ACOUSTIC EMISSION FROM FAST DISLOCATIONS IN 3D BCC IRON CRYSTALS

Petr Hora, Anna Machová,
Jan Červ, and Alena Uhnáková

Institute of Thermomechanics AS CR, v. v. i.
Prague, Czech Republic

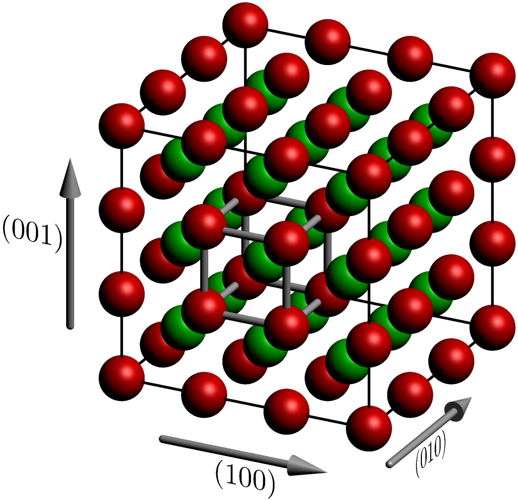
WAVE MODELLING 2018
The 2nd International Conference
on Advanced Modelling of Wave Propagation in Solids
September 17 – 21, 2018, Prague, Czech Republic

Introduction

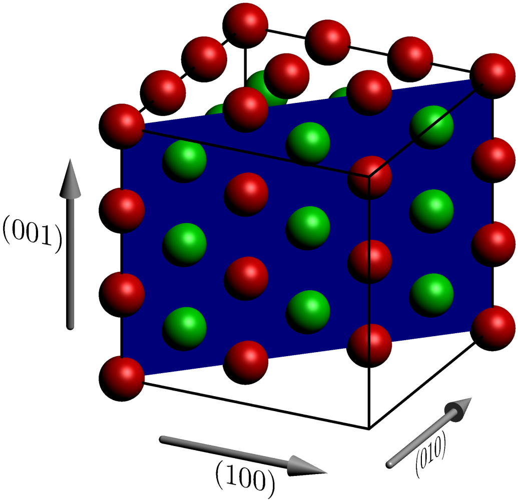
- Kinetics of dislocations emitted from a crack is studied via molecular dynamics (MD) in a 3D bcc iron crystal.
- The atomistic results show that edge dislocation segments in the middle of the crystal accelerate at the nearest vicinity of the free crystal surface.
- The dislocations in MD penetrate the surface layers in transonic or supersonic regime.
- Possible sources for such behavior are discussed in the framework of continuum models and by means of stress calculations on the atomistic level.
- Acoustic emission patterns arising from the fast dislocation motion in MD are visualized via the local kinetic energies of individual atoms and further modeled as a moving source of the stress waves in anisotropic continuum.

Problem description

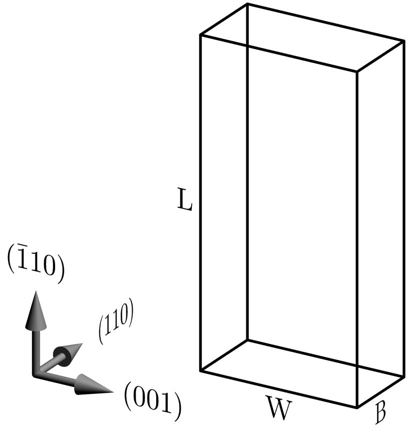
Material (bcc iron)



Orientation



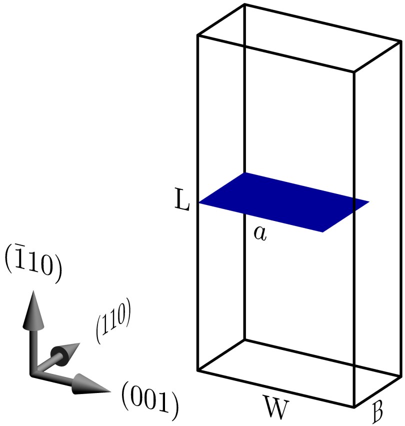
Sample geometry



$440 \times 220 \times 30$ atoms

$439 a_0 \sqrt{2}/2 \times 219 a_0/2 \times 29 a_0 \sqrt{2}/2$

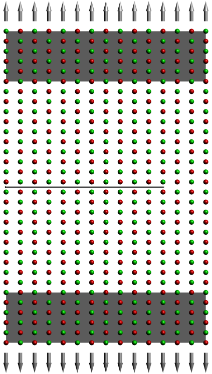
Edge crack description

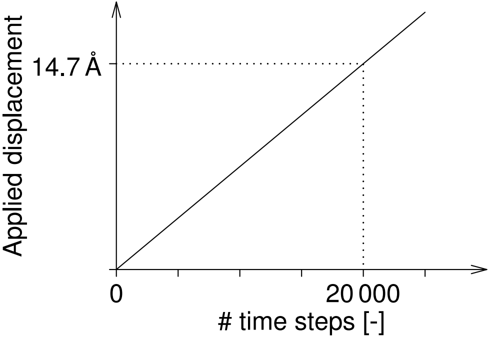


Length $0.8 \times W$

Initial crack atomic interactions over crack plane are not allowed

Kinematic loading





Temperature: 0 K
Tension mode: I
Observation planes: (110) two layers
Distributed in 6 surface layers

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

$$E = \frac{1}{2} \sum_{i \neq j = 1}^{N} V\left(r_{ij}\right) \; - \; \sum_{i=1}^{N} \left(\sum_{j \neq i = 1}^{N} \phi\left(r_{ij}\right) \right)^{1/2}$$

$V\left(r_{ij}\right)$ - pair repulsive potential

$\phi\left(r_{ij}\right)$ - many-body cohesive potential

Integration of equations of motion

Newtonian equations of motion are solved by the central difference method.

