STRESS WAVE RADIATION FROM BRITTLE CRACK EXTENSION BY MD AND FEM

Petr Hora, Vladimír Pelikán, Olga Červená,
Alena Uhnáková and Anna Machová

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

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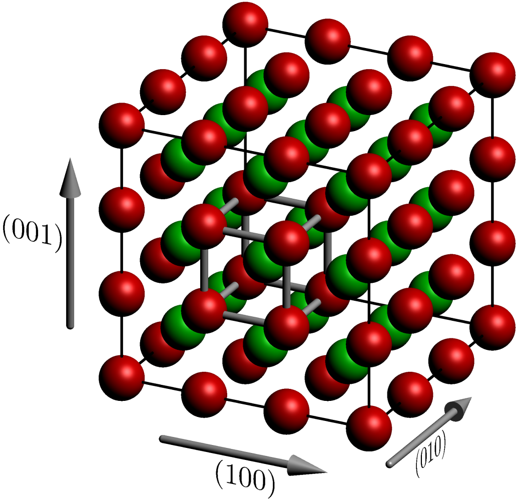
Introduction

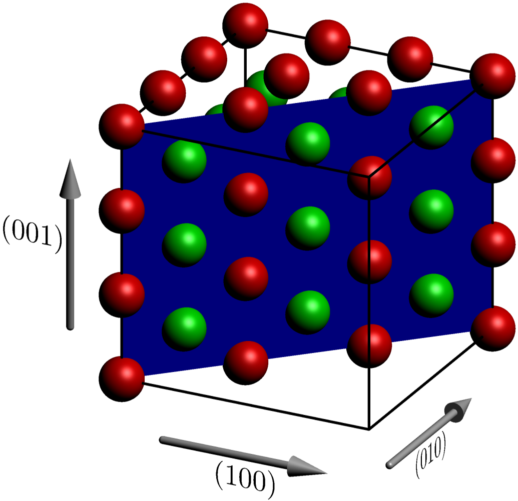
- We present results for molecular dynamic (MD) and finite element (FEM) simulations in 3D bcc iron crystals, with embedded central through crack (001)[110] of Griffith type, loaded in mode I.
- The sample geometry and border conditions in MD were chosen in such a way as to invoke a cleavage crack extension.
- Acoustic emission (AE) sources caused by the crack were analysed on both the atomistic and continuum level with FEM.

Problem description

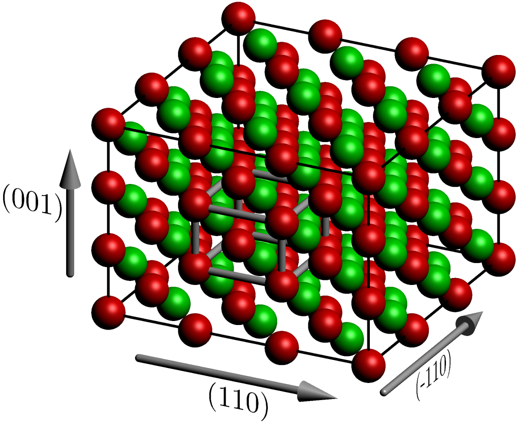
Material (bcc iron)



