DUCTILE-BRITTLE BEHAVIOR OF MICROCRACKS IN 3D

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Introduction

A large effort to understand ductile-brittle behavior in iron-based materials has been devoted in the recent past in the framework of continuum and atomic models and as well in experiments.

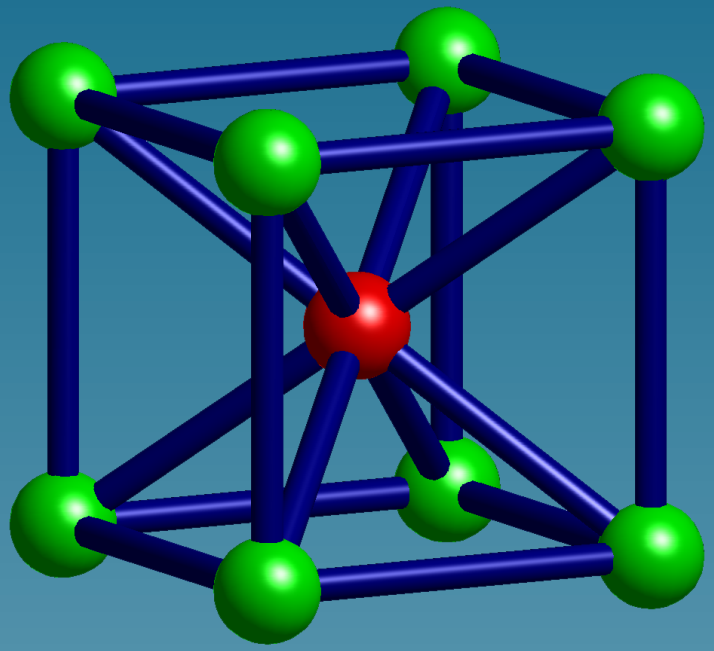
The models consider usually plane strain conditions (2D) along the crack front. Here, good agreement can be reached between continuum predictions and atomistic simulations of the ductile-brittle behavior at the crack tip.

However, free sample surface (where plane stress conditions are expected in the normal direction) may influence the ductile-brittle behavior.

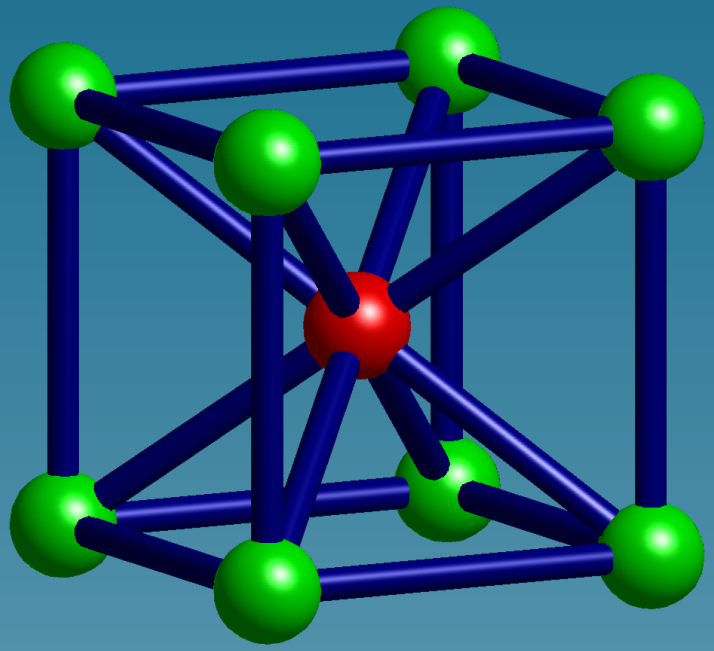
Such studies require 3D simulations.

Problem description

bcc iron crystal



bcc iron crystal



Thick sample (prevailing plane strain):

$400 \times 400 \times 400 + 399 \times 399 \times 399 \rightarrow 128$ million atoms

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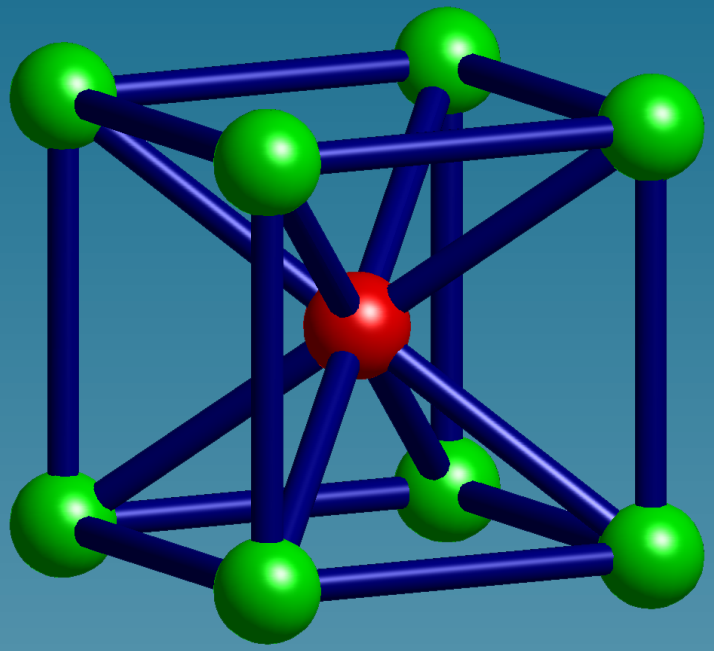


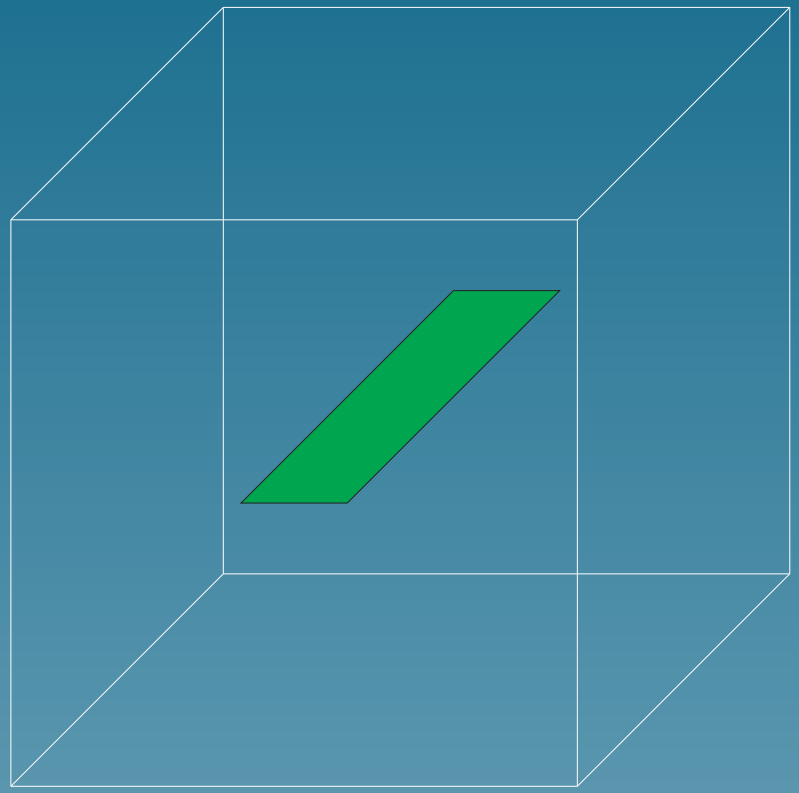
Thick sample (prevailing plane strain):

