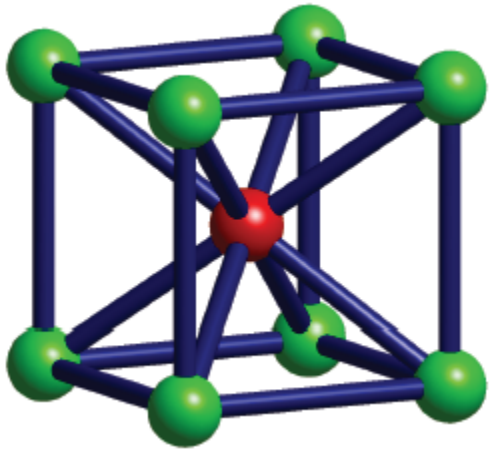
Crack orientation versus ductile-brittle behavior in 3D atomistic simulations

Alena Spielmannová, Anna Machová and Petr Hora
Institute of Thermomechanics AS CR, v.v.i.

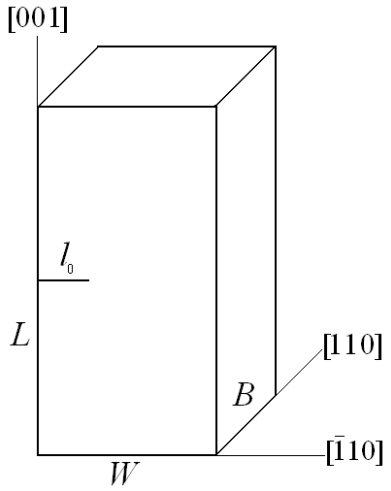


This work was supported by the Institute Research Plan AV0Z207605114 and by the grant GA CR No 101/07/0789.

Introduction

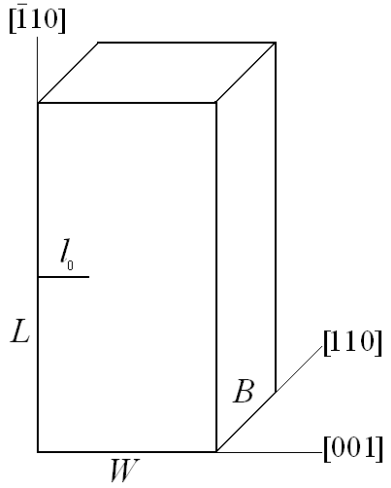
- MD simulation in 3D enable to study crack processes both on the inclined and oblique slip planes at arbitrary temperature
- 3D samples containing more than 1 million atoms
- Interatomic N-body potentials for Fe-Fe interaction from the paper by Ackland et al, Phil. Mag. A Vol. 75 (1997), p.713
- Bcc iron crystals with two different edge cracks loaded in tension mode **I**
  - (001)[110]
  - (-110)[110]
- The atomistic samples have the same crystallographic orientation and similar geometry as in our recent experiments on the single crystals Fe(3wt.%Si)

Edge (001)[110] crack



- The sample consists of 150 planes in the (-110) direction (width *W*), 600 planes in the [001] direction (length *L*) and 30 planes in the [110] direction (thickness *B*)
- Total number of atoms in the sample is $N = 1\ 350\ 000$
- The initial crack length corresponds to $l_0 = 46\ d_{110}$, where $d_{110} = a0\sqrt{2}/2$ is the interplanar distance in the [110] direction and $a_0 = 2.8665$ Å is the lattice parameter
- Edge crack lies on a (001) plane, crack front is oriented along [110] direction and the direction of potential crack extension is in [-110] direction

Edge (-110)[110] crack



- The sample consists of 440 planes in the direction (length L), 220 planes in the [001] direction (width W) and 30 planes in the [110] direction (thickness B)
- Total number of atoms in the sample is N = 1 452 000
- Initial crack length corresponds to $l_0 = 66\ d_{001}$, where $d_{001} = a_0/2$
- Edge crack lies on a (-110) plane, crack front is oriented along [110] direction and the direction of potential crack extension is [001]

MD Simulation in 3D

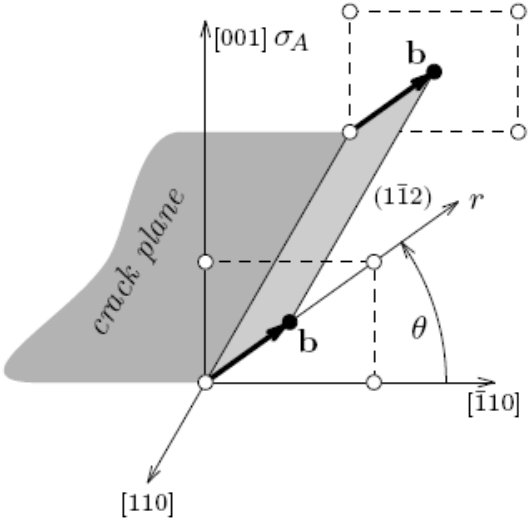
- Interatomic interactions across the initial crack faces are not allowed
- Before loading, surface relaxation was performed in the samples
- The relaxed unloaded samples were heated during 1000 time steps by prescribing random atomic velocities according to Boltzmann distribution
- At the time step 1000 *h* (the average temperature in the system corresponded T ~ 300 *K*) the samples were gradually (linearly) loaded in time in the <001> directions or in the <110> directions respectively by prescribing external forces distributed at individual atoms lying in several surface layers

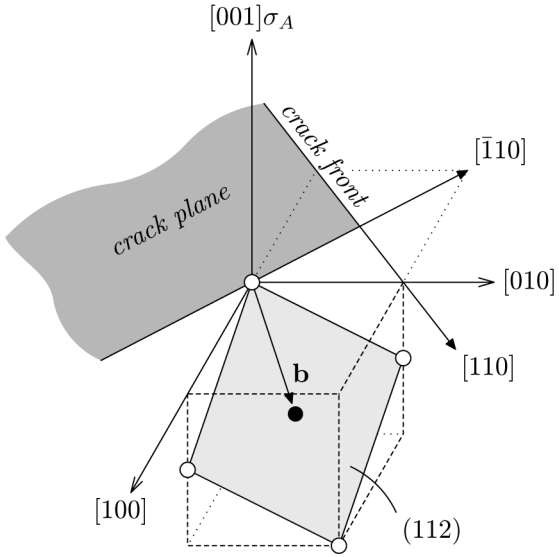
MD Simulation in 3D

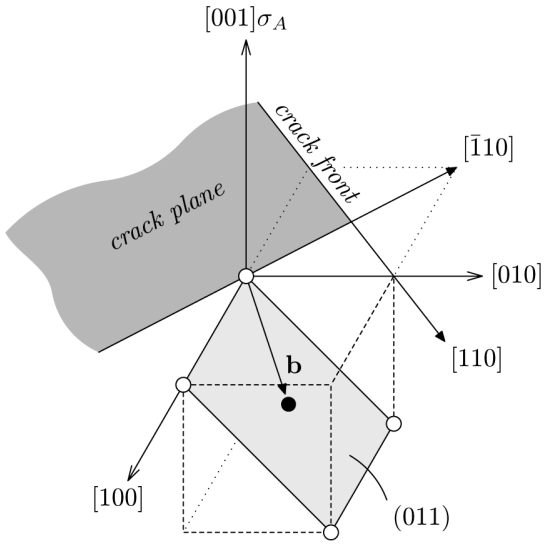
- Newtonian equations of motion for individual atoms have been solved by a central difference method using time integration step h = 10^{-14} s (sequence processing was used)
- Each time step – monitoring of the total number of existing interactions and global energy balance in the system
- Two different loading rates
  - Fast loading (4.5 *GPa* per 2000 *h*) → plane strain conditions prevail along the crack front
  - Slow loading (4.5 *GPa* per 4000*h*) → plane stress conditions prevail along the crack front

Results: Crack (001)[110]

- Oriented in easy twinning direction (τ_{twin} =9.3 GPa ; τ_{disl} = 16.3 GPa)
- Fast loading
  - Twinning on the inclined slip systems <111>{112} prevails
  - Further generation of dislocations on the oblique {110} slip planes and of twins on the oblique slip systems <111>{112}
- Slow loading
  - generation of dislocations on the oblique {110} slip planes and of twins on the oblique slip systems <111>{112}
  - twinning on the inclined slip systems <111>{112} does not occur
- Fracture correlated with twinning