Time integration step:

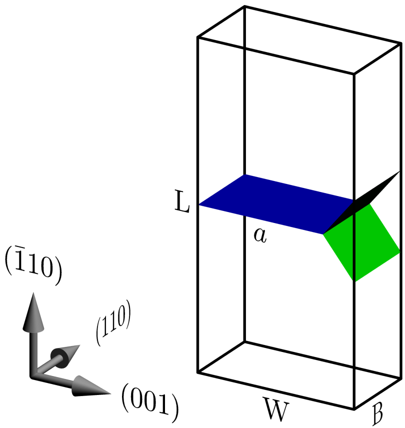
$$1 \times 10^{-14}\ \mathrm{s}$$

MD simulation

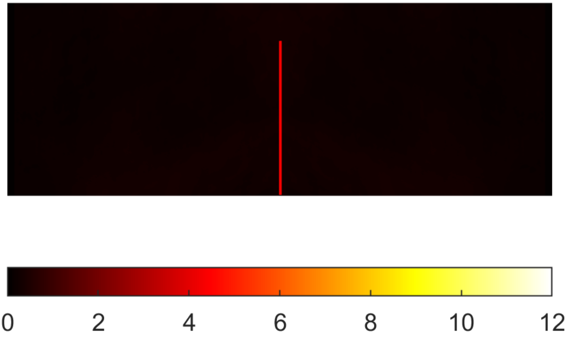
1. Generation of the crystal containing the crack.
2. Surface relaxation,
   i.e. set system to equilibrium state
   (minimum potential energy and kinetic energy nearly zero).
3. Kinematic loading, free 3D MD simulation

Simulation code has been written in *Fortran 90*.

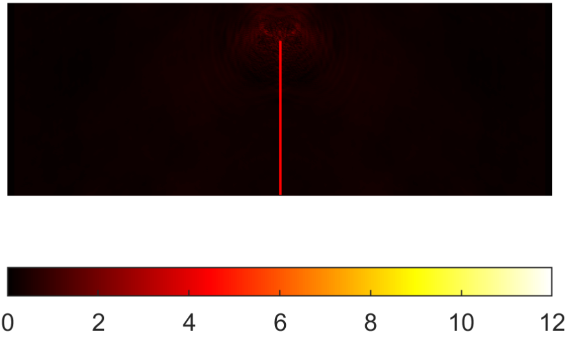
The inclined slip systems: $[\bar{1}11](\bar{1}1\bar{2})$ and $[1\bar{1}1](\bar{1}12)$