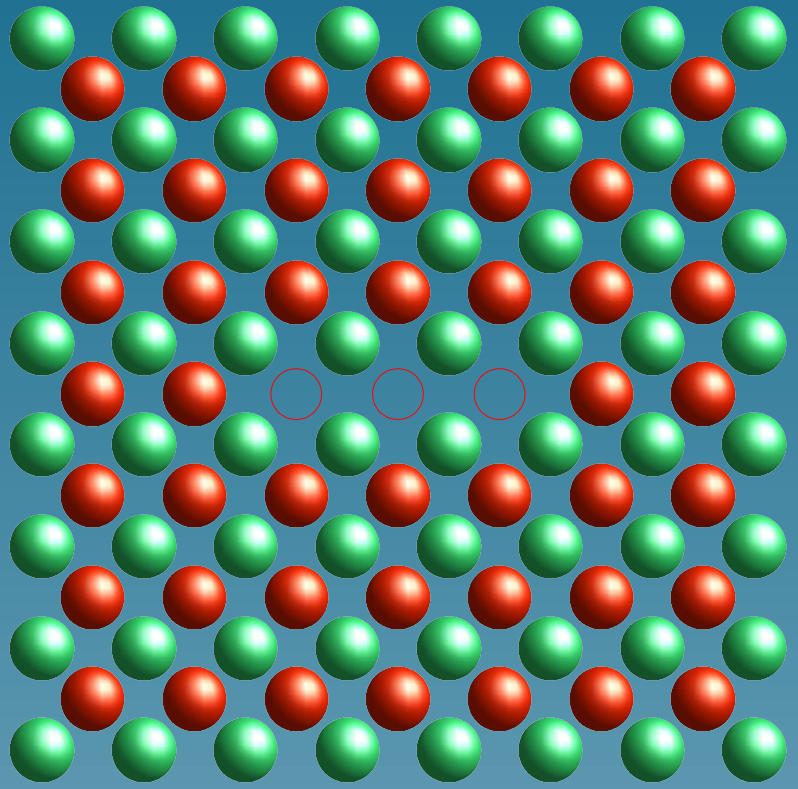
$$400 \times 400 \times 400 + 399 \times 399 \times 399 \rightarrow 128 \text{ million atoms}$$

Thin sample (prevailing plane stress):

$$1000 \times 1000 \times 50 + 999 \times 999 \times 49 \rightarrow 100 \text{ million atoms}$$

Crack description





Size: $79 \times 399 \times 1$ (thick sample), $199 \times 49 \times 1$ (thin sample)

Method: extraction (removal) central atoms

Program realization: bond restriction, i.e. atomic interactions over crack plane are not allowed.

Type of loading

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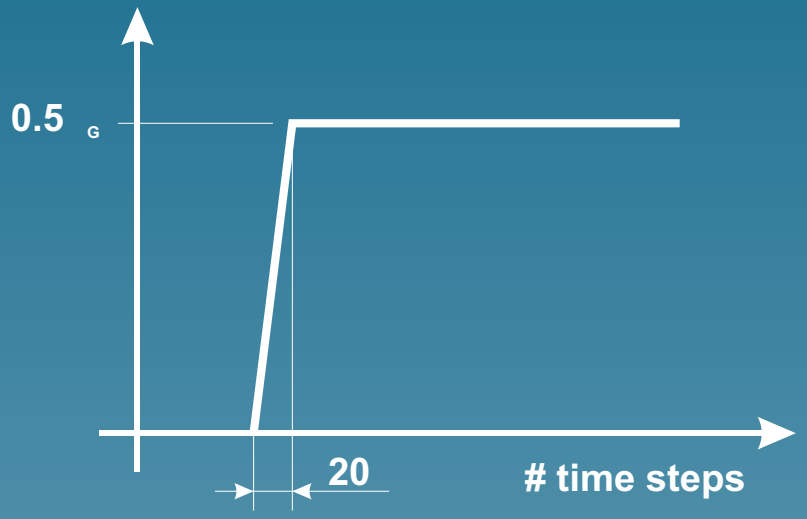
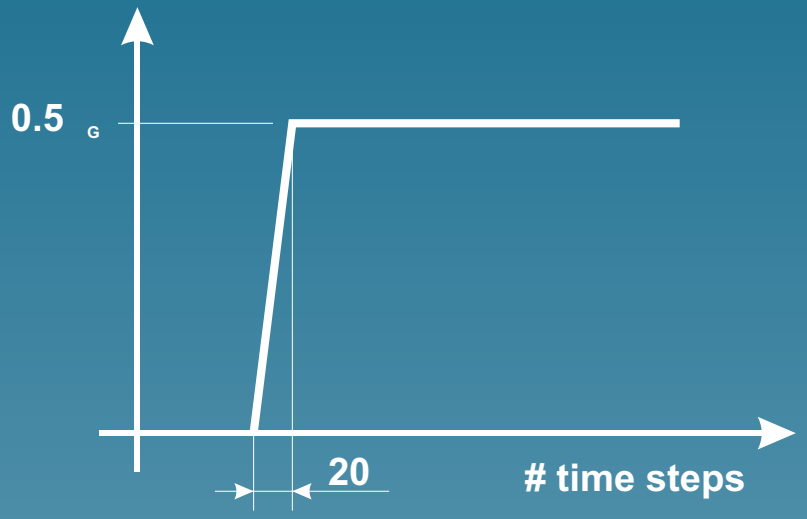