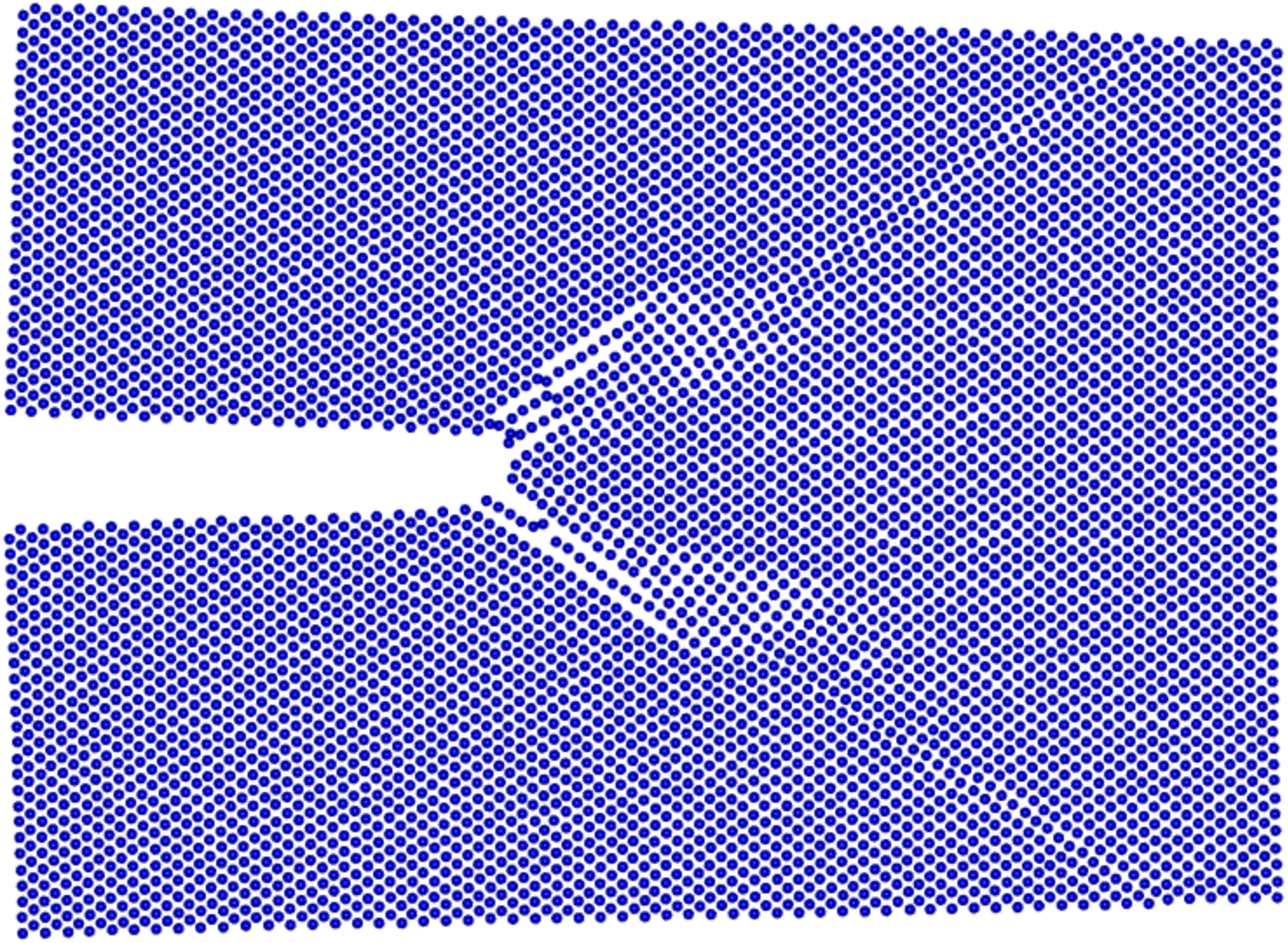




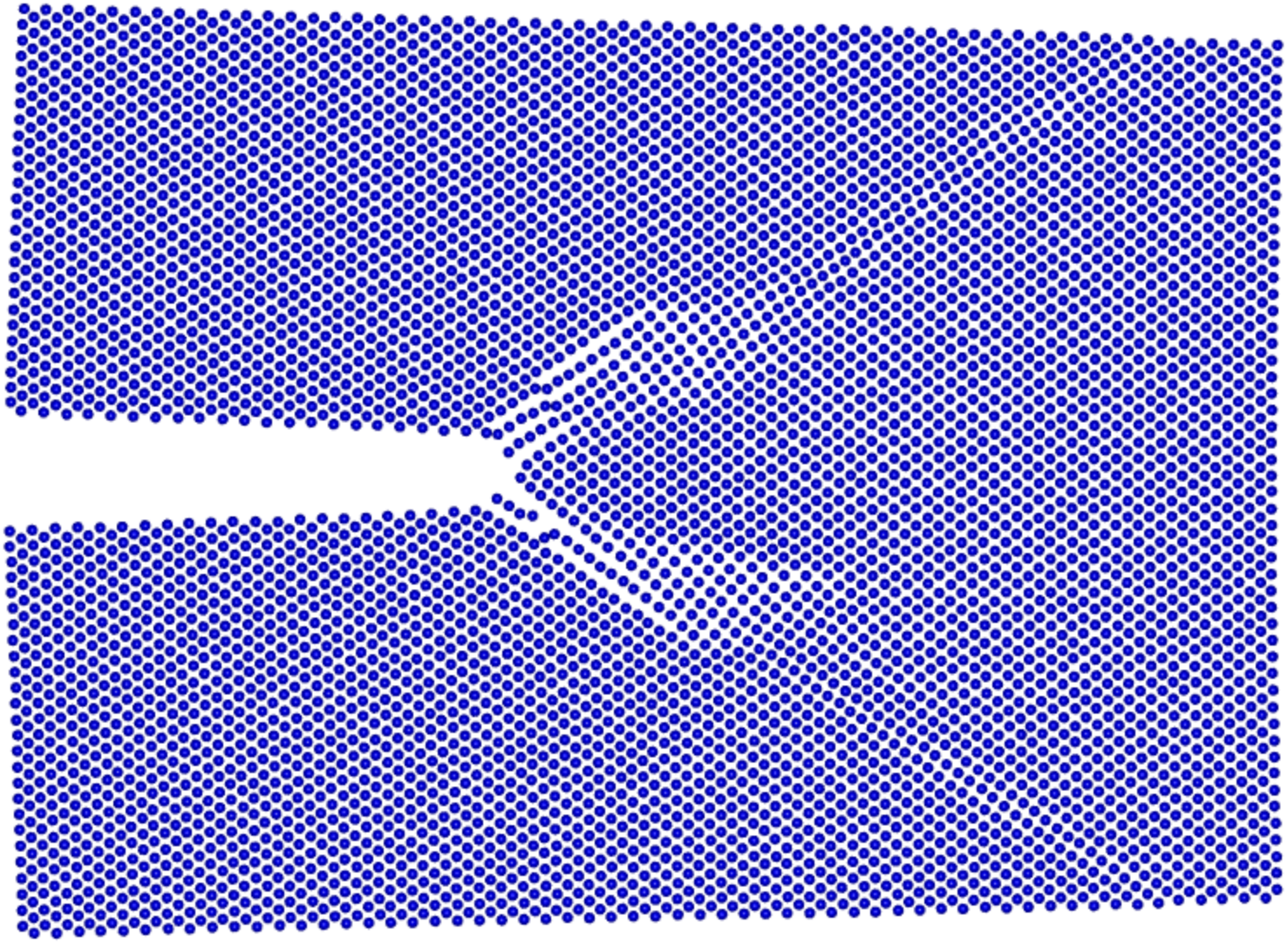


Slip patterns along the crack front under fast loading
(time step 3600)