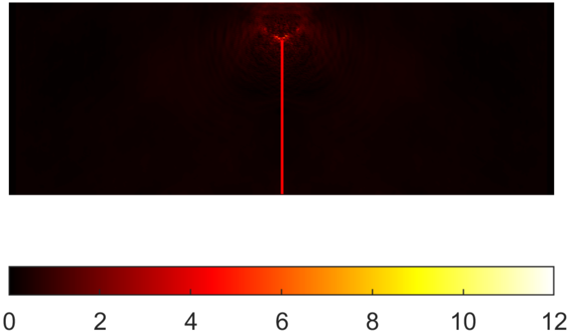
Kinetic energy, time step: 11000



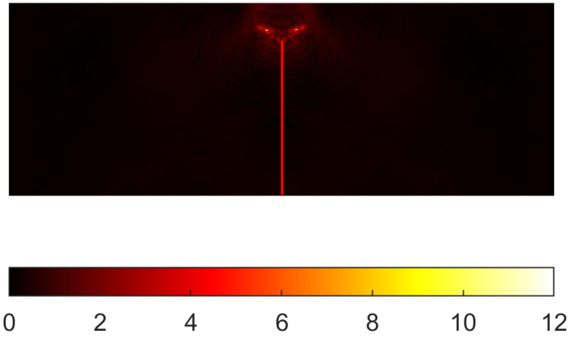
Kinetic energy, time step: 11500



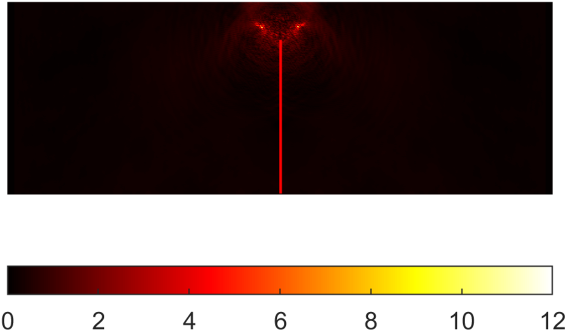
Kinetic energy, time step: 11550



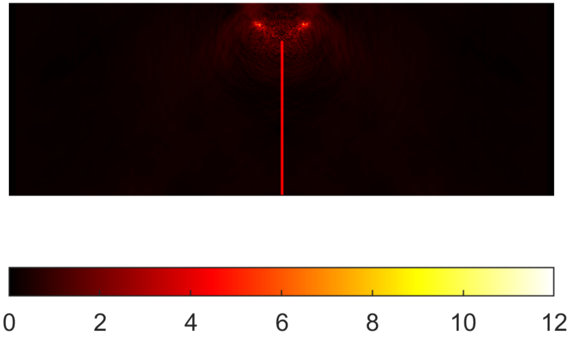
Kinetic energy, time step: 11600



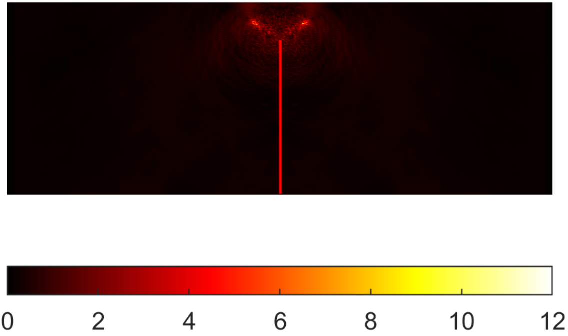
Kinetic energy, time step: 11620



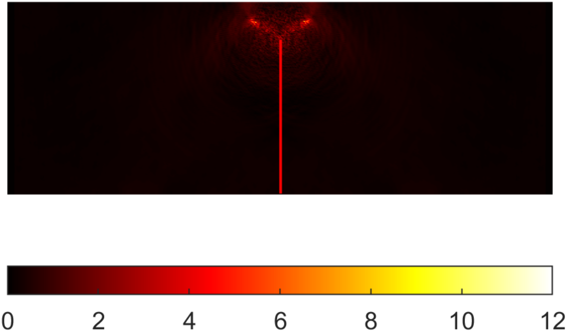
Kinetic energy, time step: 11640



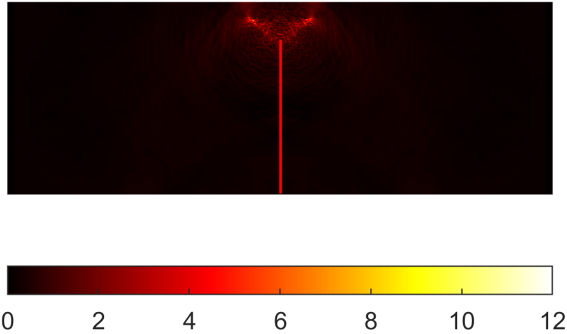
Kinetic energy, time step: 11650



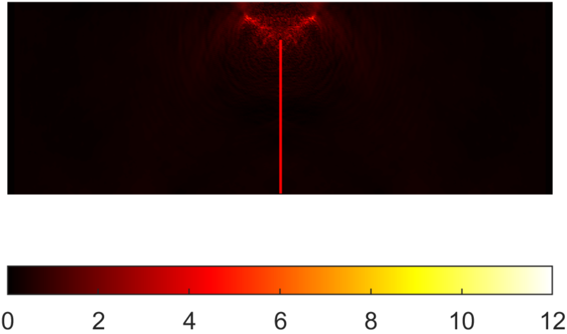
Kinetic energy, time step: 11660



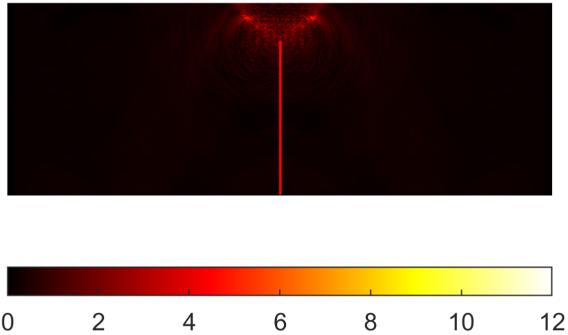