Impact: 0 K only

Type of loading



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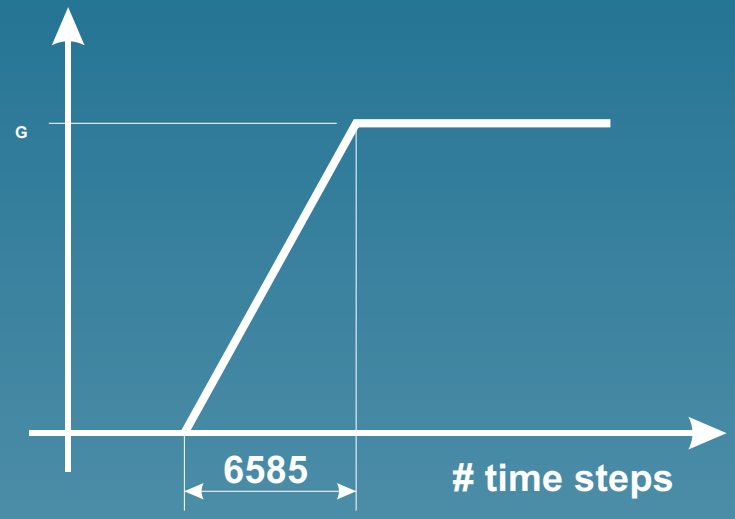
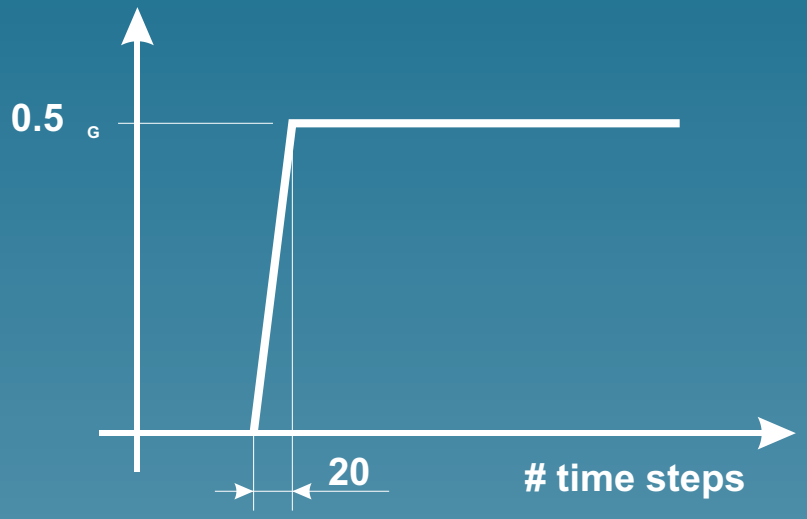


Quasistatic: 0 K and 300 K

Type of loading



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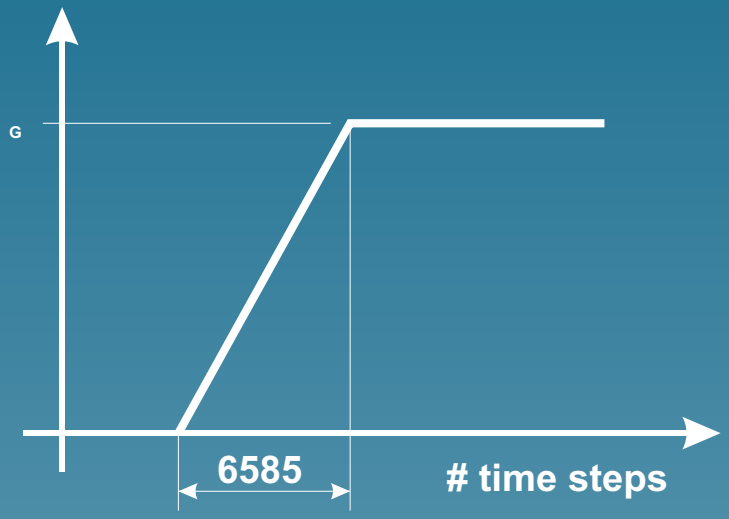

Quasistatic: 0 K and 300 K

Tension MODE I

Many-body interatomic potential

G.J.Ackland, D.J.Bacon, A.F.Calder, T.Harry:
Computer simulation of point defect properties in dilute Fe-Cu alloy using a many-body interatomic potential.
Philosophical Magazine A, 1997, Vol. 75, No. 3, 713–732

The energy of an assembly of N atoms is given by

$$E = \frac{1}{2} \sum_{i \neq j=1}^{N} \underbrace{V(r_{ij})}_{\substack{\text{repulsive} \\ \text{potential}}} - \sum_{i=1}^{N} \left(\sum_{j \neq i=1}^{N} \underbrace{\phi(r_{ij})}_{\substack{\text{cohesive} \\ \text{potential}}} \right)^{1/2}$$

Integration of equations of motion

Newtonian equations of motion are solved by

the central difference method.

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the central difference method.

Time integration step:

$$1 \times 10^{-14} \text{ s}$$

(even for heating)

Simulation steps

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1. Generation of the crystal containing the crack.

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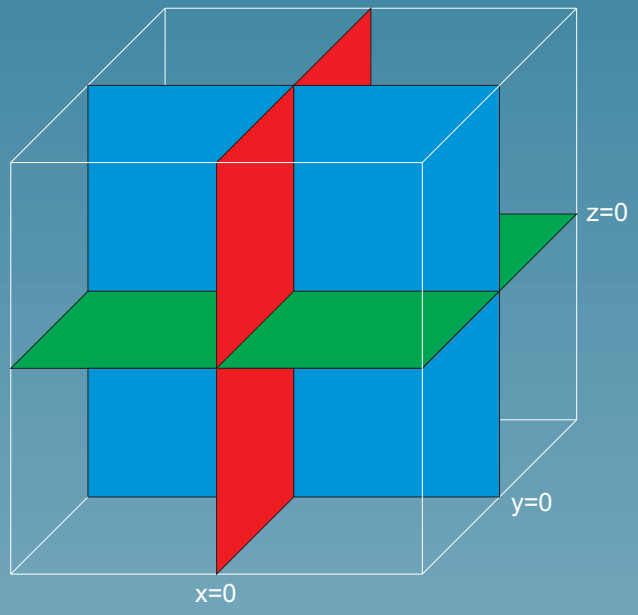
2. Fixation,
   i.e. atoms in plane $x = 0$, $y = 0$, $z = 0$ can move only in a given plane.



3. Surface relaxation,
   i.e. set system to equilibrium state
   (minimum potential energy and kinetic energy nearly zero).