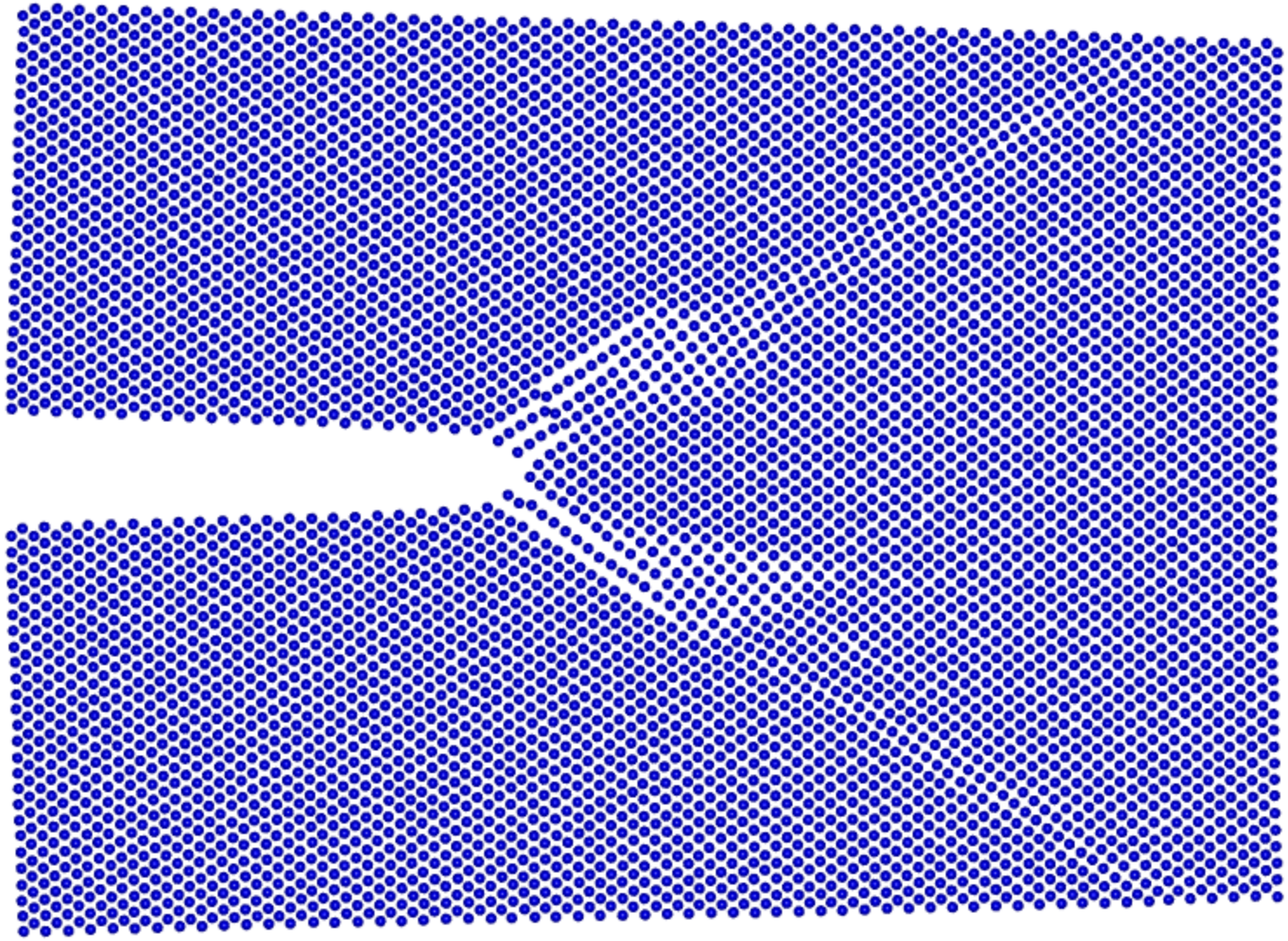
Layer 1



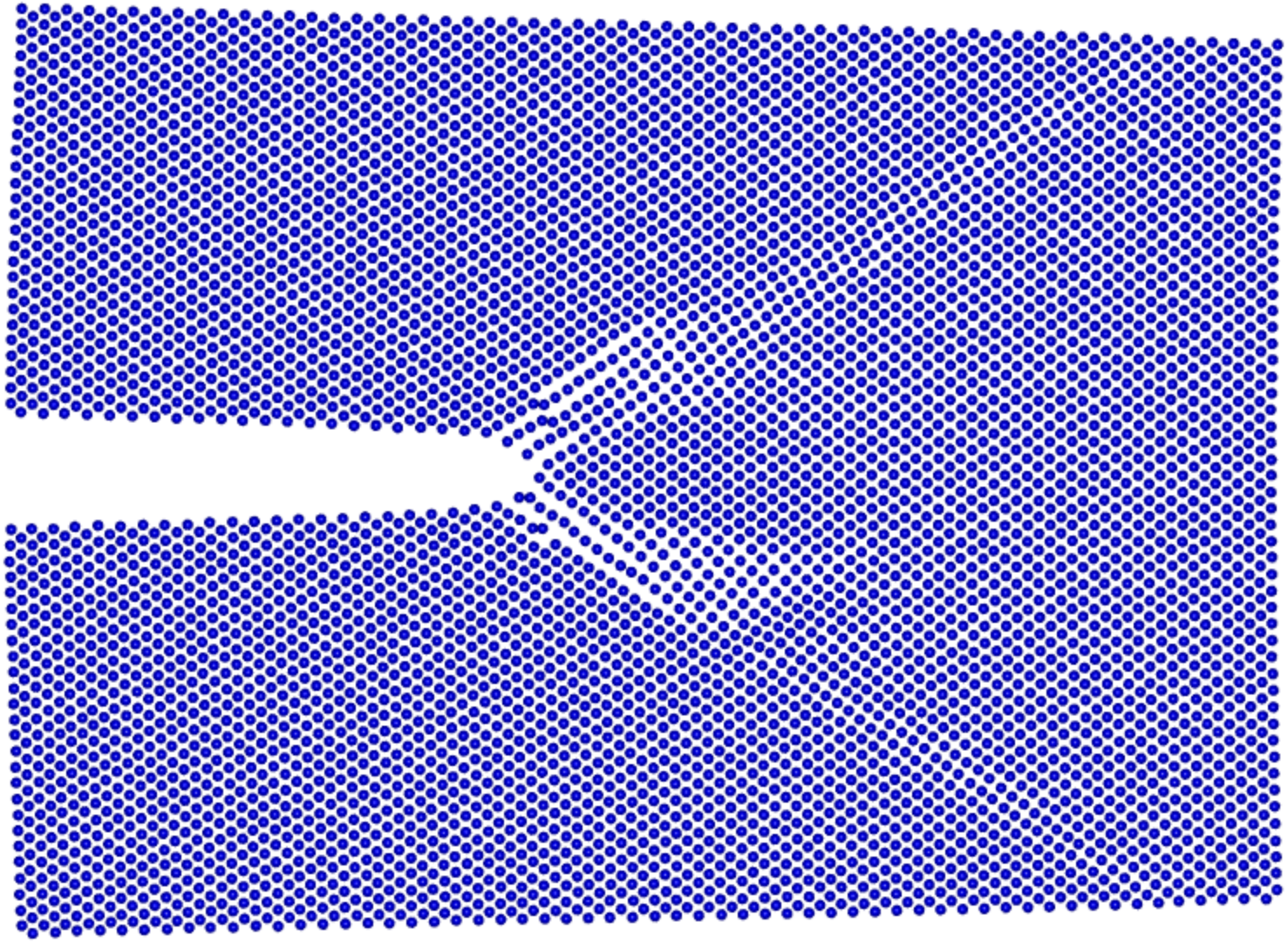
Layer 2



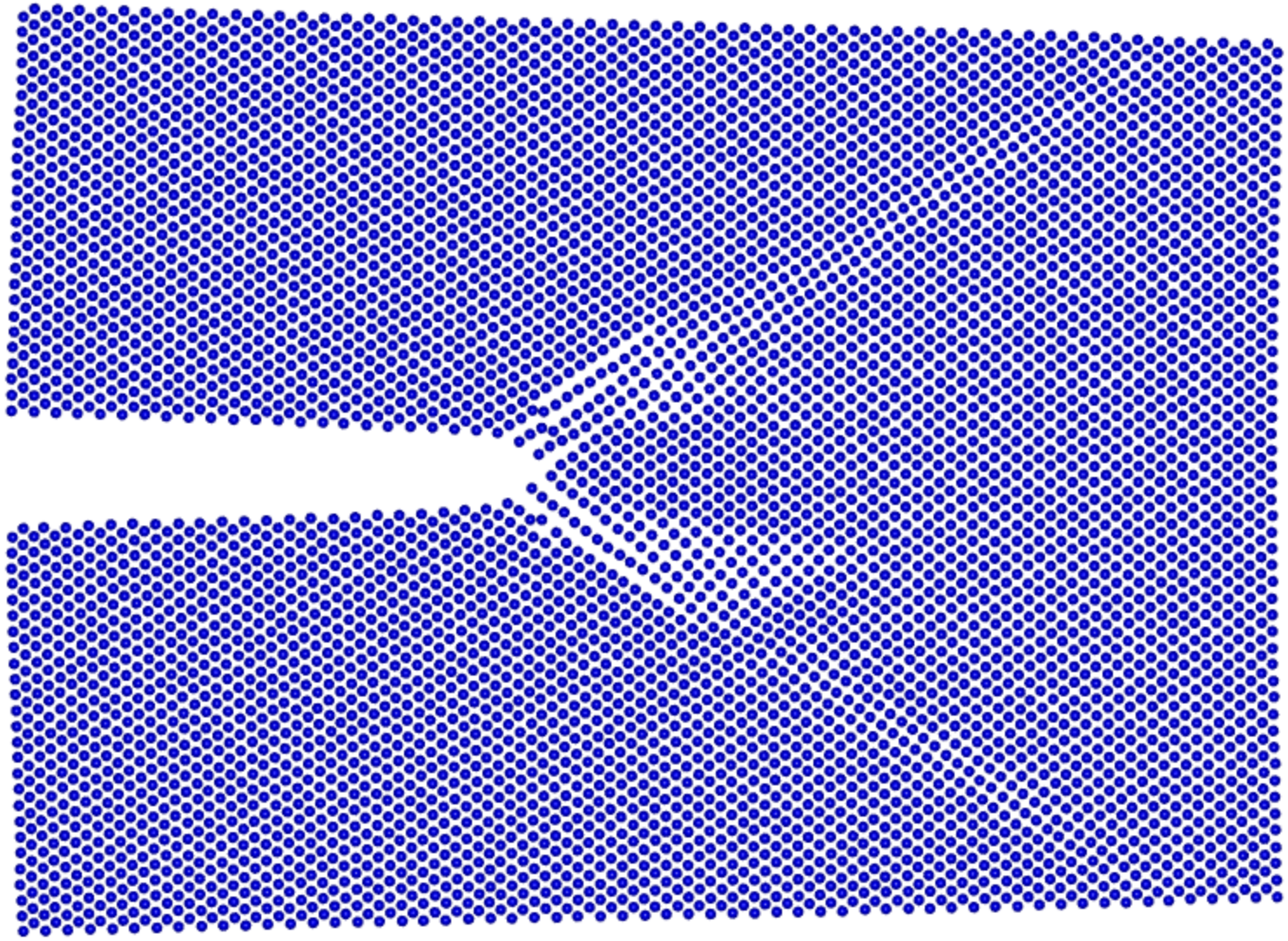
Layer 3



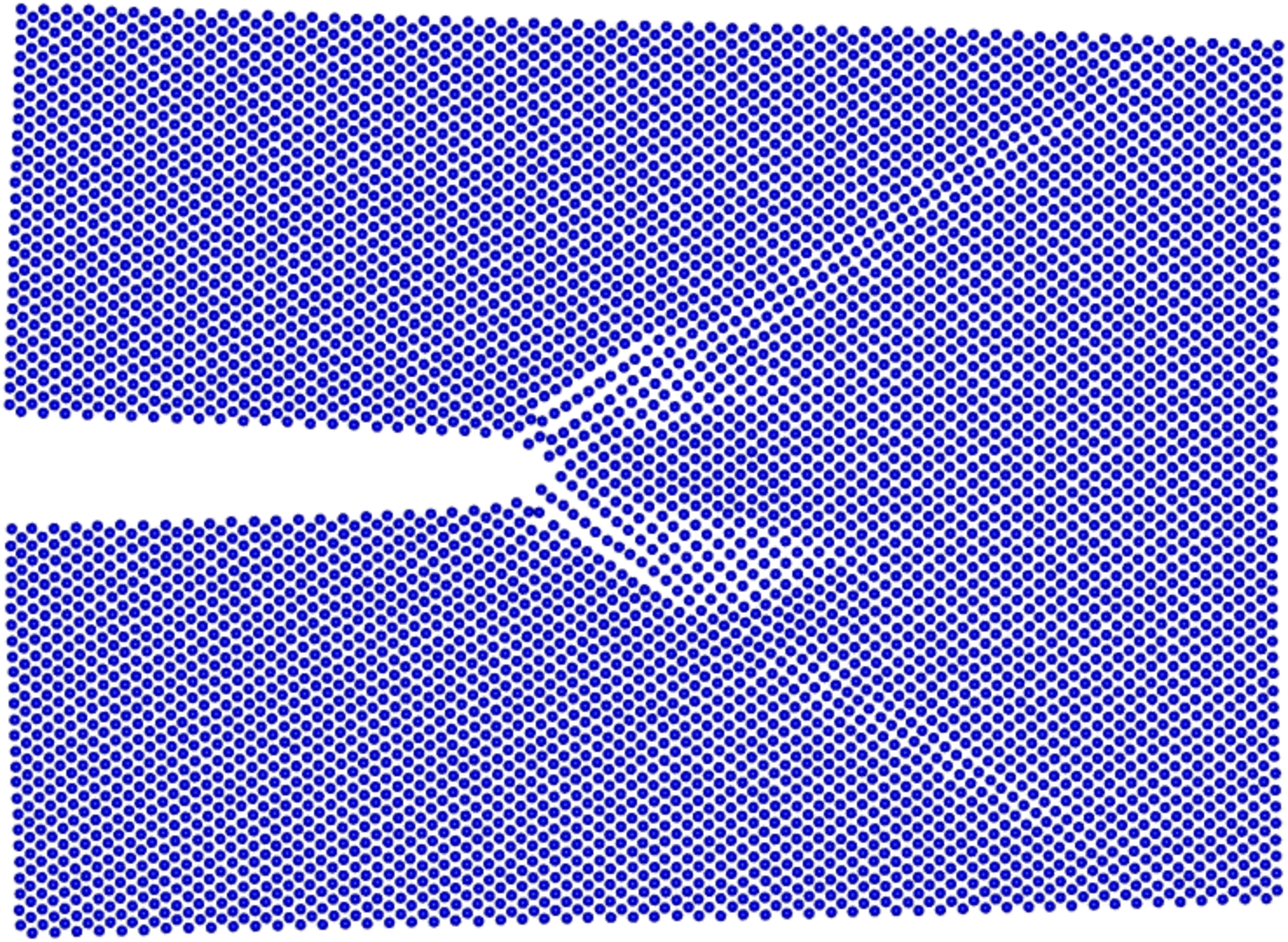
Layer 4



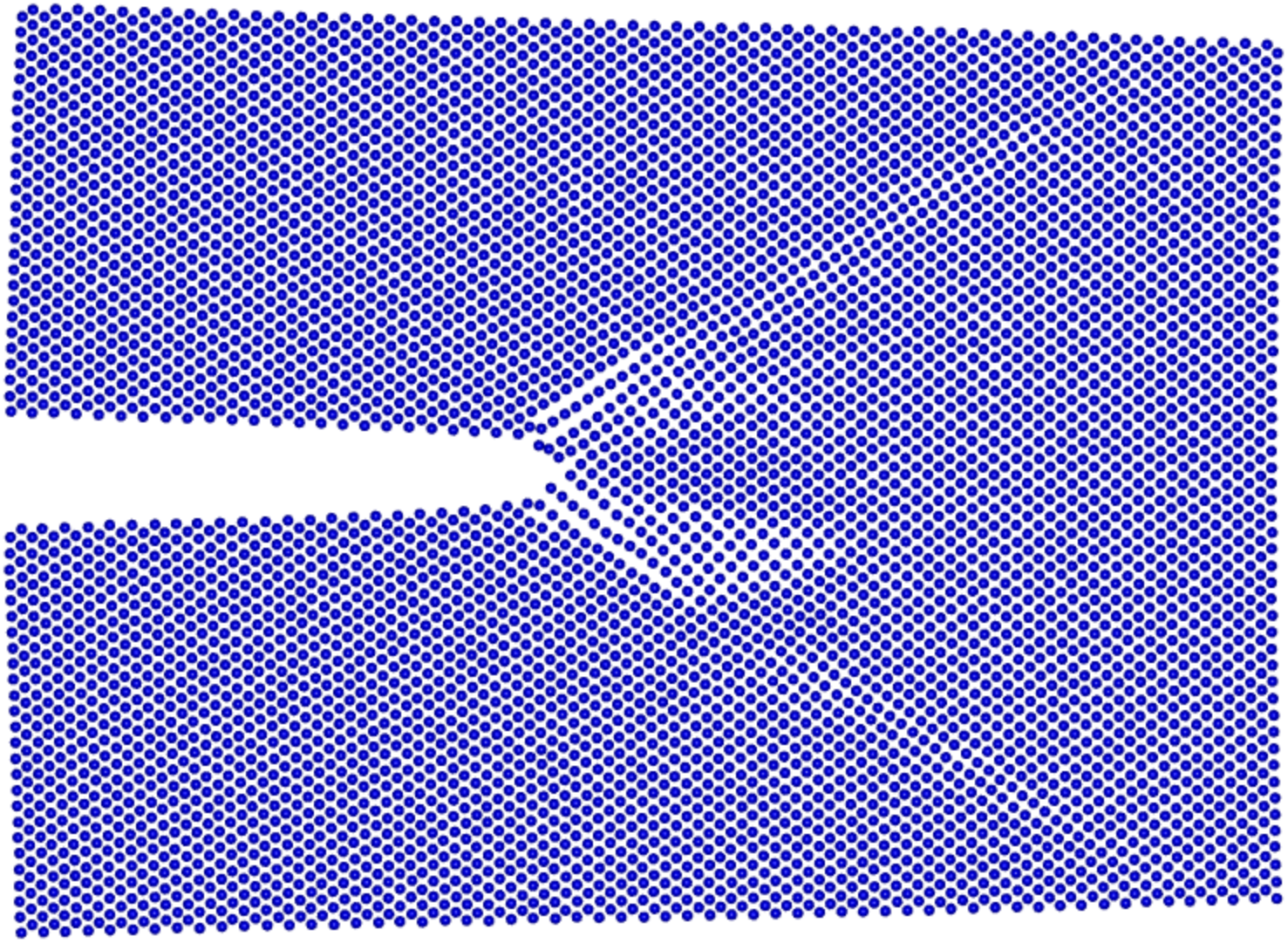
Layer 5



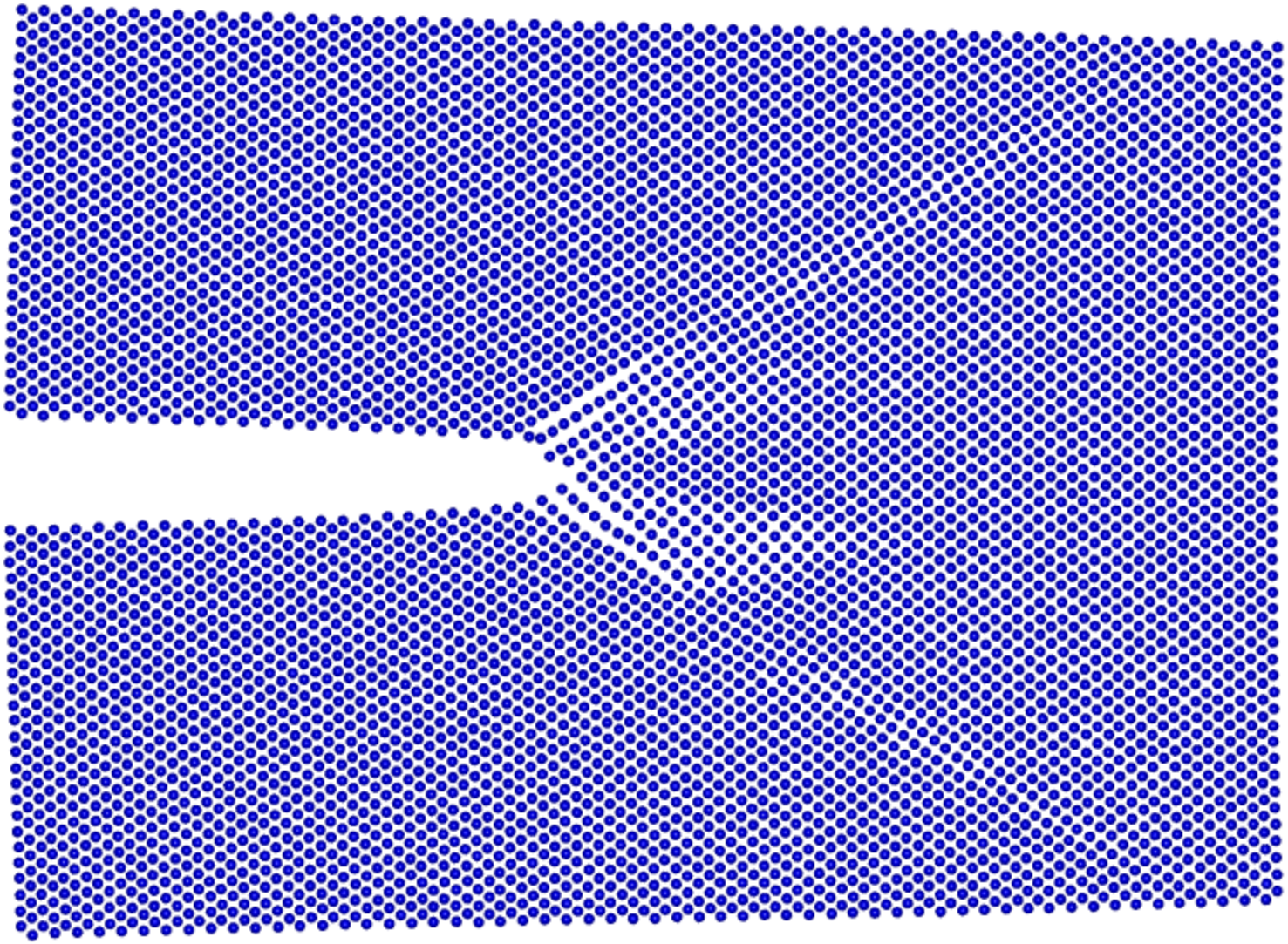
Layer 6



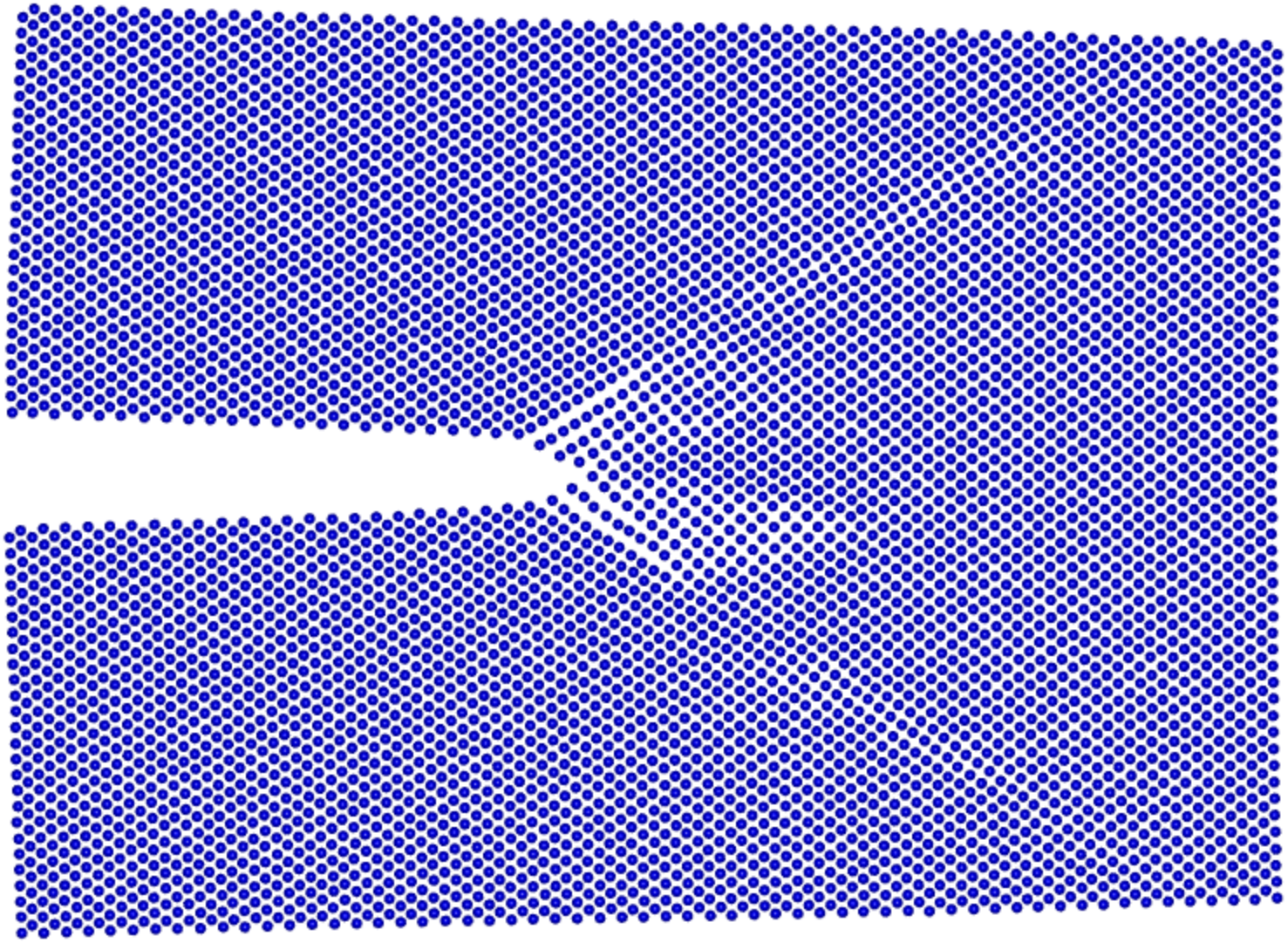
Layer 7



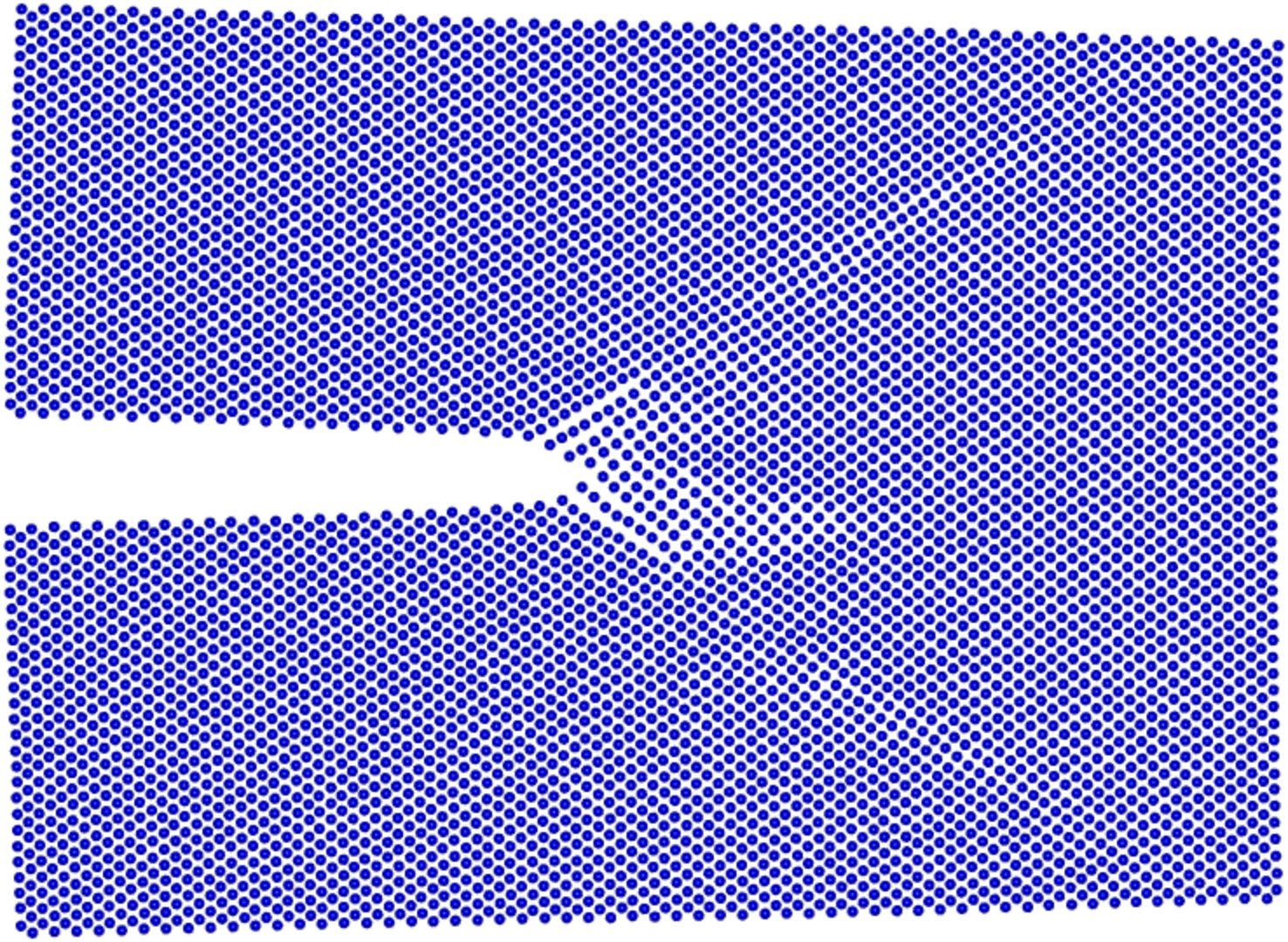
