SLIP PROCESSES AND FRACTURE IN IRON CRYSTALS

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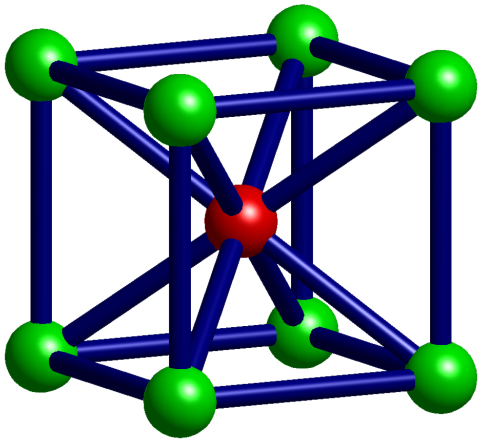

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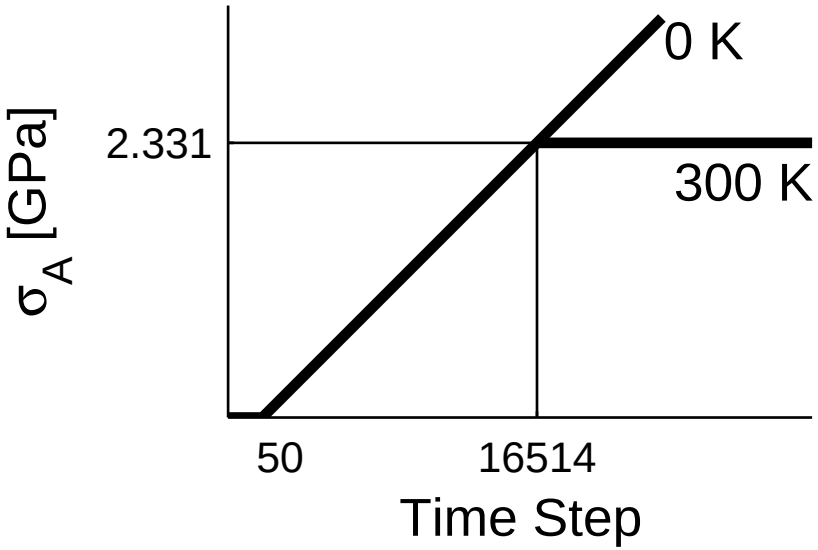
MD simulations in 3D

Interatomic interactions in bcc iron are described by an N-body potential from the paper by Ackland et al, Phil.Mag. A 75 (1997) 713. In the present contribution, two different crack orientations (crack plane/crack front) are treated: a pre-existing Griffith (through) **central crack** $(001)[010]$ and an **edge crack** $(001)[110]$ (through, pre-existing). The relatively long cracks are embedded in thin bcc iron crystals of different orientations and loaded in tension **mode I**.

The samples were loaded symmetrically in the $\langle 001 \rangle$ directions by prescribing external forces F_{ext} distributed homogeneously at individual atoms lying in several surface layers. Newtonian equations of motion for the individual atoms have been solved by a central difference method using time integration step $h = 1 \times 10^{-14}$ s. Each time step $t = nh$ we monitored the total number of existing interactions and global energy balance in the system.

Central $(001)[010]$ crack

The crystal with basic cubic orientation $\{100\}$ consists of 1999 planes in the $[100]$ direction, 100 planes along the crack front in the $[010]$ direction and 1999 planes in the $[001]$ direction. The central pre-existing (through) crack has been placed in the middle of the crystal. The crack is introduced by removing part of atoms from the central (001) plane. The initial half crack length in the $[100]$ direction is $l_o = 100a_o$, where $a_o = 2.8665\text{Å}$ is the lattice parameter. The initial half crack opening is $c_o = a_o$. The total number of atoms in the crystal is $N = 98\,892\,298$. Parallel processing in MPI has been used for these simulations.



Edge $(001)[110]$ crack

The simulated crystal has the same orientation and similar geometry as in our fracture experiments by Landa et al, Czech. J. Phys. 48 (1998) 1589: edge crack lies on a (001) plane, crack front is oriented along the $[110]$ direction and the direction of potential crack extension is $[\bar{1}10]$. The crystal contains 600 planes (001) (along the length L), 100 planes $(\bar{1}10)$ (along the width W) and 20 planes (110) along the crack front (thickness B). The initial edge crack of the length $l_o = 30a_o/\sqrt{2}$ was placed in the middle of the crystal and it was created by cutting of interatomic bonds across the crack plane. Half of the initial crack opening is $c_o = a_o/4$. The boundary correction factors are similar in simulations and in experiments. The simulated crystal was initially heated up to average temperature of 300 K during 1000 time steps. After that, the crystal was gradually (linearly) loaded during 3200 time steps up to an applied stress level of 8.42 GPa. The total number of atoms in the system is $N = 600\,000$ and single processing has been used in this case.