   Pendulum method:
   J.B.Gibson, A.N.Goland, M.Milgram, G.H.Vineyard:
   Phys. Rev., **120**, p.1229, 1960

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4. Heating,
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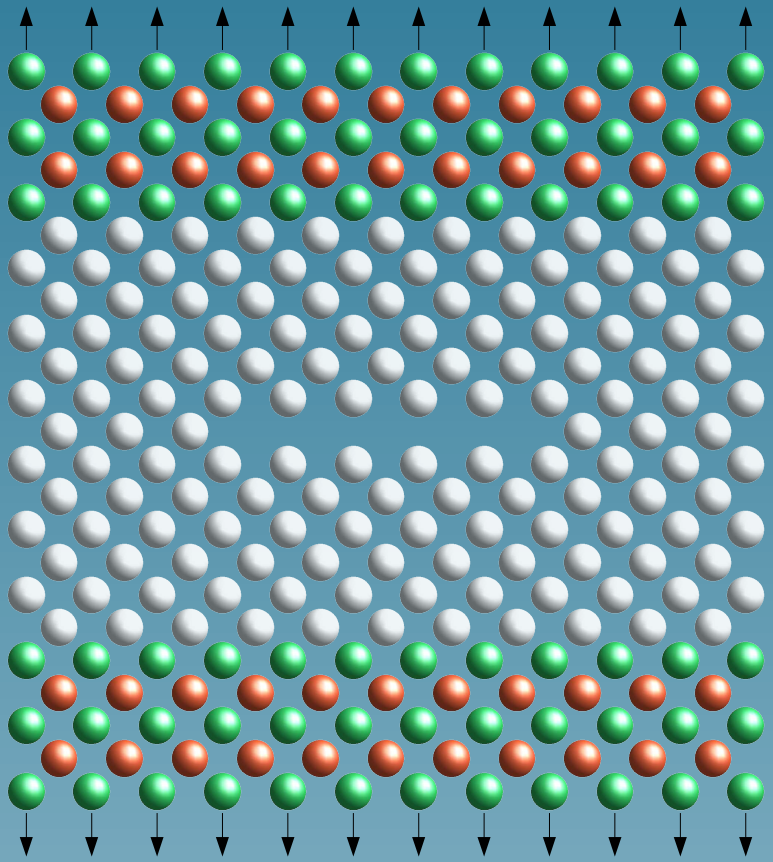
4. Heating,
   gradual Maxwell heating, i.e. scaling of atomic velocity.

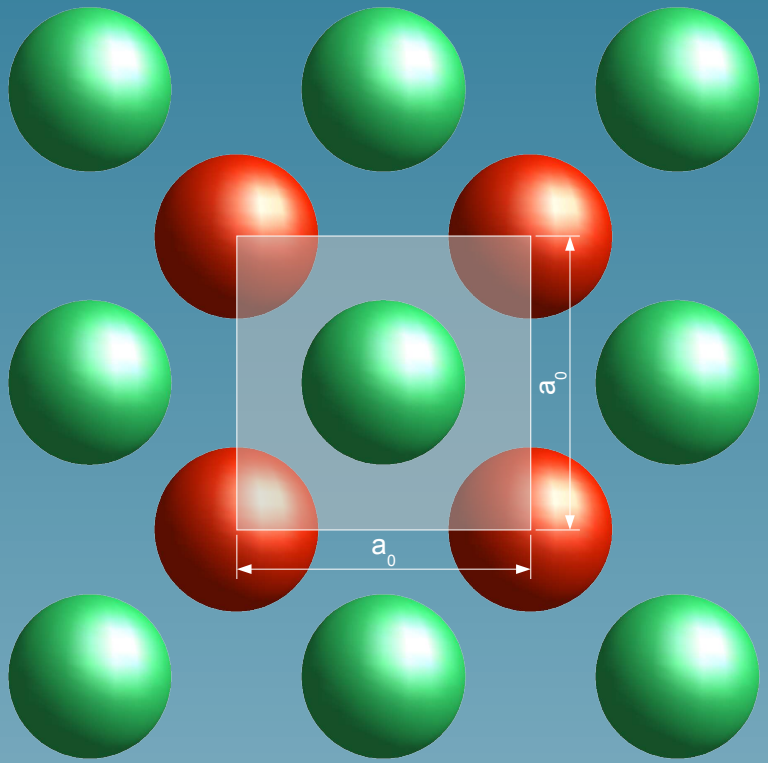
5. Remove fixation.

6. Loading

   symmetric loading,

   distributed in 5 surface layers





Simulation technique

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Simulation code has been written in *Fortran 90*.

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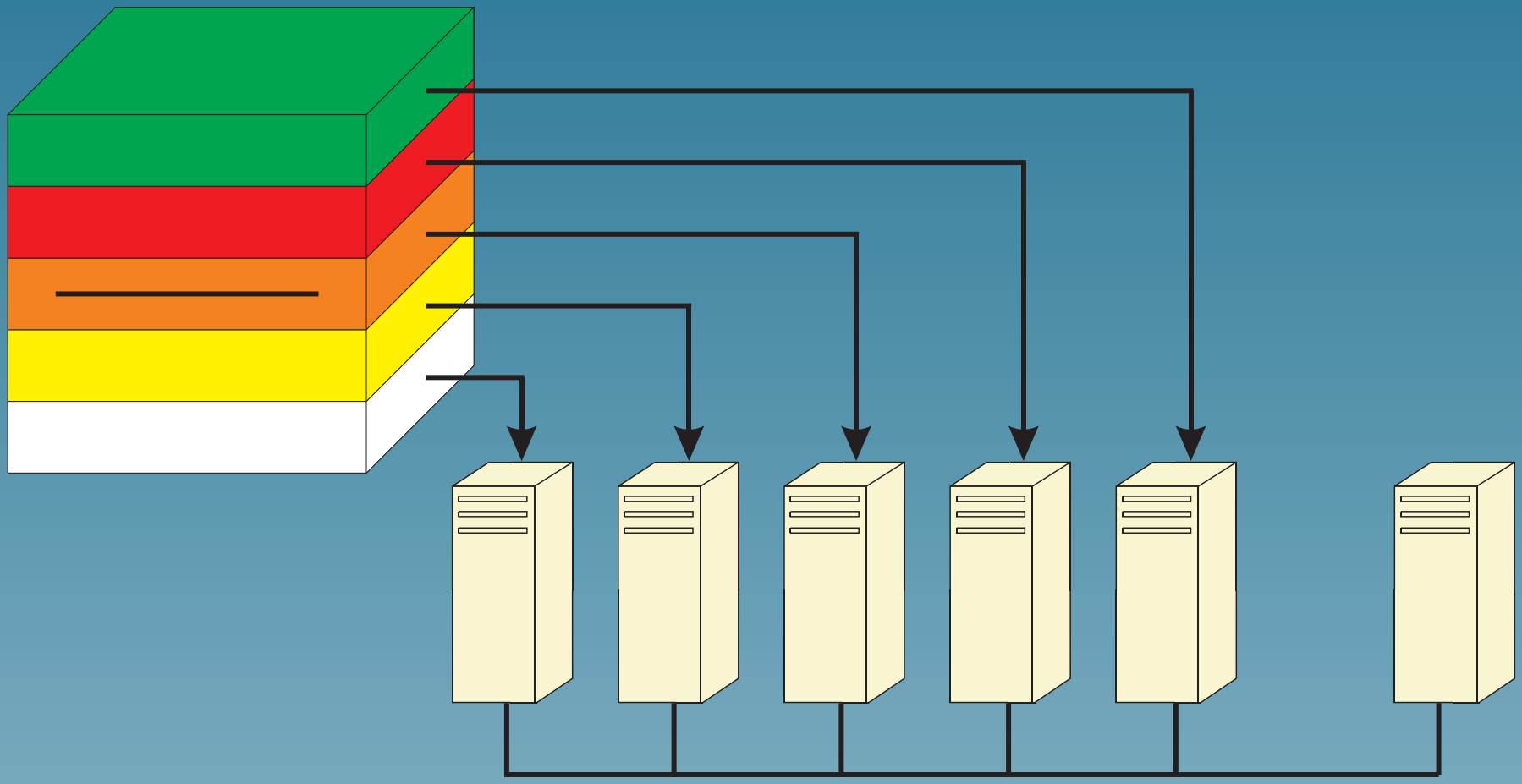
Parallel task