Layer 8



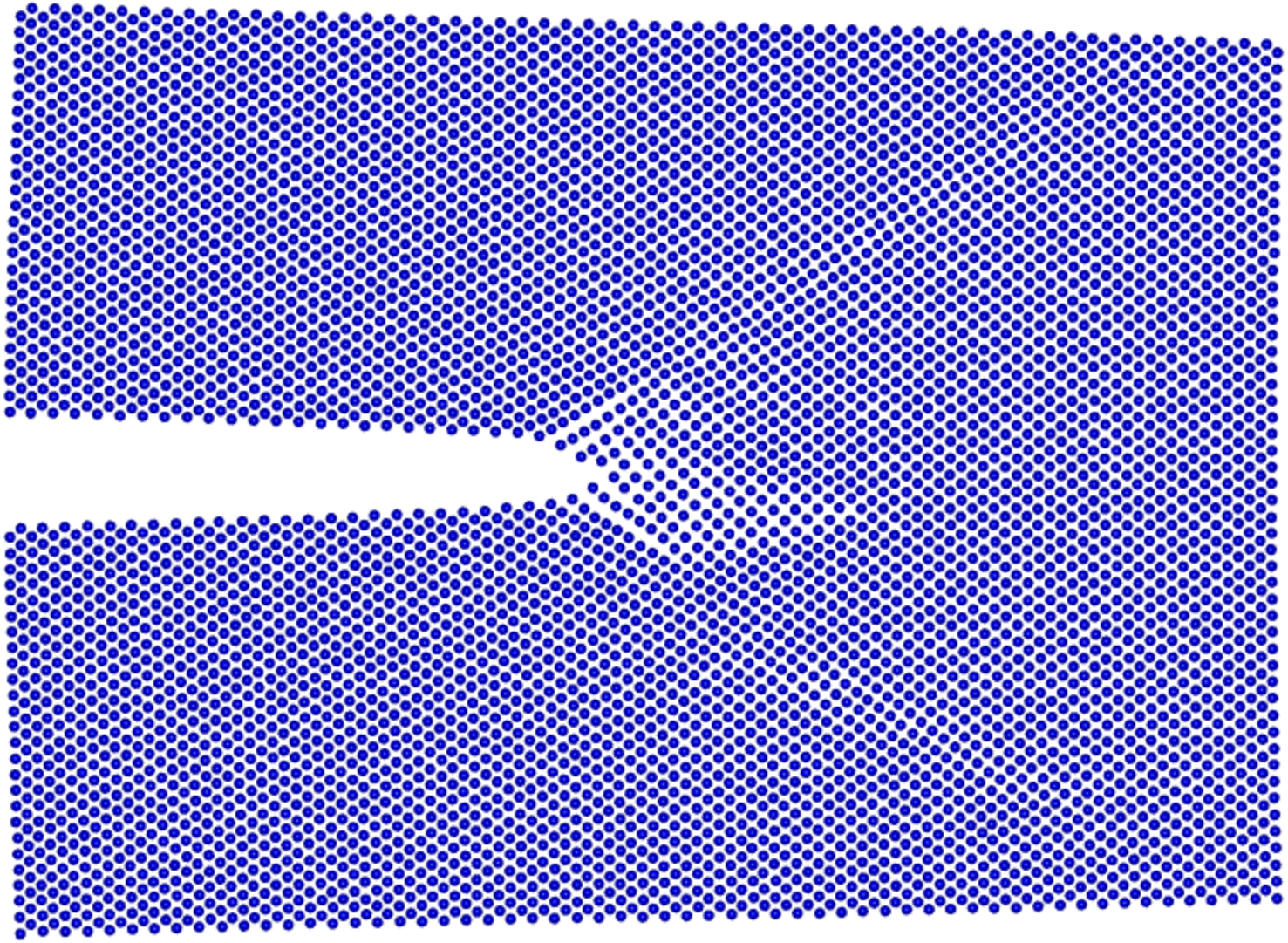
Layer 9



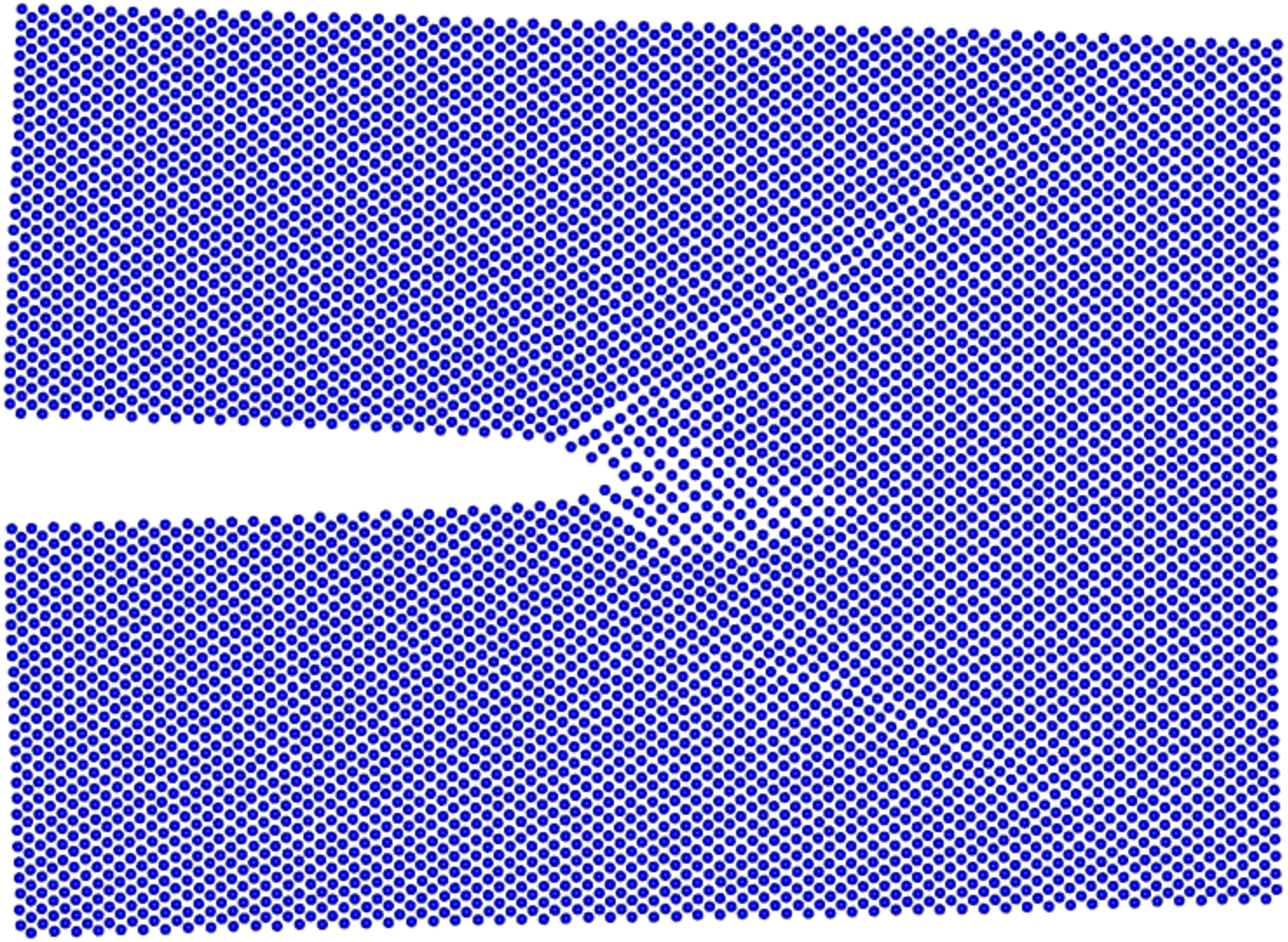
Layer 10



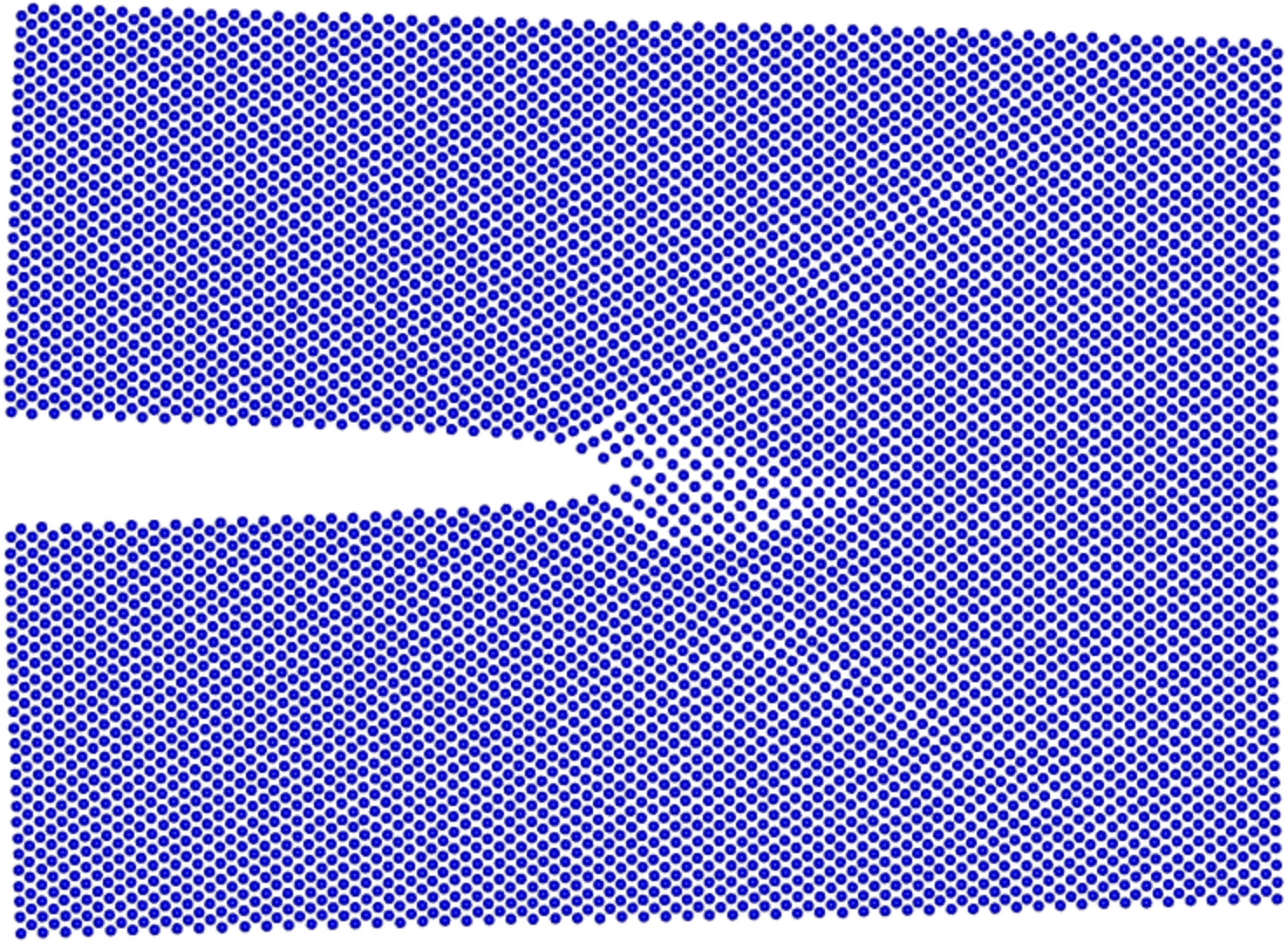
Layer 11



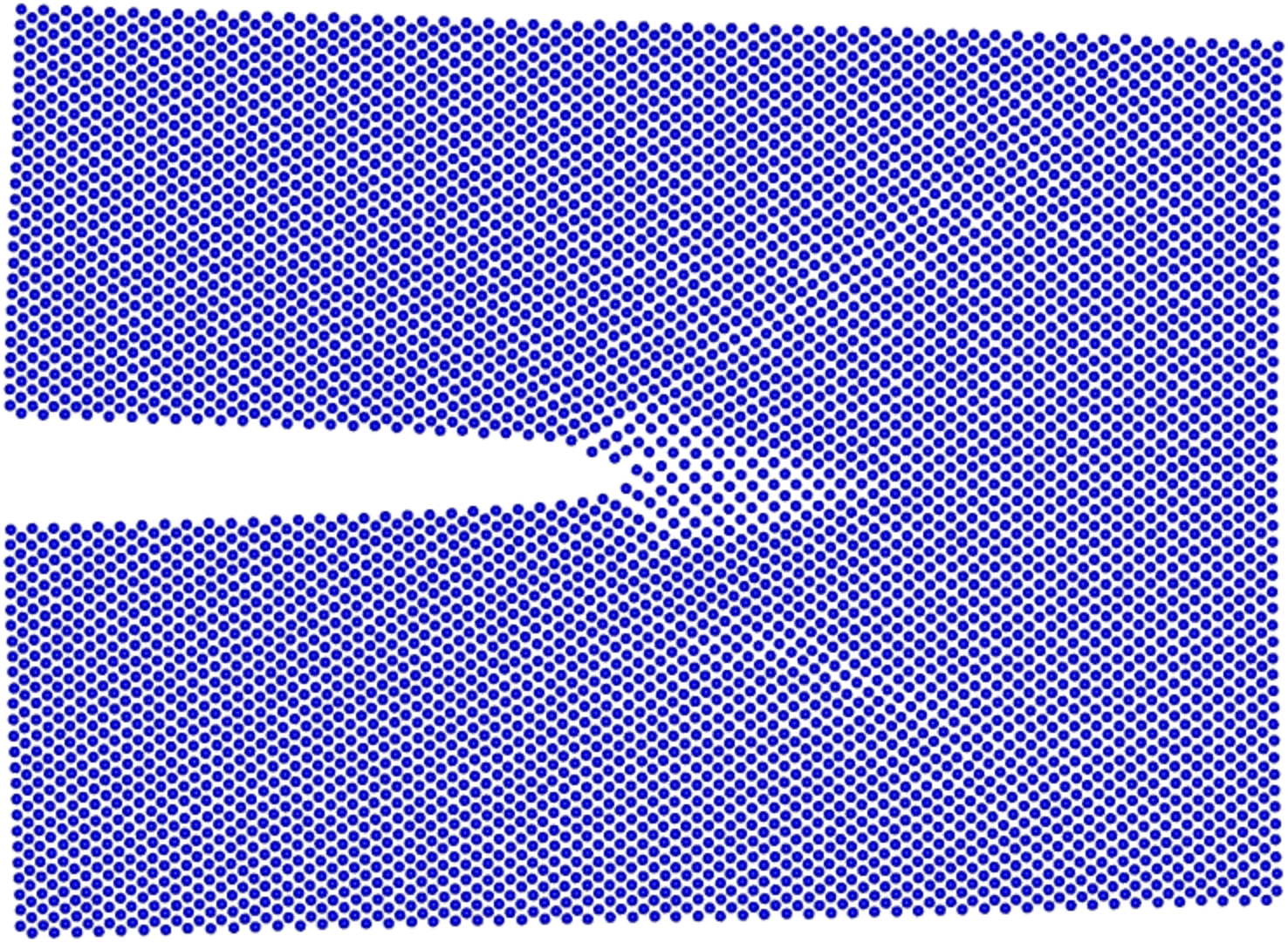
Layer 12



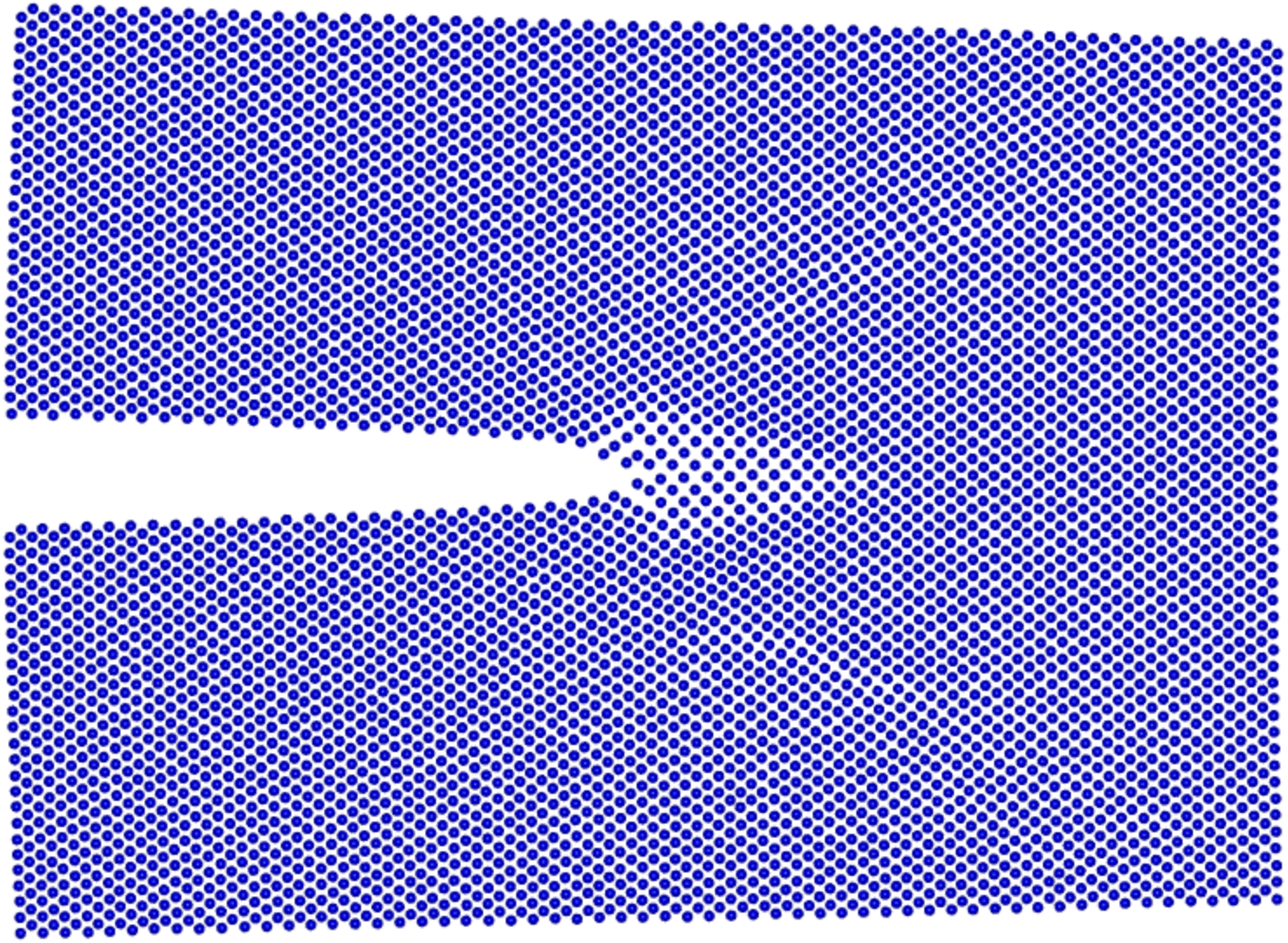
Layer 13



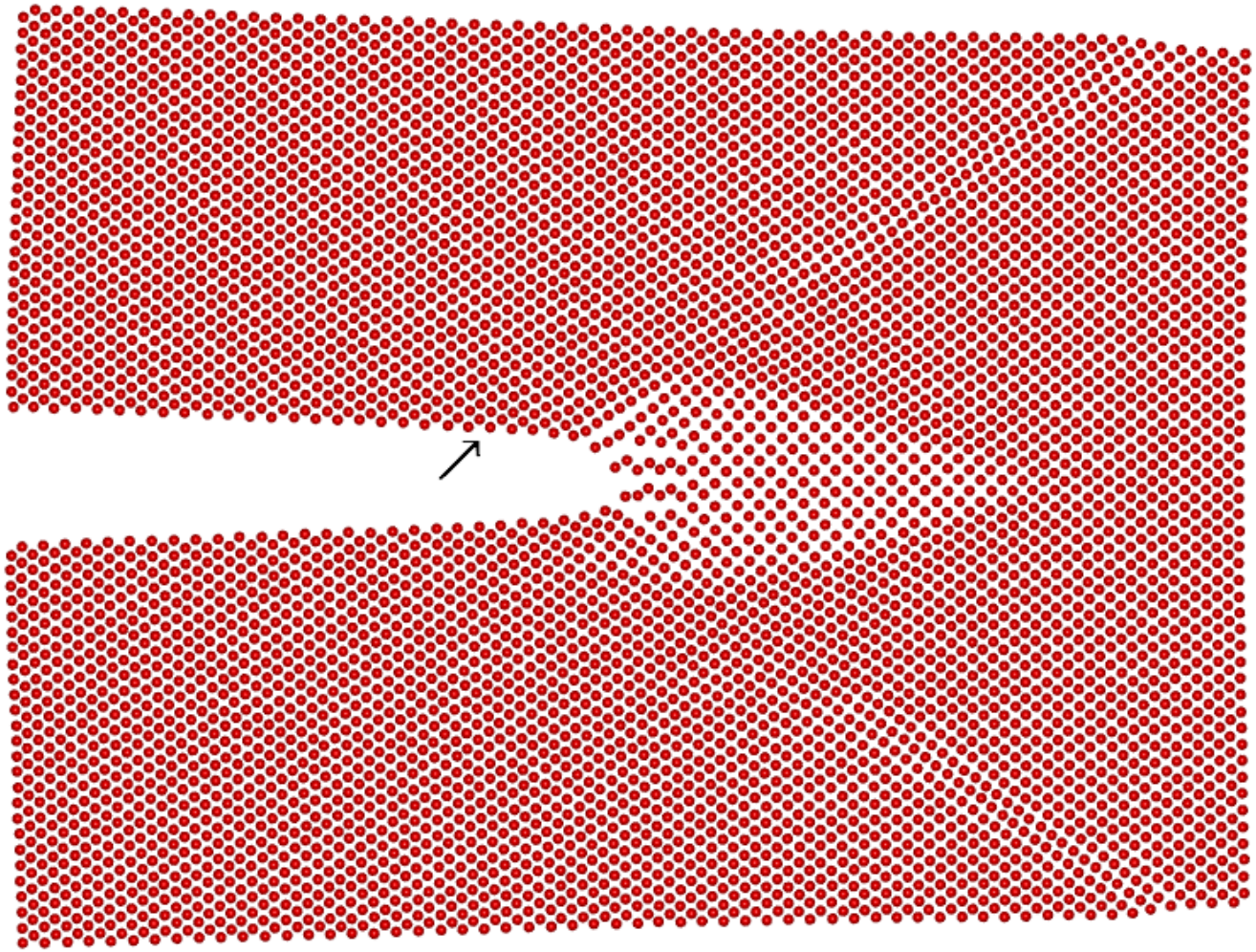
Layer 14



Layer 15

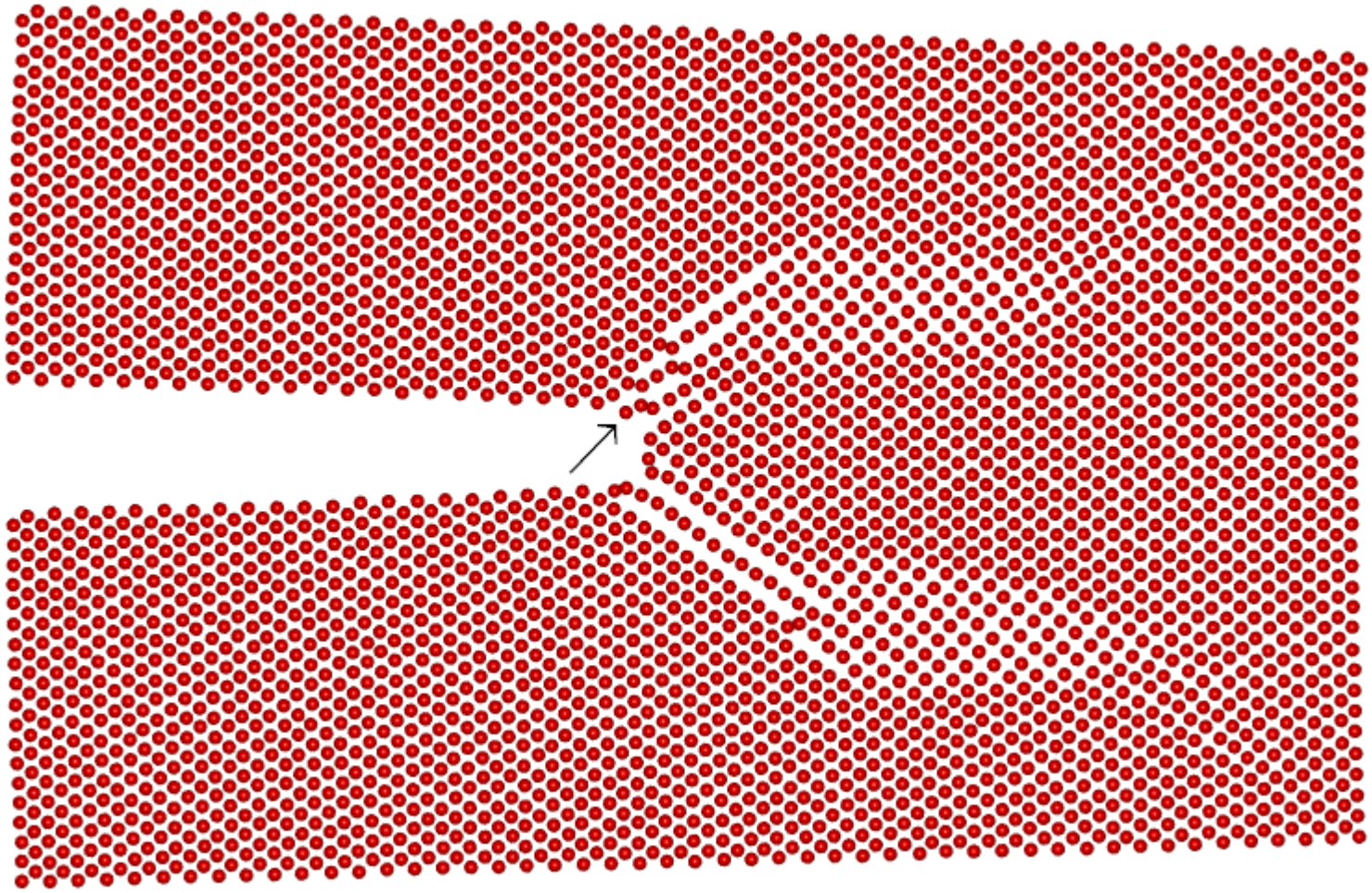