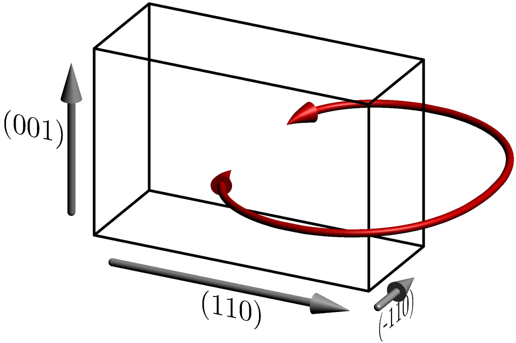
Orientation



Orientation



Size and boundary conditions

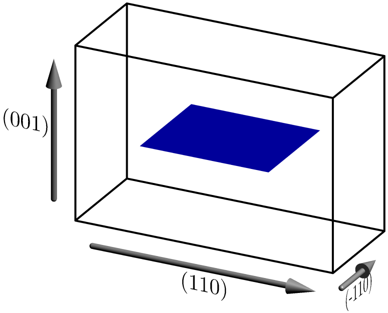


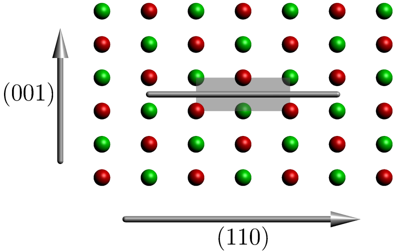
Plane strain

300 × 150 × 15 atoms

$299a_0\sqrt{2} \times 149.5a_0\sqrt{2} \times 14.5a_0\sqrt{2}$

Crack description

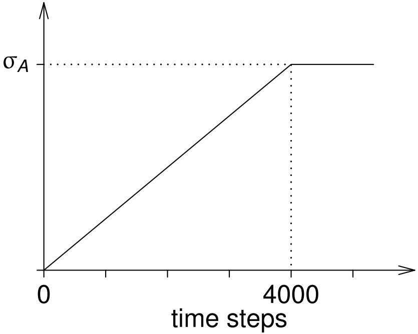




Size $178a_0\sqrt{2} \times 14.5a_0\sqrt{2}$

Method bond restriction,
i.e. atomic interactions over crack plane are not allowed.

Type of loading



Temperature: 0 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

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

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

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

Integration of equations of motion

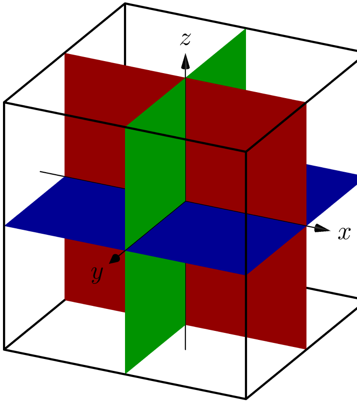
Newtonian equations of motion are solved by the central difference method.

Time integration step:

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

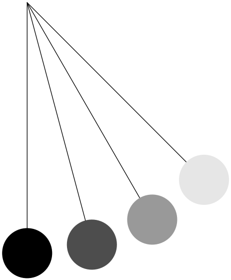
Simulation steps

1. Generation of the crystal containing the crack.
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).

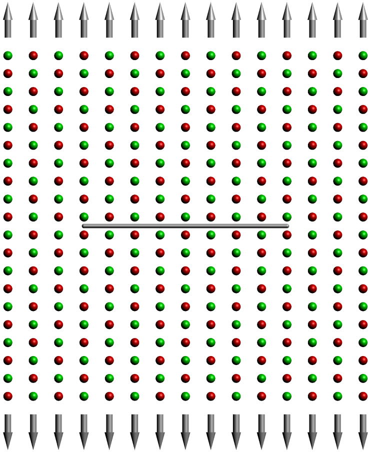
   Pendulum method:

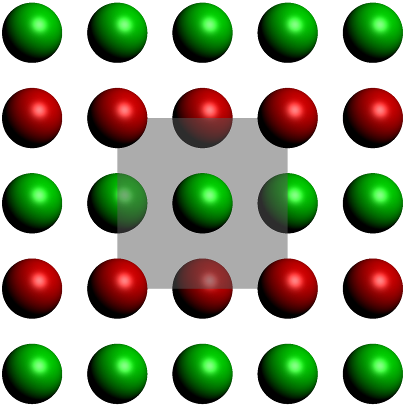


   J.B.Gibson, A.N.Goland, M.Milgram, G.H.Vineyard:
   Phys. Rev., **120**, p.1229, 1960

4. Remove fixation.

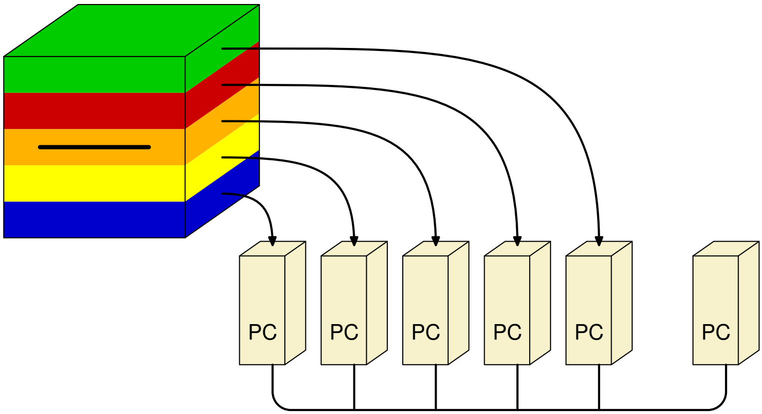
5. Loading
   symmetric loading,
   distributed in 2 surface layers