Simulation code has been developed under system MPI
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Used MPI-functions:

- MPI_INIT, MPI_FINALIZE,
- MPI_COMM_RANK, MPI_COMM_SIZE,
- MPI_SEND, MPI_RECV, MPI_BCAST,
- MPI_ISSEND, MPI_IRECV,
- MPI_WAIT.

Memory requirement:

$$6 \times 8 + 2 \times 8 = 64 \text{ bytes/atom},$$

thick sample: 8 GB $\rightarrow$ 12 nodes 1 GB RAM

thin sample: 6.4 GB $\rightarrow$ 10 nodes 1 GB RAM

Memory requirement:

$$6 \times 8 + 2 \times 8 = 64 \text{ bytes/atom},$$
thick sample: 8 GB $\rightarrow$ 12 nodes 1 GB RAM
thin sample: 6.4 GB $\rightarrow$ 10 nodes 1 GB RAM

Disk requirement:

$$6 \times 8 = 48 \text{ bytes/atom},$$
thick sample: 6 GB
thin sample: 4.8 GB

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$$6 \times 8 = 48 \text{ bytes/atom},$$
thick sample: 6 GB
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Hash: cell index method (link cell method)

M.P.Allen, D.J.Tildesley:
Computer Simulation of Liquids.
Oxford University Press, New York, 1987

D. Frenkel, B. Smit:
Understanding Molecular Simulations.
Academic Press, New York, 1996

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32 CPU's
Dual Pentium III
700 MHz
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Fast Ethernet

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Fast Ethernet

MINOS
32 CPU's
Dual Athlon MP1900+
1.6 GHz
512 MB/CPU
16 x 40 GB
Gigabit

SKIRIT
32 CPU's
Dual Pentium III/XEON
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512 MB/CPU
16 x 18 GB
Fast Ethernet, Myrinet

Results

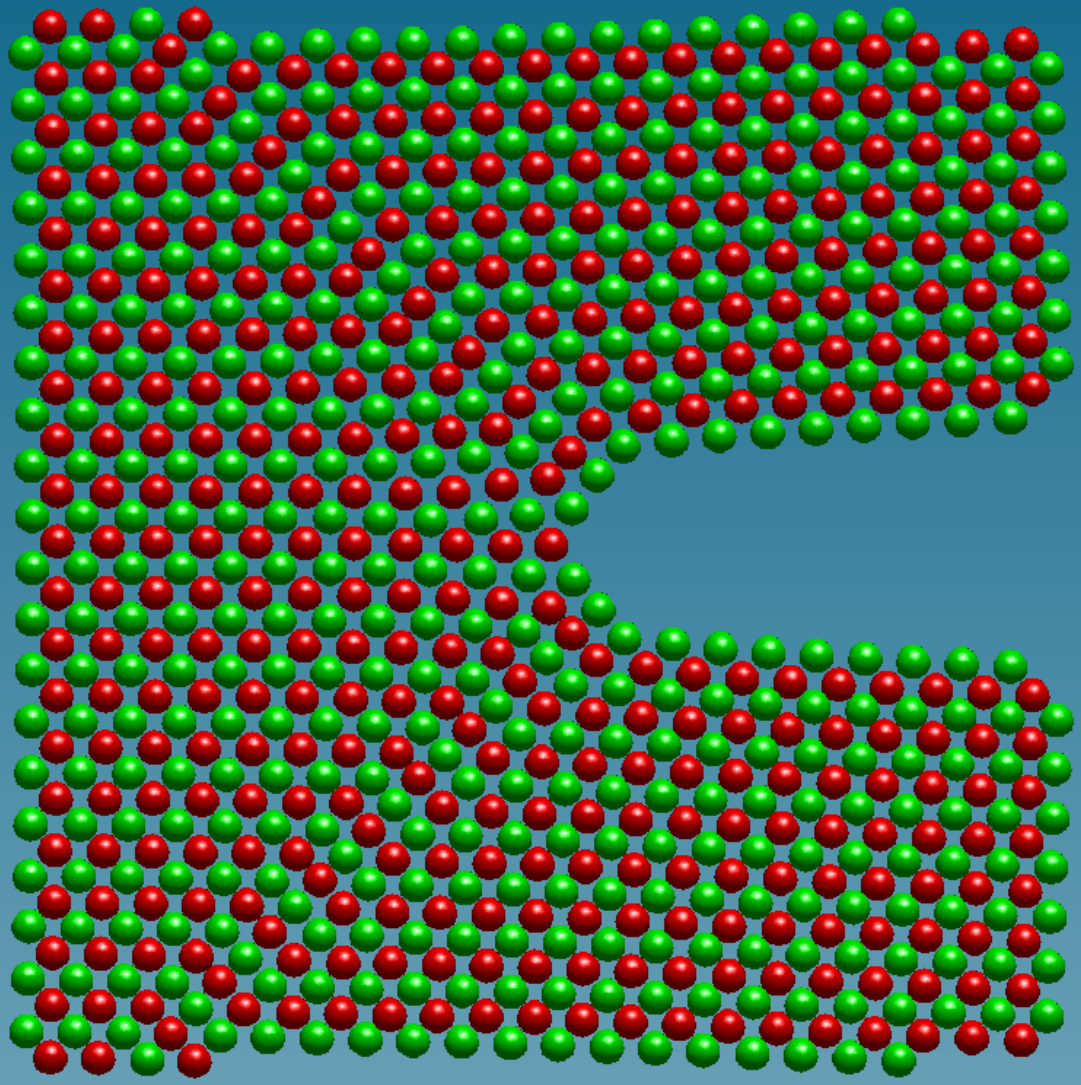
Thin sample under quasi-static loading at 0 K