Twinning under fast loading - time step 3750

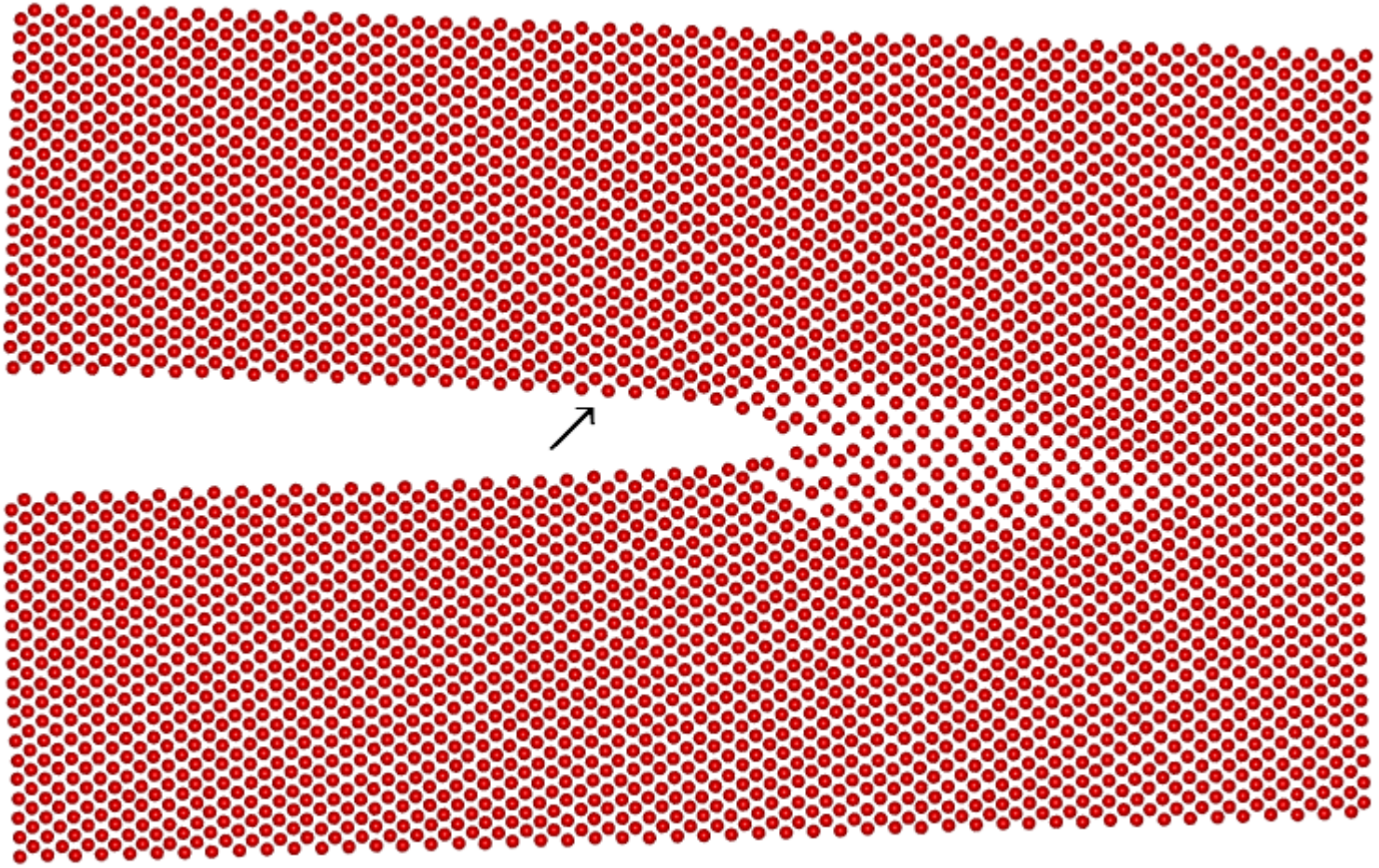


Twinning in 3D under fast loading
Time step 3750

Oblique twinning and dislocation emission under slow loading, surface layer, time step 4600



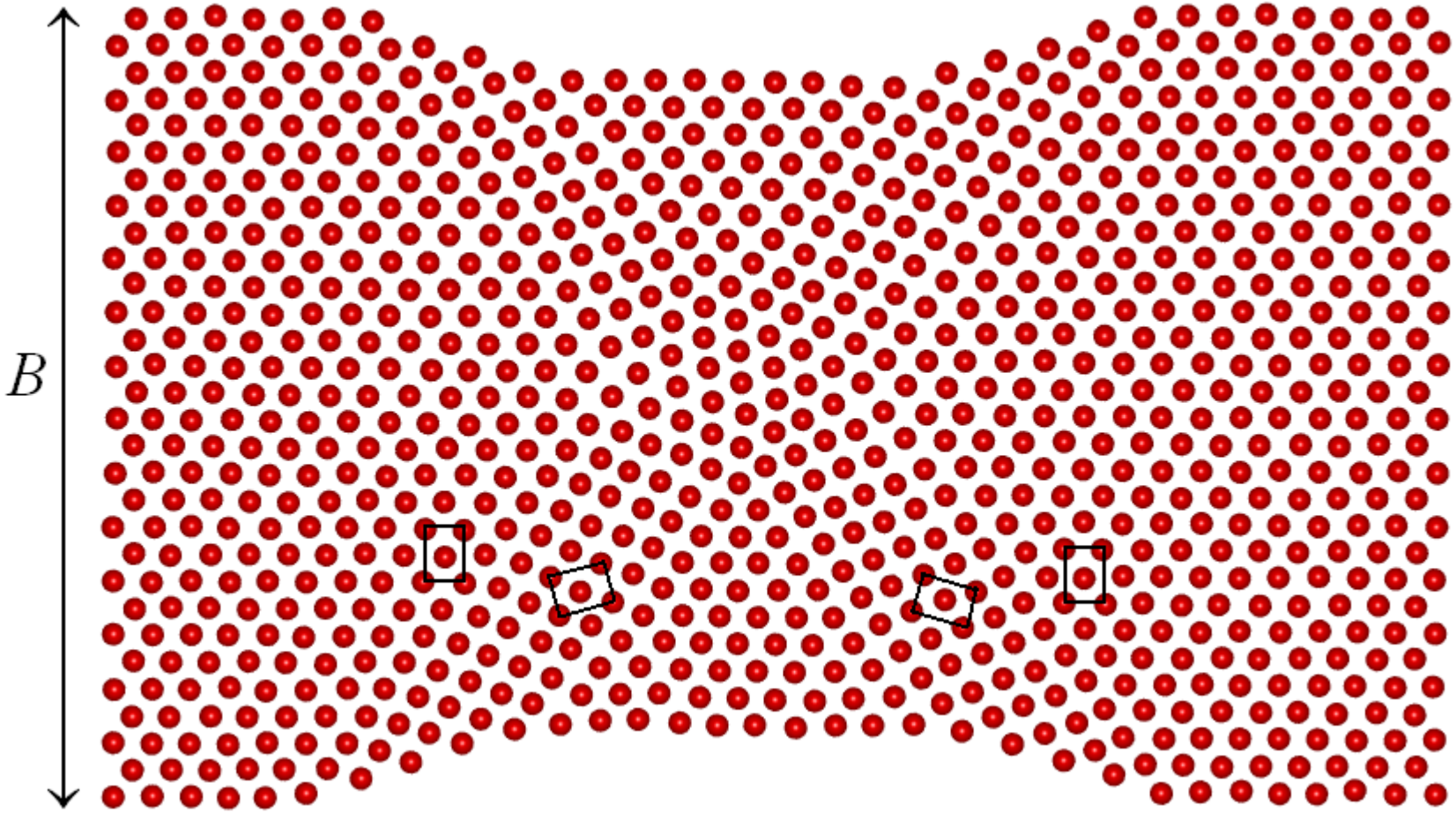
Twinning under slow loading
Middle layer, time step 4600



Plastic zone of the experimental sample with crack orientation (001)[110] under slow loading