Simulation technique

Simulation code has been written in *Fortran 90*.
Parallel task



Simulation code has been developed under system MPI (Message Passing Interface).

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:

$$6\times8 + 2\times8 = 64 \text{ bytes/atom} \rightarrow 165 \text{ MiB}$$

Disk requirement:

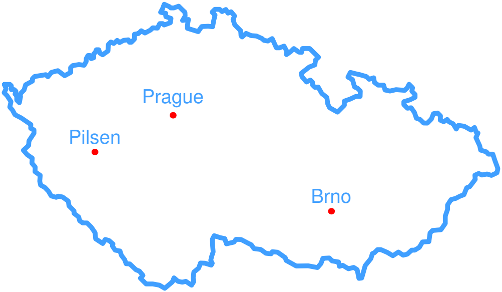
$$6\times8 = 48 \text{ bytes/atom} \rightarrow 124 \text{ MiB}$$

Hash: cell index method (link cell method)

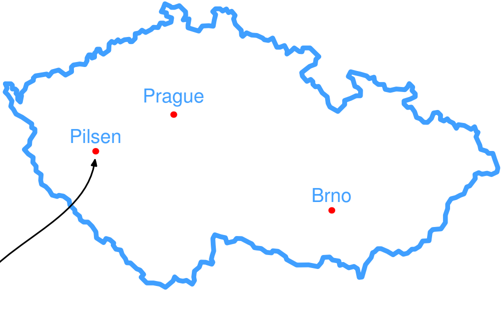
M.P.Allen, D.J.Tildesley:
Computer Simulation of Liquids.
Oxford University Press, New York, 1987

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

Where was it computed?

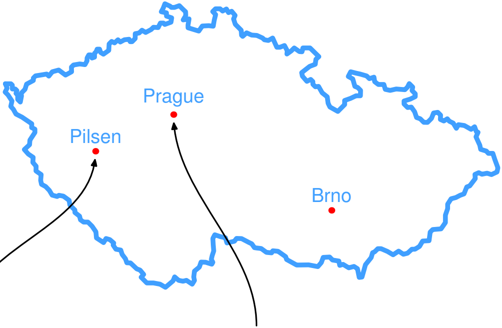


Where was it computed?



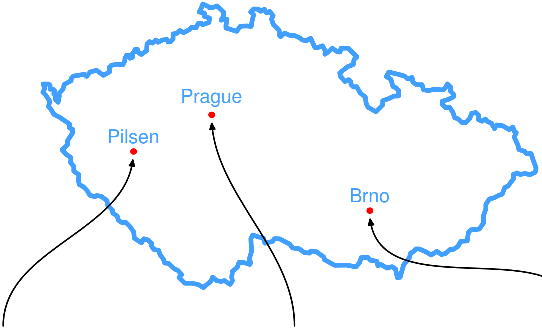
MINOS
49 nodes
2x 6-cores Xeon E5645
2.4 GHz
24 GiB
2x 600 GiB (15 k rpm, SAS)
1 Gb Ethernet, Infiniband

Where was it computed?



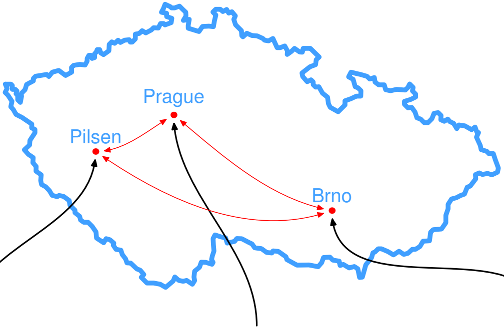
MINOS	TARKIL
49 nodes	28 nodes
2x 6-cores Xeon E5645	2x Quad Core Intel Xeon X5570
2.4 GHz	2,93 GHz
24 GiB	24 GiB
2x 600 GiB (15 k rpm, SAS)	2x 300 GiB (15 k rpm, SAS)
1 Gb Ethernet, Infiniband	1 Gb Ethernet, Infiniband 4x QDR

Where was it computed?



