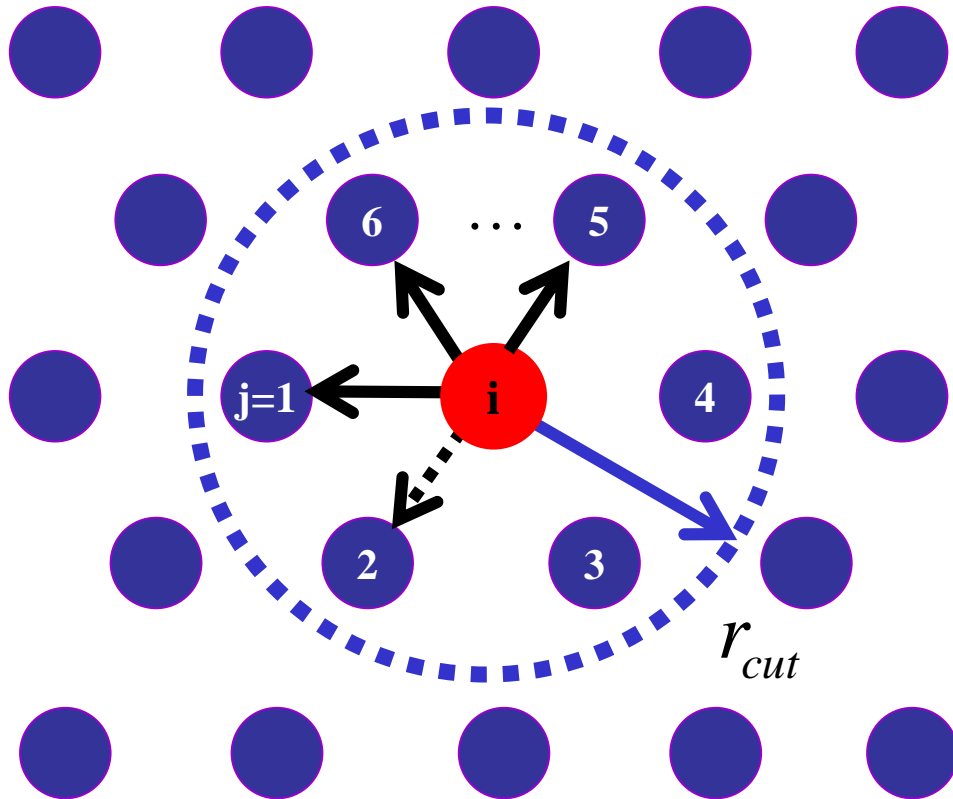
Positions at t_0

(3) Obtain forces from potential

$$F = -\frac{d\phi(r)}{dr} \qquad f_i = F\frac{x_i}{r}$$

Potential

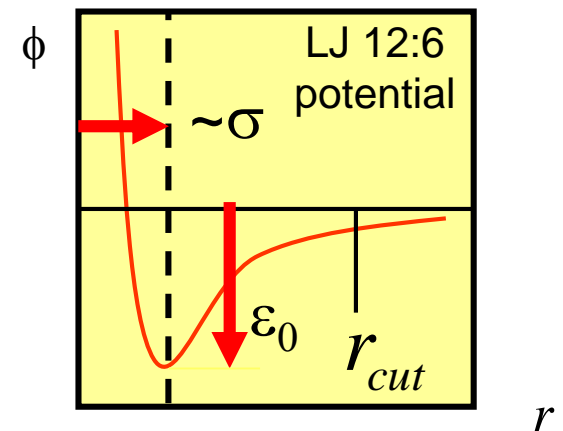$$\phi(r) = 4\varepsilon\left(\left[\frac{\sigma}{r}\right]^{12} - \left[\frac{\sigma}{r}\right]^{6}\right)$$
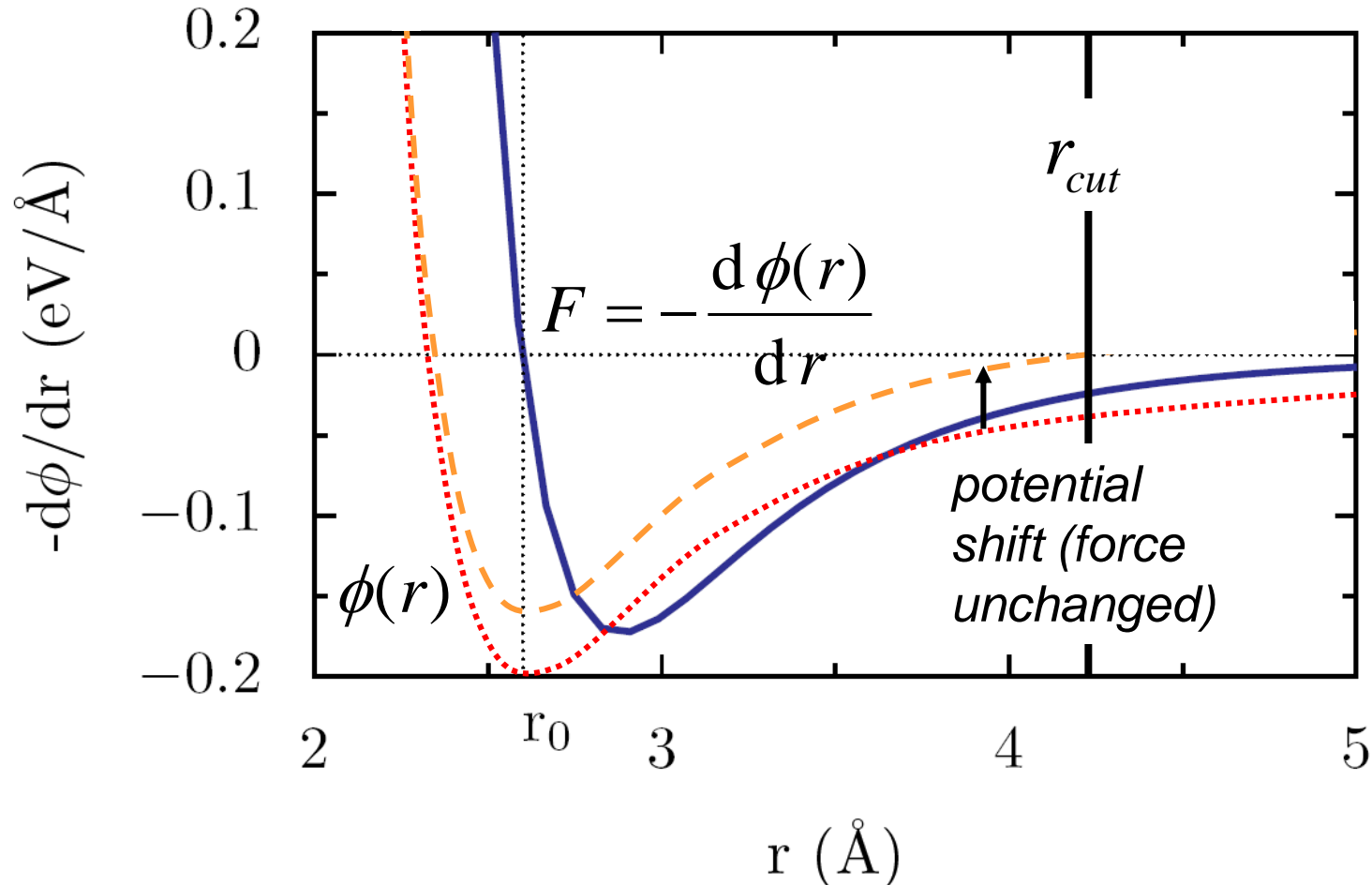
Cutoff radius

$$U_i = \sum_{j=1}^{N} \phi(r_{ij})$$

$$U_i = \sum_{j=1..N_{neigh}} \phi(r_{ij})$$

LJ 12:6 potential

$\sim\sigma$

ε_0

r_{cut}

r_{cut}

ϕ

r

Cutoff radius = considering interactions only to a certain distance
Basis: Force contribution negligible (slope)

Derivative of LJ potential ~ force

Beyond cutoff: *Changes in energy (and thus forces) small*