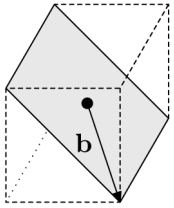
A. Spielmannová, M. Landa, A. Machová, P. Haušild and P. Lejček: *Influence of crack orientation on the ductile – brittle behavior in Fe-3wt%Si single crystals*, Materials Characterization (2006), doi: 10.1016/j.matchar.2006.09.001 (article in press)

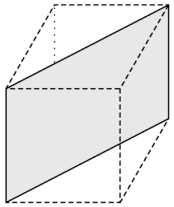
Twinning from the oblique planes {112}
Cross-section in front of the crack (001)[110]
Slow loading, time step 4600

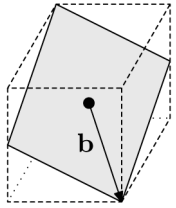


Recognition of slip patterns in perfect samples by Block Like Shear simulations

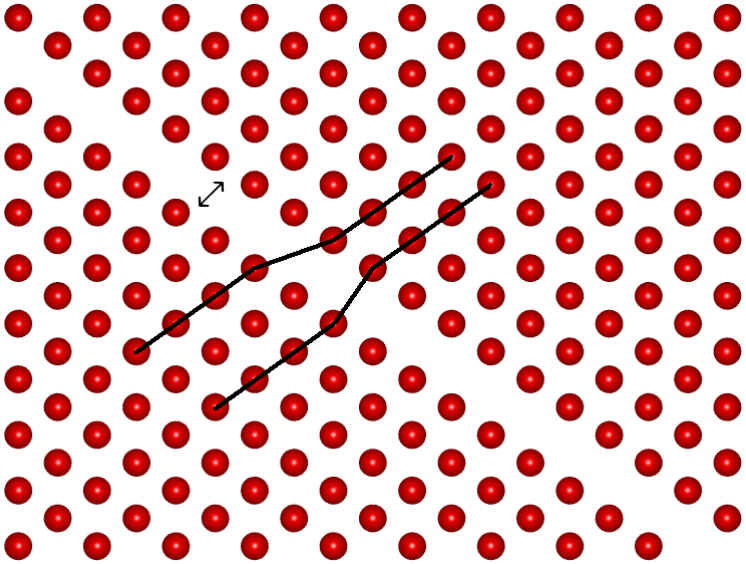
$\Delta u = b$

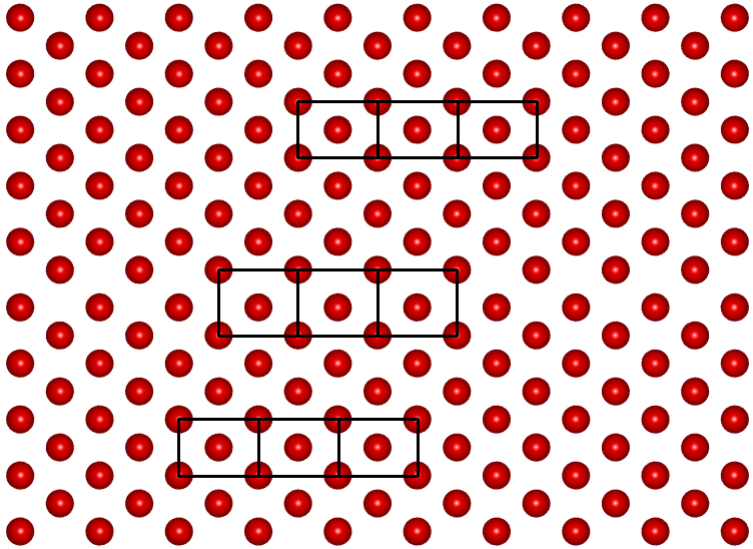






$\Delta u = b/3$



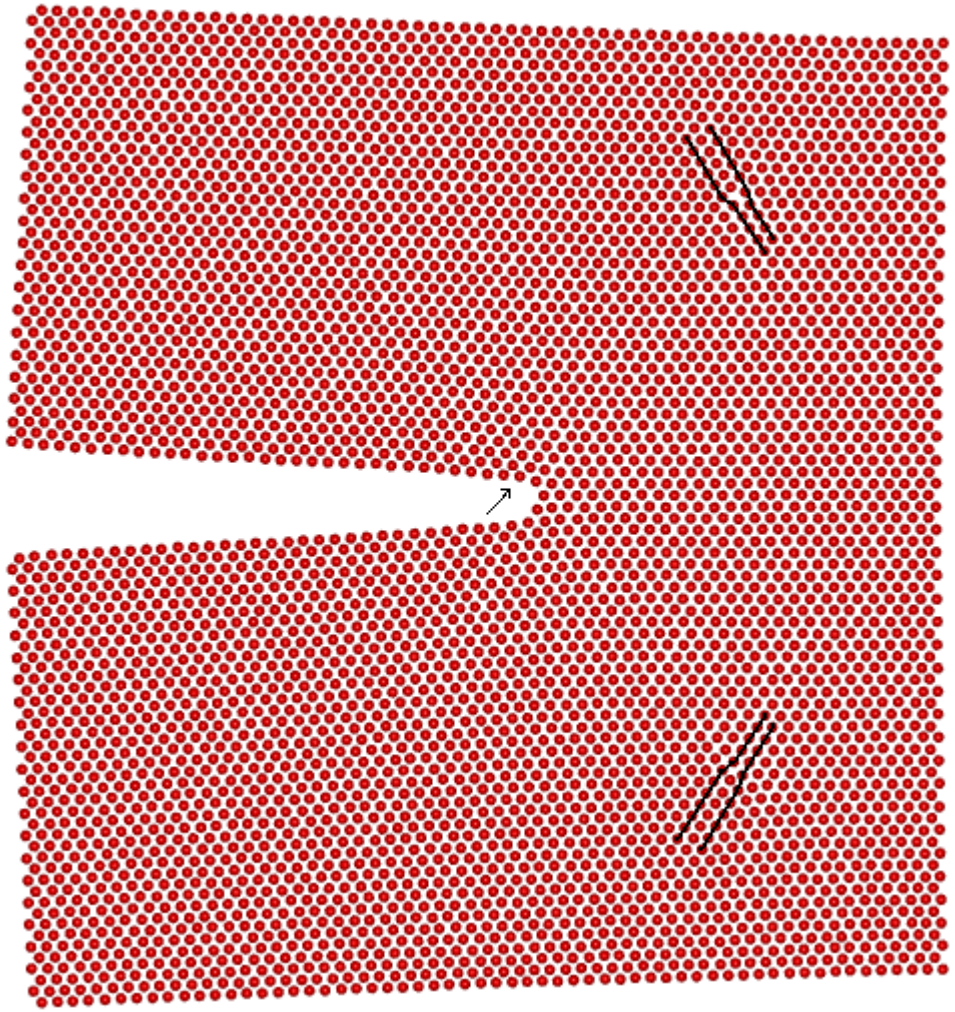


Results: Crack (-110)[110]