Kinetic energy, time step: 11680



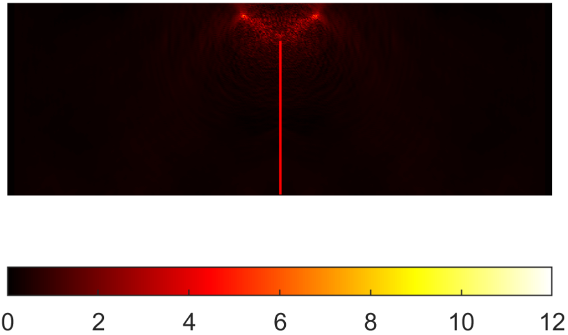
Kinetic energy, time step: 11700



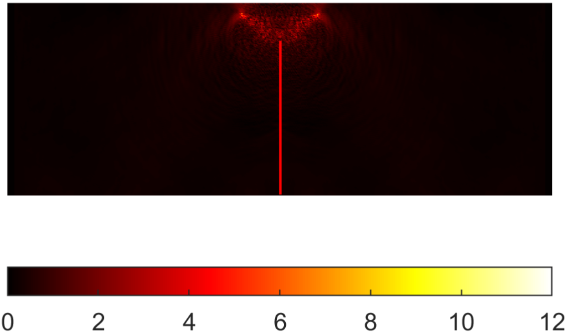
Kinetic energy, time step: 11720



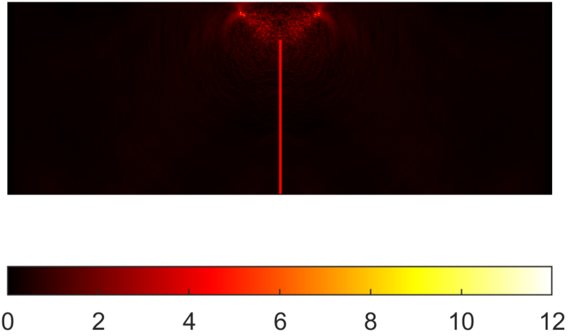
Kinetic energy, time step: 11740



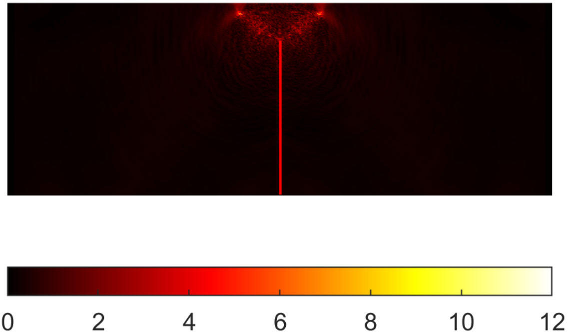
Kinetic energy, time step: 11750



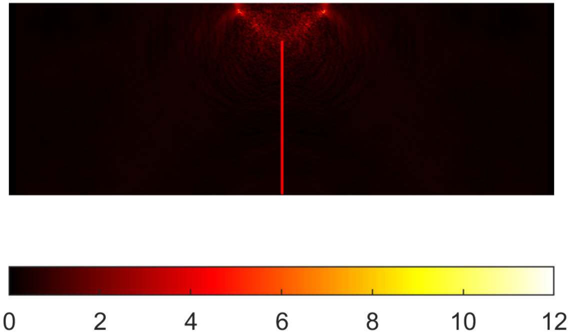
Kinetic energy, time step: 11760



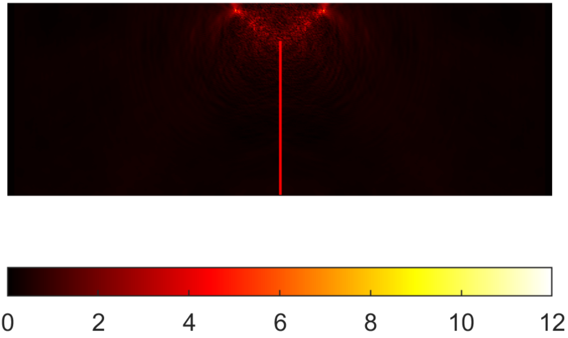
Kinetic energy, time step: 11780



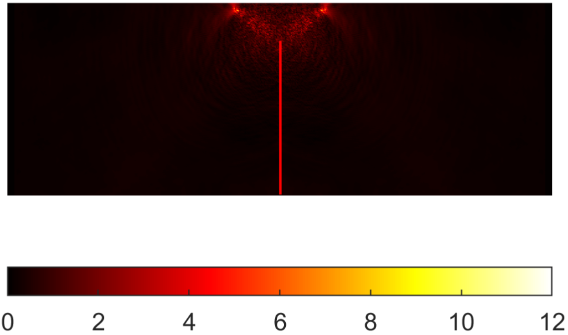
Kinetic energy, time step: 11800



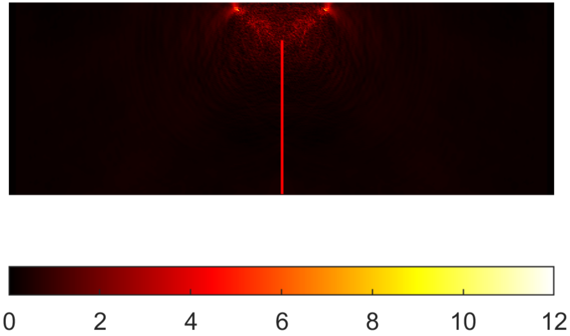