MINOS	TARKIL	MANDOS
49 nodes	28 nodes	14 nodes
2x 6-cores Xeon E5645	2x Quad Core Intel Xeon X5570	4x AMD Opteron 6274
2.4 GHz	2,93 GHz	2.5 GHz
24 GiB	24 GiB	256 GiB
2x 600 GiB (15 k rpm, SAS)	2x 300 GiB (15 k rpm, SAS)	870 GiB, 27 TiB
1 Gb Ethernet, Infiniband	1 Gb Ethernet, Infiniband 4x QDR	1 Gb Ethernet, Infiniband

Where was it computed?



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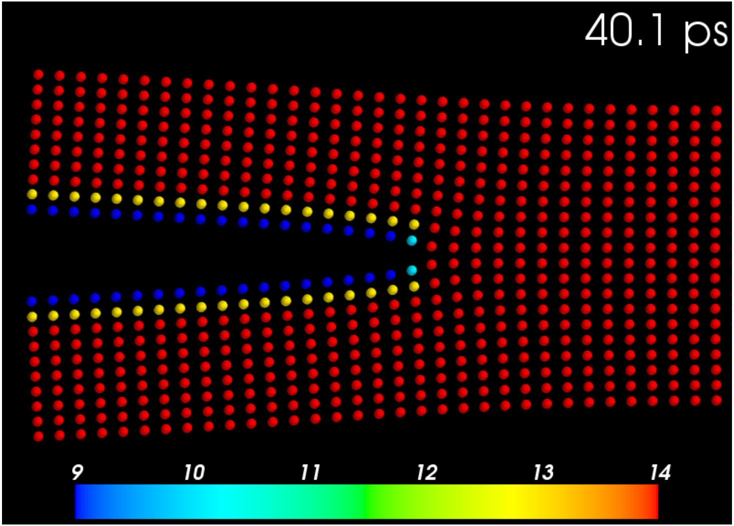
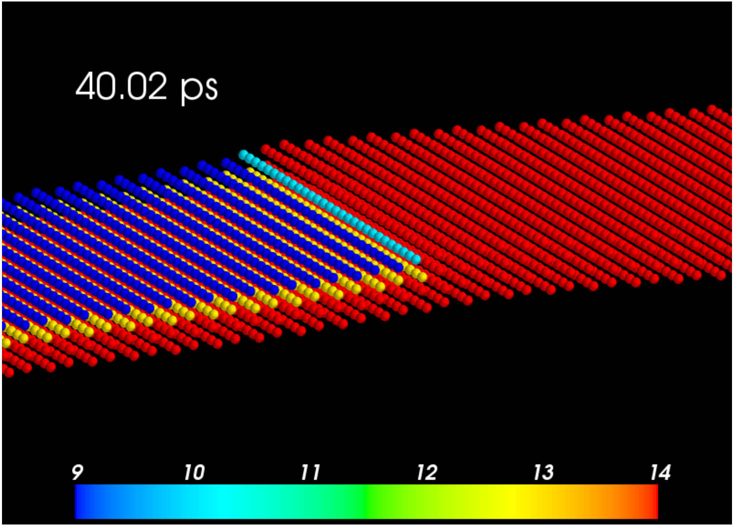
1 Gb Ethernet, Infiniband	1 Gb Ethernet, Infiniband 4x QDR	1 Gb Ethernet, Infiniband