Brittle crack initiation has been observed in the middle of the sample under applied stress intensity

$$K_{IA} \approx 1.1 K_G$$

Thick sample under impact loading at 0 K

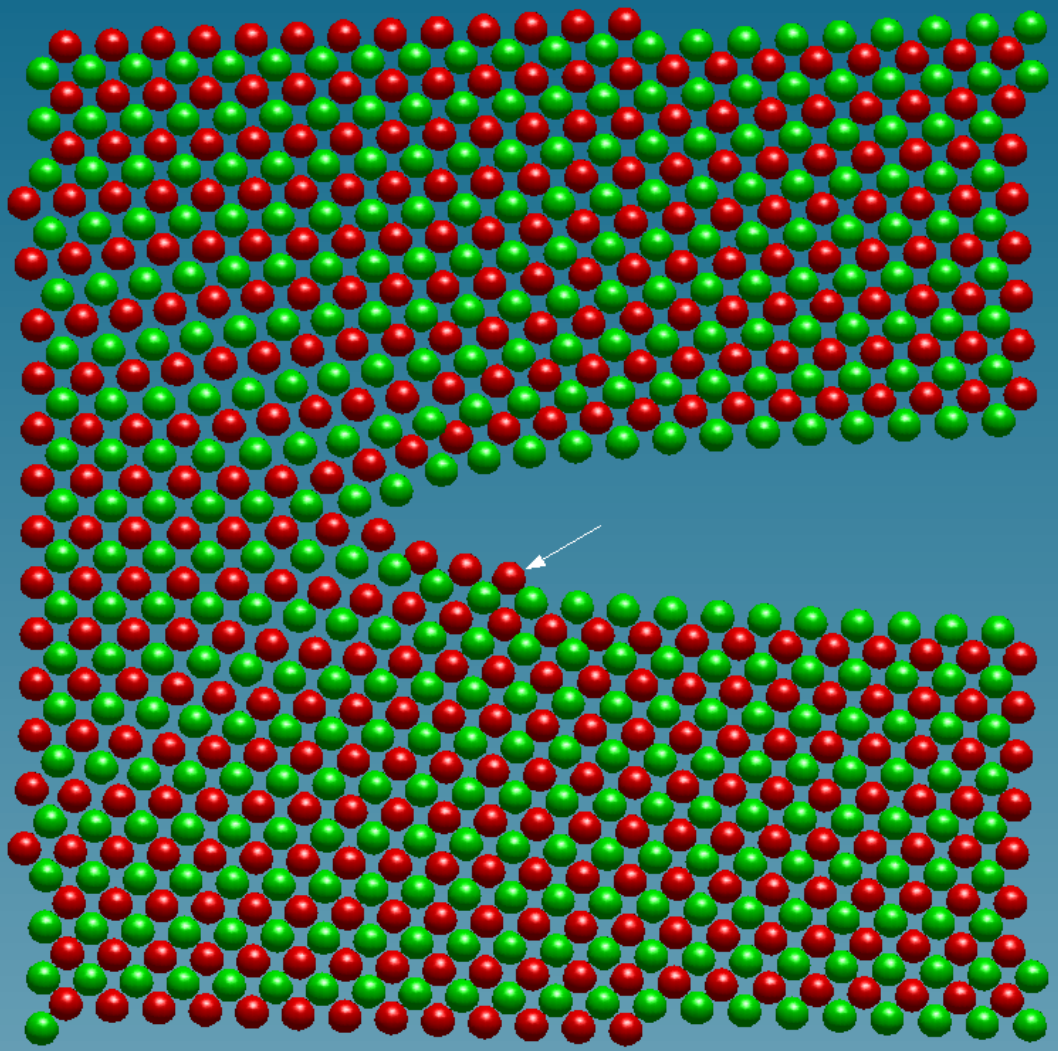
- Twin formation and crack initiation after twinning
  near the free sample surface perpendicular to crack front.
- In the middle of the sample only stacking faults at the crack front
  (without crack initiation).
- At time step 4000, the situation along the crack front
  is already complicated, since it is influenced
  by the back reflections of the incident loading waves
  from the free sample surfaces.



Twinning at the left crack front near the free surface.
Loading $\sigma_A = 0.5\sigma_G$, time step 4000.