Kinetic energy, time step: 11810



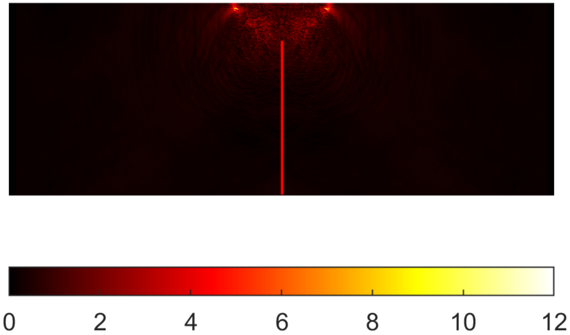
Kinetic energy, time step: 11820



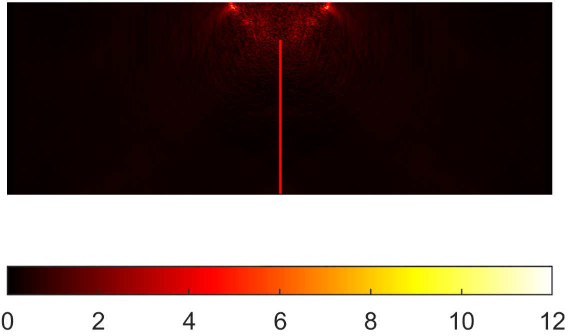
Kinetic energy, time step: 11830



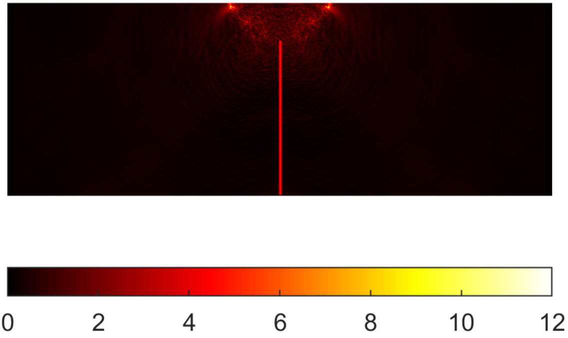
Kinetic energy, time step: 11840



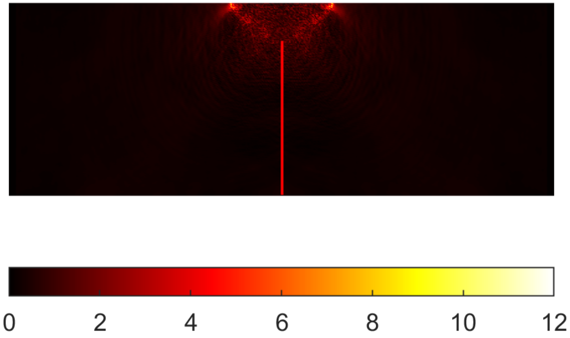
Kinetic energy, time step: 11850



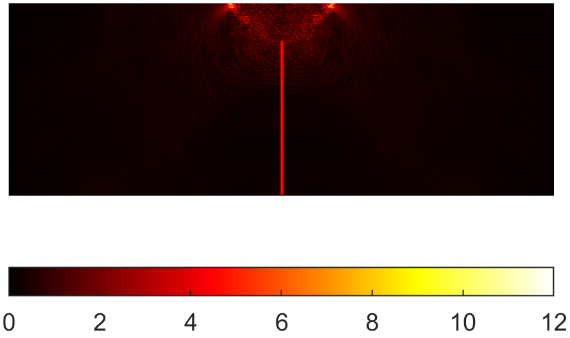
Kinetic energy, time step: 11861



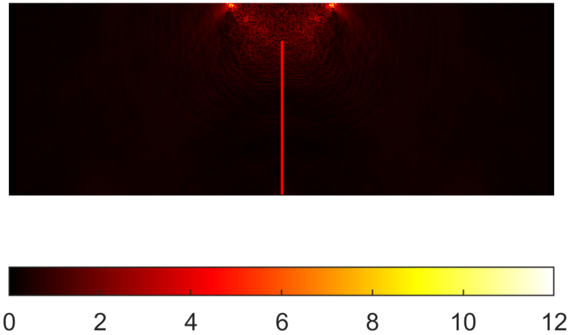
Kinetic energy, time step: 11870



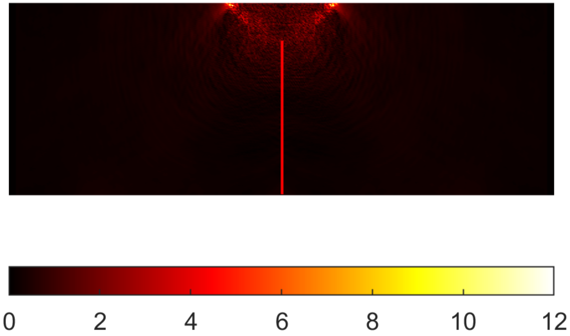
Kinetic energy, time step: 11880



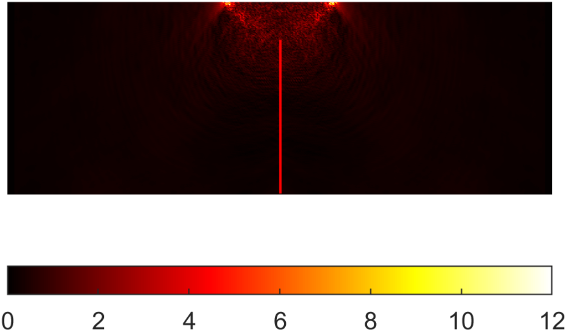
Kinetic energy, time step: 11885