Results - MD

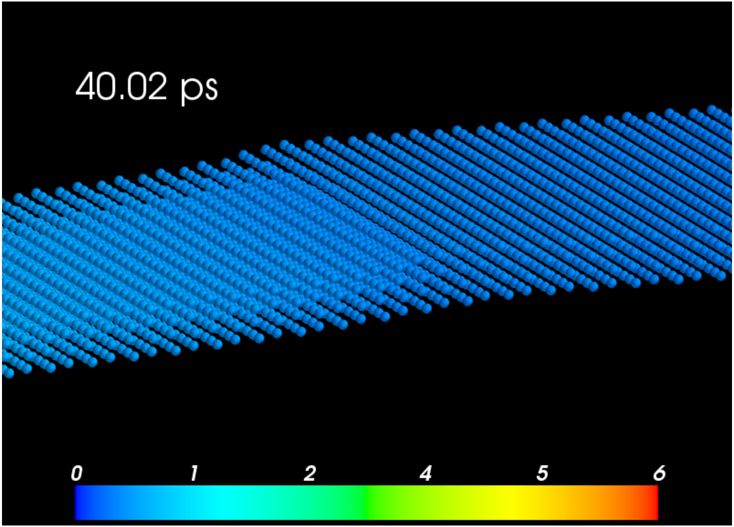
Coordination number



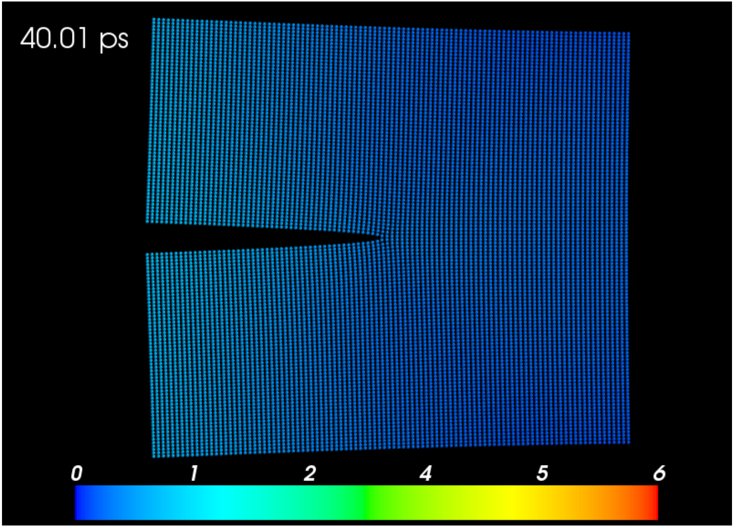
Coordination number



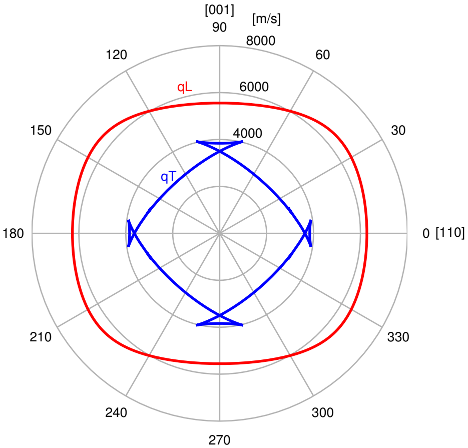
Kinetic energy



Kinetic energy



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



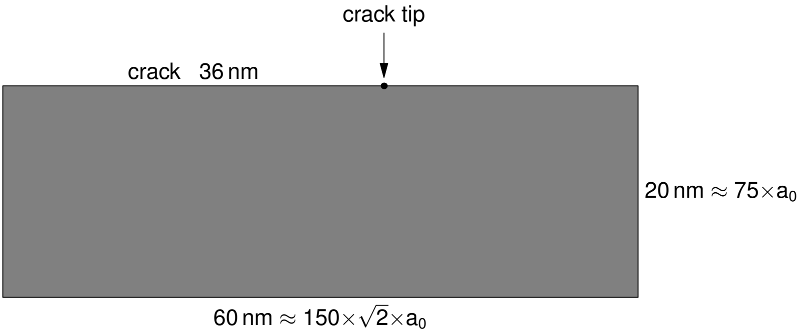
FEM analysis

- COMSOL Multiphysics
- Structural Mechanics Module
- Plane strain
- Shape function: Lagrange (Quadratic)