Thick sample under quasi-static loading at 0 K

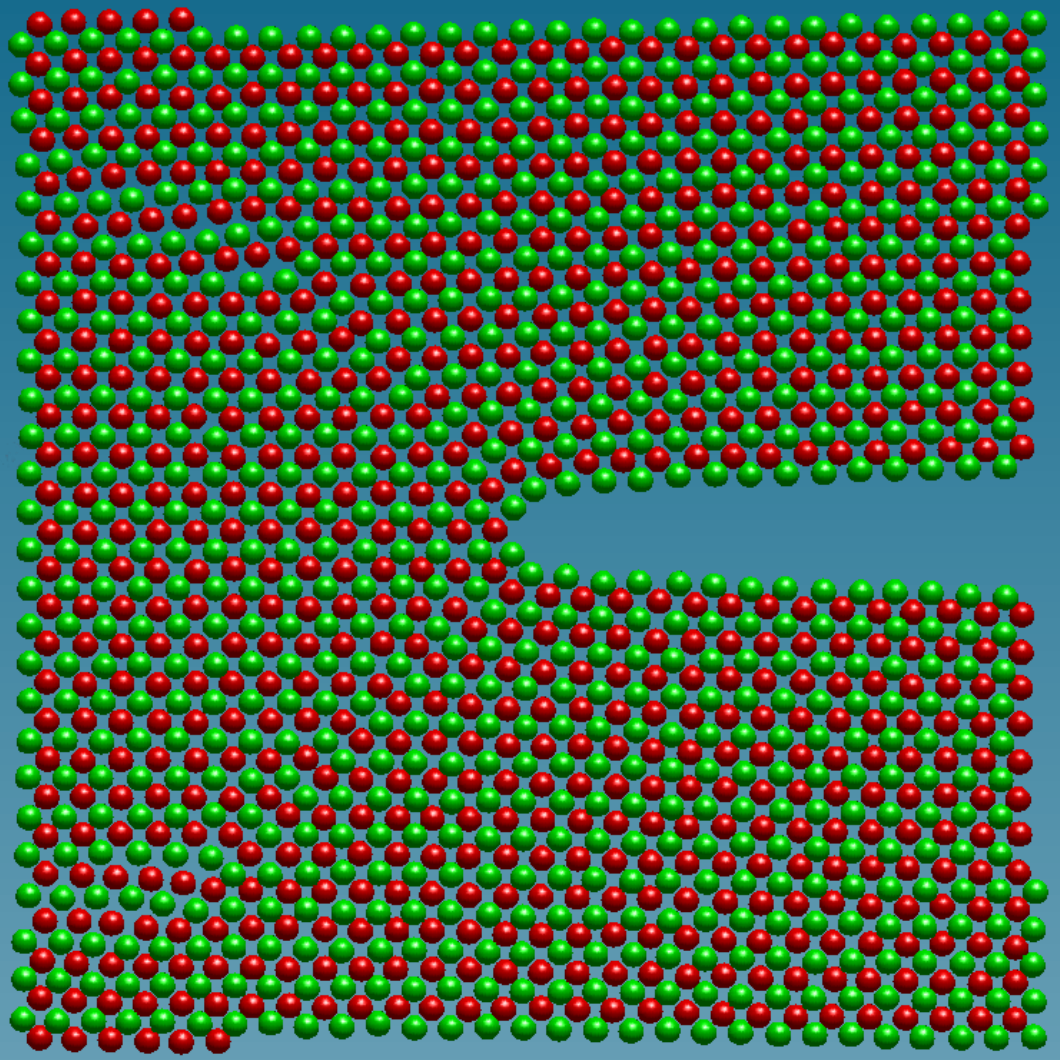
- Crack initiation already at time step 6000 near the twinned surface region.
- Crack initiation in the middle of the sample later at time step 7760.
- The presented results are in qualitative agreement
  with previous plane strain simulations
  and with experimental observations that twinning and fracture cooperates.
- The inhomogeneous crack expansion along the crack front
  can be explained by the transition plane stress (near the free surface)
  vs. plane strain (in middle of a thick crystal).



Crack initiation near the free surface.
Time step 6000.

Thick sample under quasi-static loading at 300 K

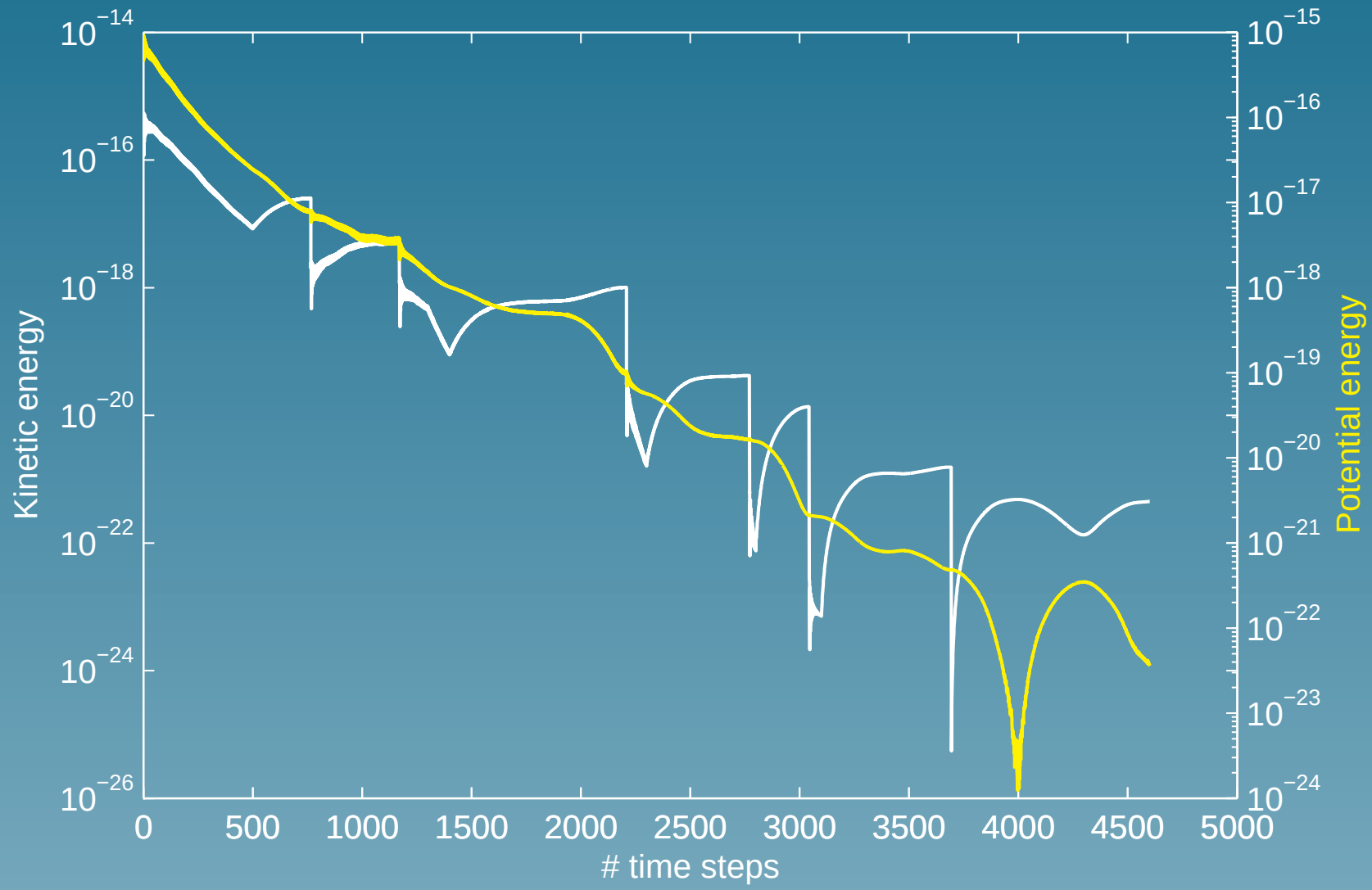
- Initially emission of dislocations on $\{112\}$ planes at the free sample surface perpendicular to the crack front in time step 5000.
- It is in a qualitative agreement with experiments on Fe-Si single crystals where dislocation emissions on $\{112\}$ planes have been observed before a ductile crack initiation.
- It also agrees with the theoretical analysis revealing that thermally activated emission of dislocation loops on oblique slip planes to the crack front is possible near the free surfaces also for bcc iron.
- At time step 6000, twin formation near the surface and also crack initiation. The initiation is more homogeneous along the crack front at 300 K in comparison with 0 K, since thermal vibration of atoms can remove the sharp transition plane stress - plane strain near the free surface.
- The observed transformation dislocation $\longrightarrow$ twin on $\{112\}$ planes is possible also according to the model by Ogawa.