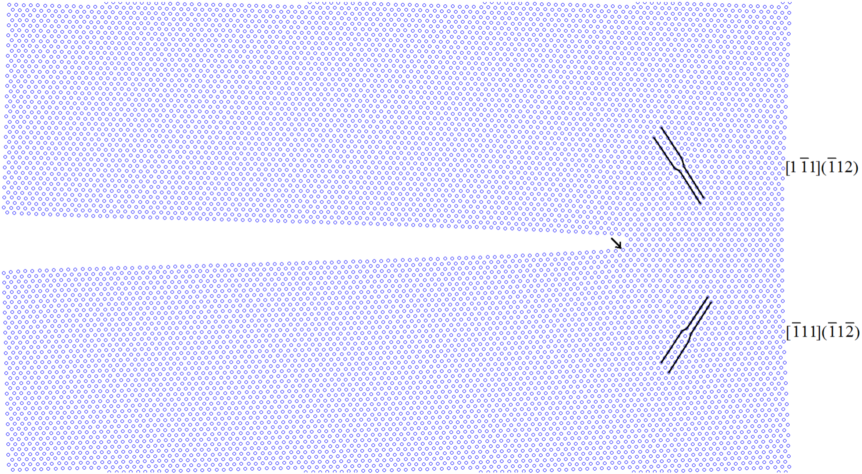
Kinetic energy, time step: 11890



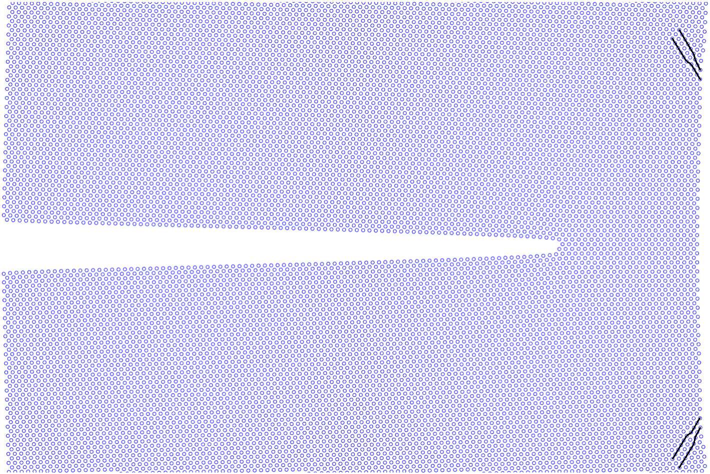
Kinetic energy, time step: 11900



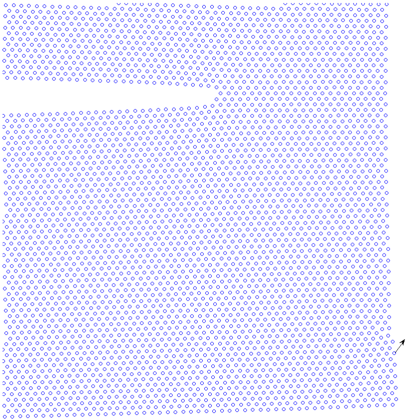
The first dislocation emission, time: 11600*h*



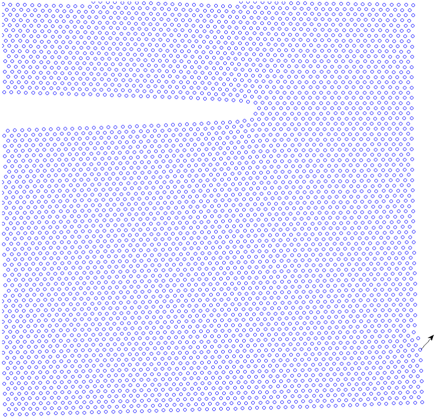
Dislocation position at time: $11880h$



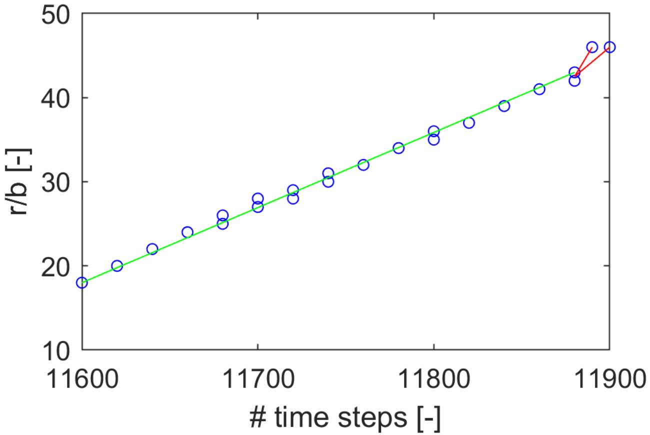
Surface steps at time: 11890h



Surface steps at time: 11900h



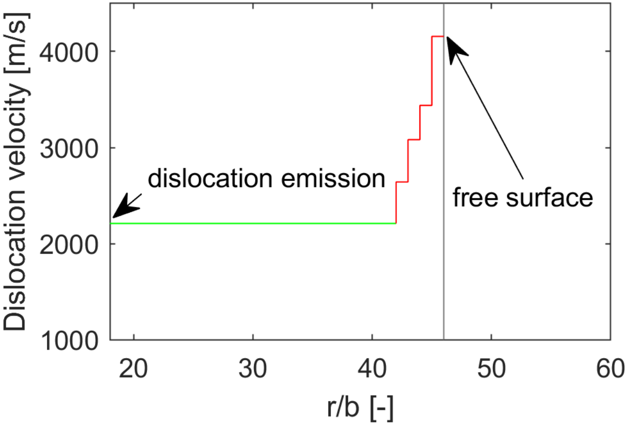
Dislocation motion



r ... distance from crack front, b ... Burgers vector magnitude

The green line corresponds to an average dislocation velocity (2210 m/s).