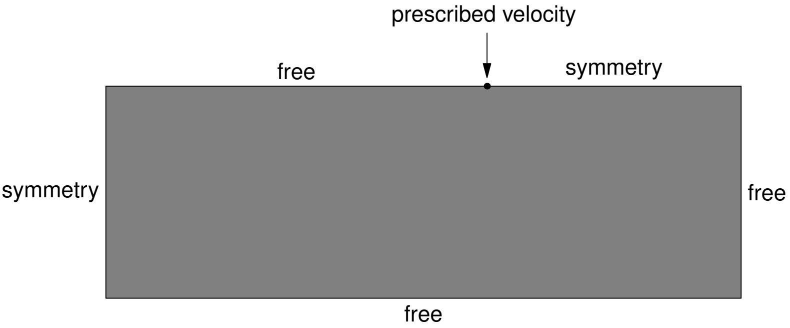
- Time analysis
- Time: 0 – 5 ps, step 0.01 ps
- Time stepping method: Generalized alpha
- Relative tolerance: 10^{-7}
- Absolute tolerance: 10^{-14}

- Mesh: Quadrilateral elements (300×100), Size: 2×2 Å
- Number of degrees of freedom: $\approx$250000

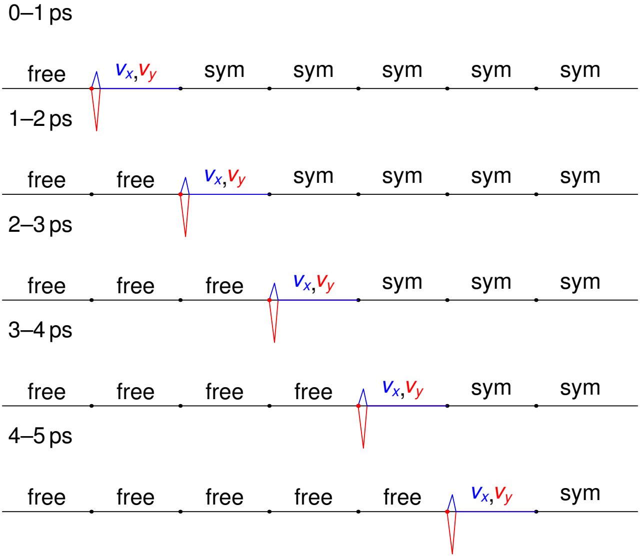
Sample



Boundary condition

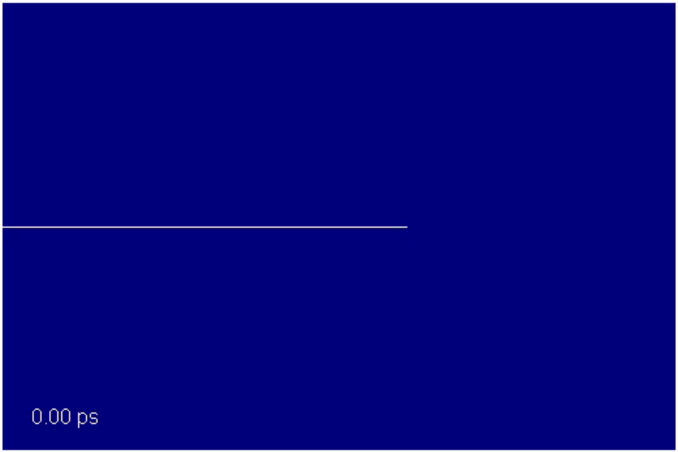


Detail of crack tip



Results - FEM

Modulus of velocity



Conclusion

- At higher applied loads, positive T-stress contributes to cleavage crack extension in MD. Under the ramp loading during 4000 time steps, the crack was initiated at the critical Griffith stress intensity.
- MD simulations show that cleavage crack initiation in the 3D bcc iron crystal forms an AE-source, where qL-waves dominate. However, qT-waves are also generated during a continuous bond breakage in the crystal, which is new knowledge from 3D modelling. The strongest pulse emission comes from stress relaxation at the crack front, after the crack initiation.
- Simplified modelling of the pulse emission by FEM shows that, besides the qL and qT-waves, Rayleigh waves can also be generated at the (001) free crack faces, in agreement with expectations according to continuum analysis.

Question time

The work was supported under grants GA CR No 101/09/1630
and AV0Z20760514.