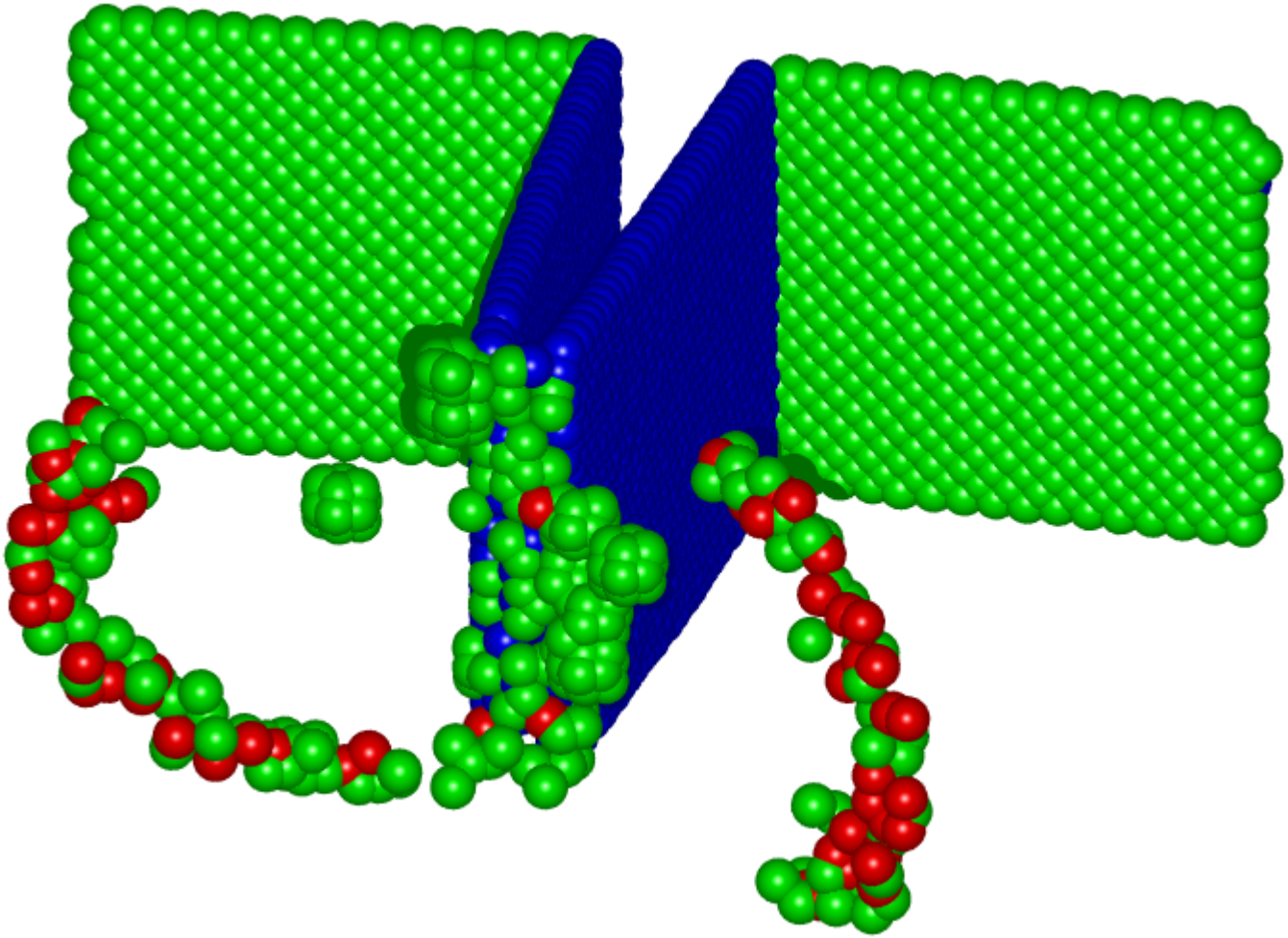
- Not sensitive to loading rate
- It emits dislocations on the inclined slip systems <111>{112} leading to crack blunting and stability of the crack
- Oriented in hard anti-twinning direction

  (τ_{twin} = 27.9 GPa; τ_{disl} = 16.3 GPa)

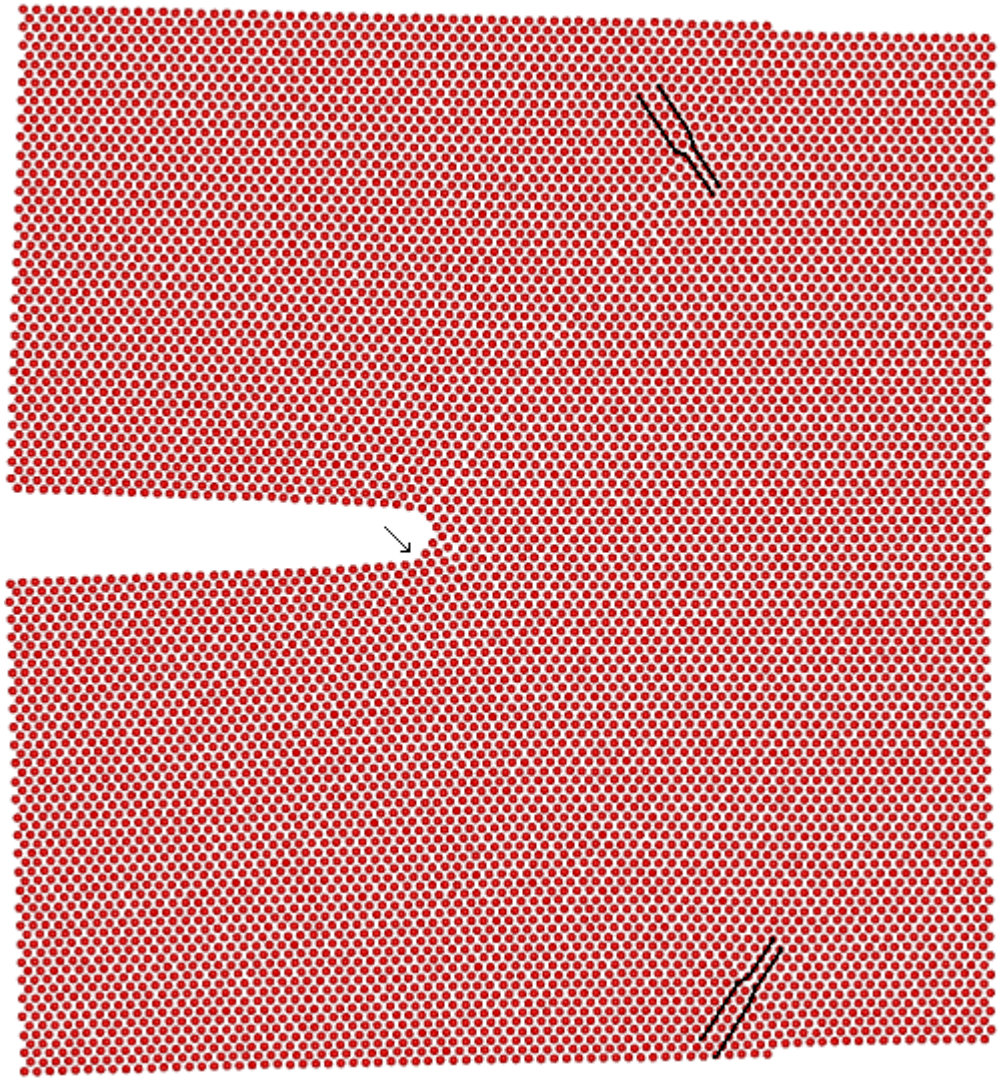
Dislocation emission under fast loading
Time step 3500, middle of the crystal



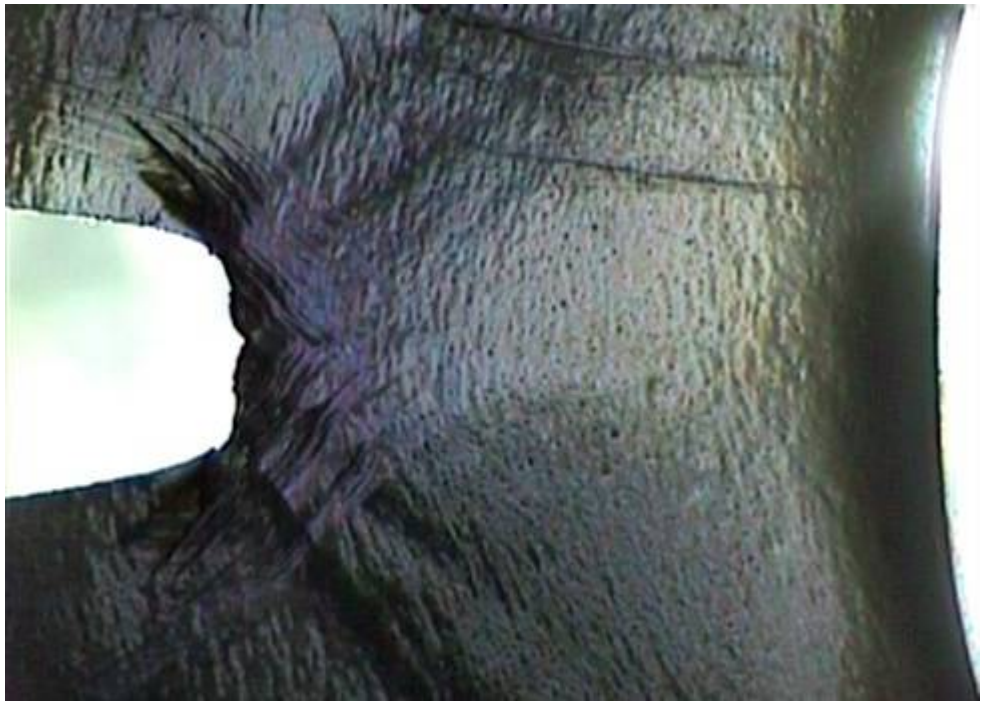
Dislocation emission by fast loading (3D)
Time step 3500



Dislocation emission by slow loading
Time step 6000



Slip patterns of the experimental sample with crack orientation (-110)[110]



A. Spielmannová, M. Landa, A. Machová, P. Haušild and P. Lejček: *Influence of crack orientation on the ductile – brittle behavior in Fe-3wt%Si single crystals*, Materials Characterization (2006), doi: 10.1016/j.matchar.2006.09.001 (article in press)

Conclusions

- Crack (001)
  - Ductile vs. brittle behavior sensitive to loading rate
  - Twinning on the slip systems <111>{112} and generation of dislocations on the oblique {110} slip planes
- Twins on the inclined {112} planes enable crack growth (it prevails under fast loading), while twinning on the oblique {112} planes causes contraction in sample thickness and hinders crack growth (typical for slow loading)
- Crack (-110)
  - Ductile behavior not sensitive to loading rate
  - Large crack blunting leading to crack stability
- The effect of the crack and slip orientation in 3D are in a qualitative agreement with our previous 2D plane strain simulations and our experimental observations