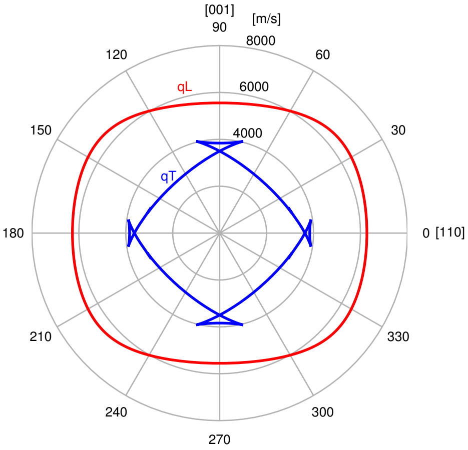
Dislocation velocity toward the free surface



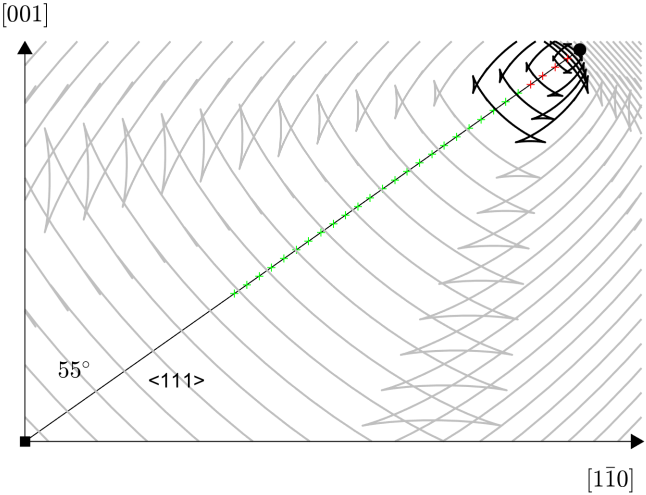
$c_T = 3007$ m/s; in the slip system $\langle 111 \rangle \{112\}$

Reconstruction of the wave pattern (AE) in anisotropic continuum

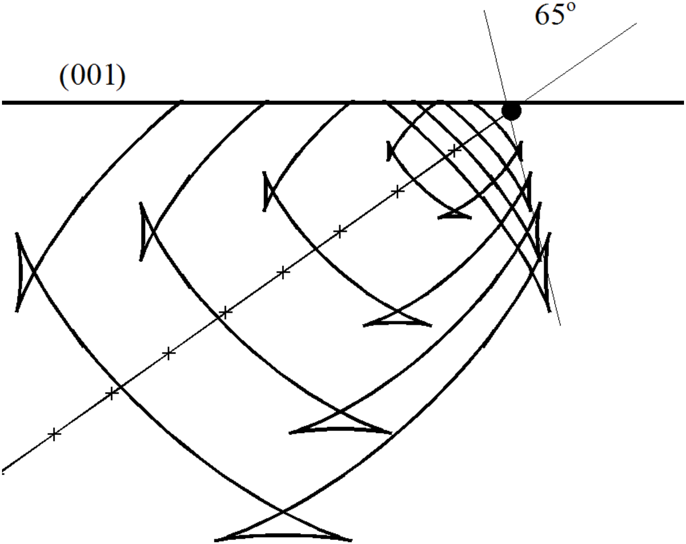
Section of the ray (wave) surfaces in the (110) plane



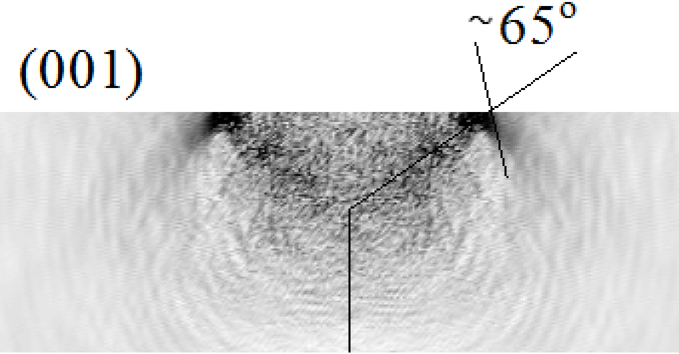
AE patterns near by the final position of the dislocation core at the free surface



Simplified reconstruction at the free surface



Comparison with a detail from MD



Conclusion

- Dislocation emission from edge crack $a/W = 0.8$ embedded in a 3D bcc iron crystal have been studied via MD by a direct graphical treatment of the atomistic configurations, further via mapping of the local kinetic energies of individual atoms (revealing the acoustic emission from dislocations) and also from the global energy balance.
- The graphical treatment of MD results show that the edge dislocation segments in the middle of the crystal after the emission move on the slip systems $\langle 111 \rangle \{112\}$ with a subsonic velocity up to a very close distance from the free surface (001) where they accelerate and penetrate the surface layers in transonic or supersonic regime.
- Analysis of the global energy balance and of the acoustic emission from the moving dislocations have been shown that dislocation motion in MD near by the free surface (001) can be accelerated to transonic regime (not supersonic), i.e. just above the velocity c_T of the transversal shear waves in the $\langle 111 \rangle$ direction.