Dislocation emission near the free surface.
Time step 5000.

Question time

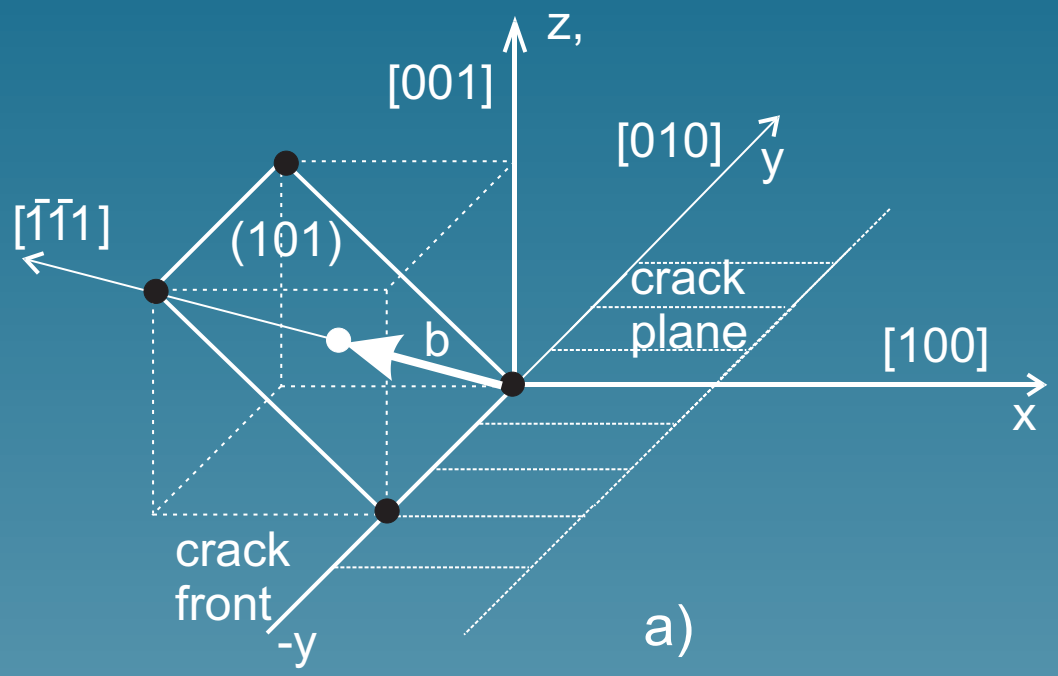
Surface relaxation



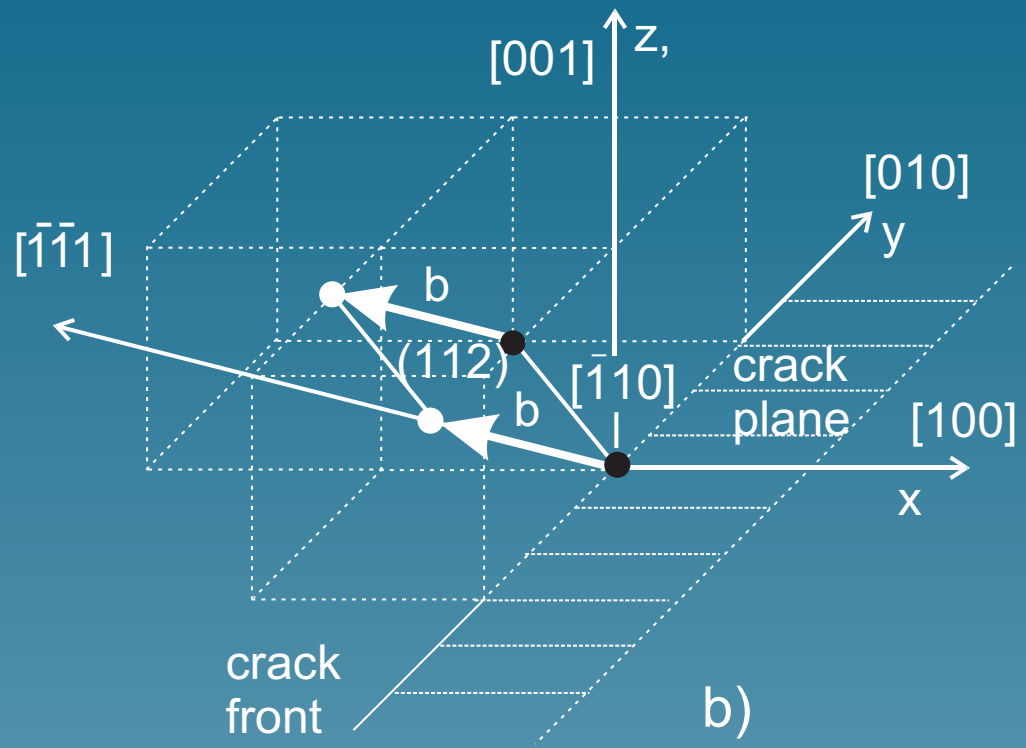
Heating

1. Maxwell heating to 0.5 K,
2. Obtaining of velocity directions,
3. Velocity scaling to 300 K,
4. Relaxed crystal scaling to 300 K,
5. Velocity assignment,
6. Stabilization (1000 time steps),
7. Energy computation.

Slip systems



The slip system (101)[-1-11] is inclined to the crack front and contains the crack front. Dislocation emission in this slip system results in the two crystalline blocks being pulled apart in the $\langle 001 \rangle$ directions, which was verified in 3D by block like shear simulations along a 101 plane in the direction of the Burgers vector $\mathbf{b} = a_o/2$[-1-11]. It causes crack blunting.



The second slip system (112)[-1-11] is oblique to the crack front and dislocation emission makes a jog in the crack front in the direction of b. Also generation of stacking faults and twinning is possible in these slip systems $\{112\}\langle 111\rangle$, without crack tip blunting. Analysis of atomic displacements from the 3D simulations and the larger Schmid factor (0.47) indicate that our shear processes occur on 112 planes.

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Heating

Slip systems