Conclusion - cont.

- Additional (complementary) stress calculations on the atomistic level reveal the reason: the dislocations in MD accelerate to transonic regime at a close distance from the free surface due to the short ranged surface tension. It complies with experimental data on surface relaxation in bcc iron.
- The transonic regime $(V_{disl} = 1.35c_T - 1.38c_T)$ following from this study does not concern the dislocations in macroscopic experimental specimens under a low external loading. Here, the surface stress itself (without any external loading) may only cause an increment in dislocation velocity (of about 400 m/s by this study). It concerns a very short distance 1-3 lattice parameter from the free surface (001). The range of surface relaxation (and consequently the range of surface stress) in bcc iron differs in the individual crystallographic directions.
- This study indicates that the existence of an initial surface tension can facilitate disappearing of dislocations at the free crystal surfaces.

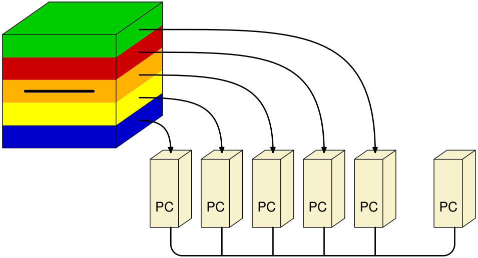
Thank you for your attention

The work was supported by the Institute Research Program RVO: 61388998
and by the projects of the Czech Science Foundation GACR 17-22615S and GACR 17-12925S.
The work of P. Hora was supported by the European Regional Development Fund under Grant No.CZ.02.1.01/0.0/0.0/15_003/0000493 (Centre of Excellence for Nonlinear Dynamic Behavior of Advanced Materials in Engineering).

Future

- Parallel task

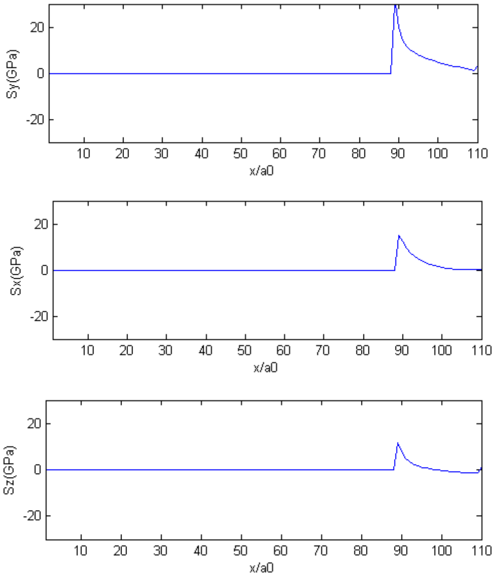
  Simulation code using MPI (Message Passing Interface).



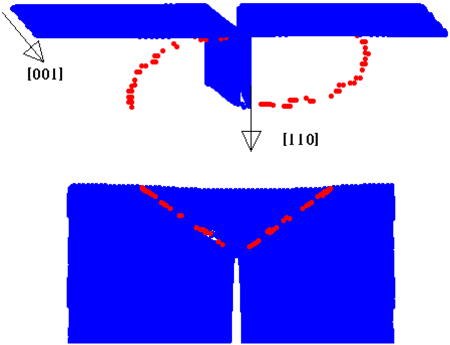
- Surface relaxation

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

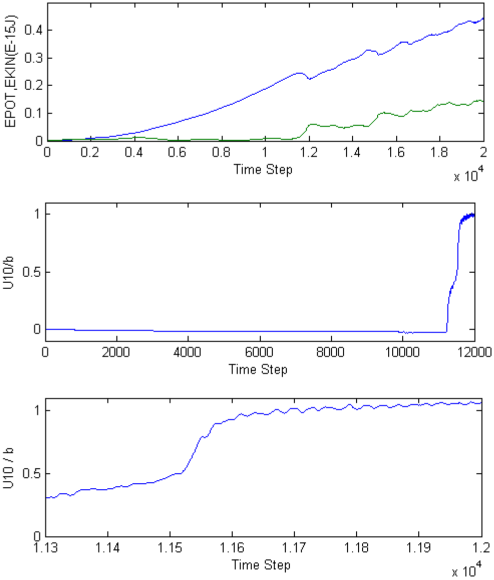
Stress components in the middle of the sample



3D visualization of the first emitted dislocations



The energy balance, the relative shear displacement



Decrease of the stress concentration at the crack tip