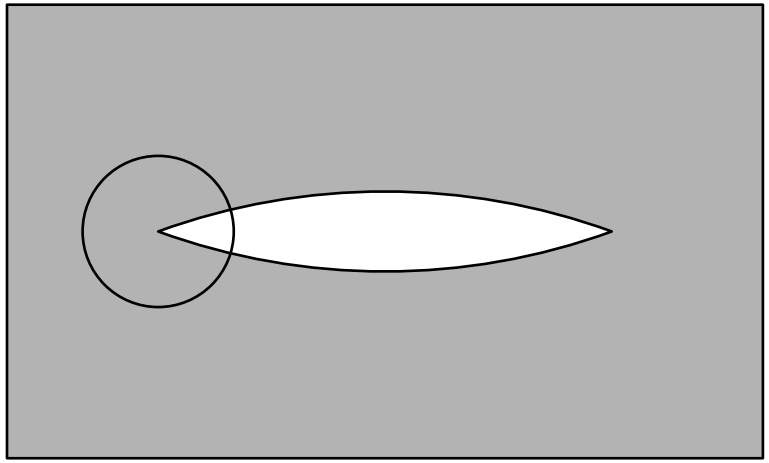
Results
Central crack

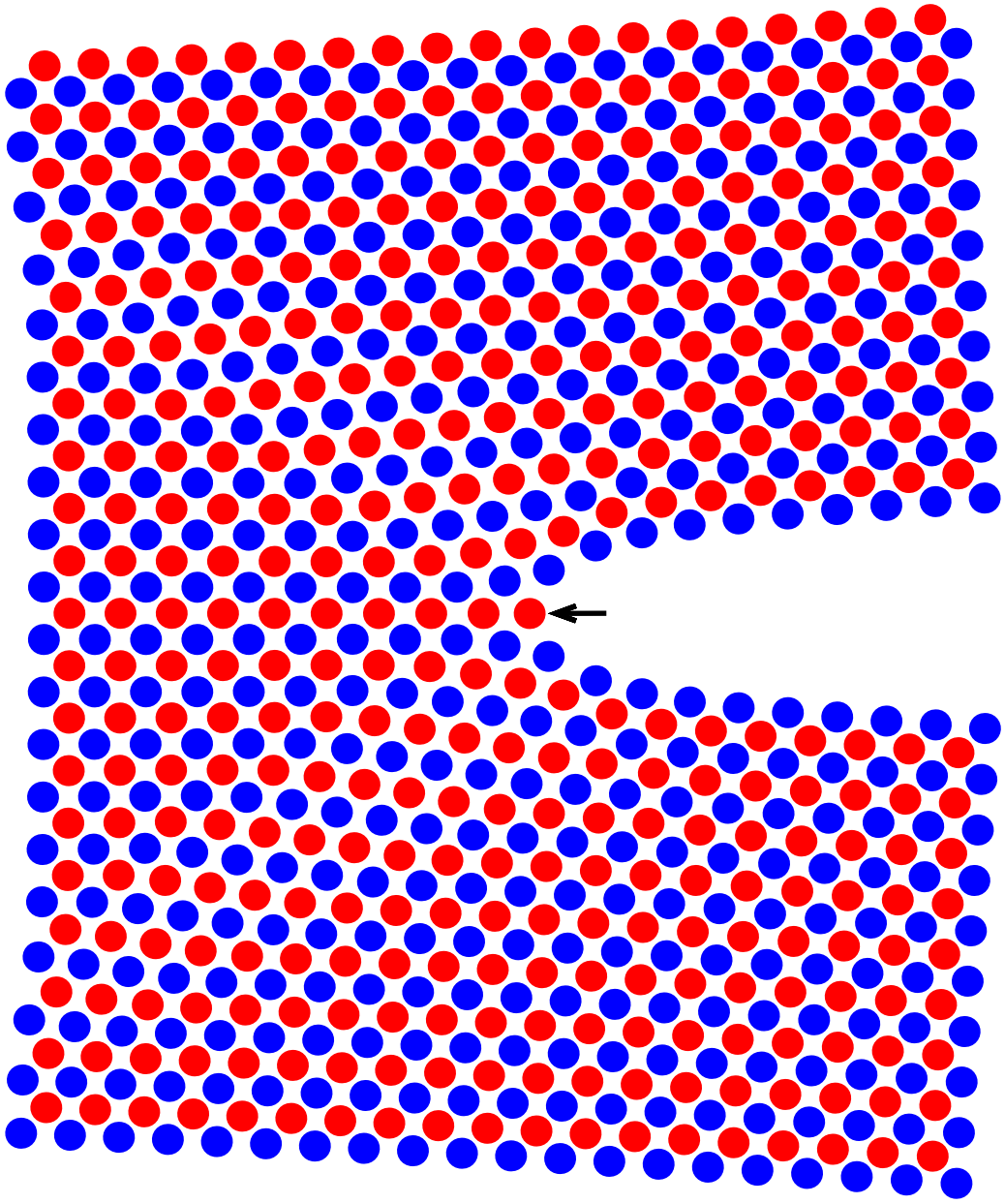
Brittle crack initiation at 0 K

at time step $23\,340$ in the middle of the crystal, $K_{MD} = 0.879$ MPam$^{1/2}$, the critical Griffith stress intensity expected according to anisotropic LFM for cleavage mechanism of crack initiation: $K_G = 0.817$ MPam$^{1/2}$ for plane strain, $K_G = 0.793$ MPam$^{1/2}$ for plane stress.

Detail at the left crack front before crack initiation

Atomic configuration after crack initiation, the arrow shows the original crack tip point





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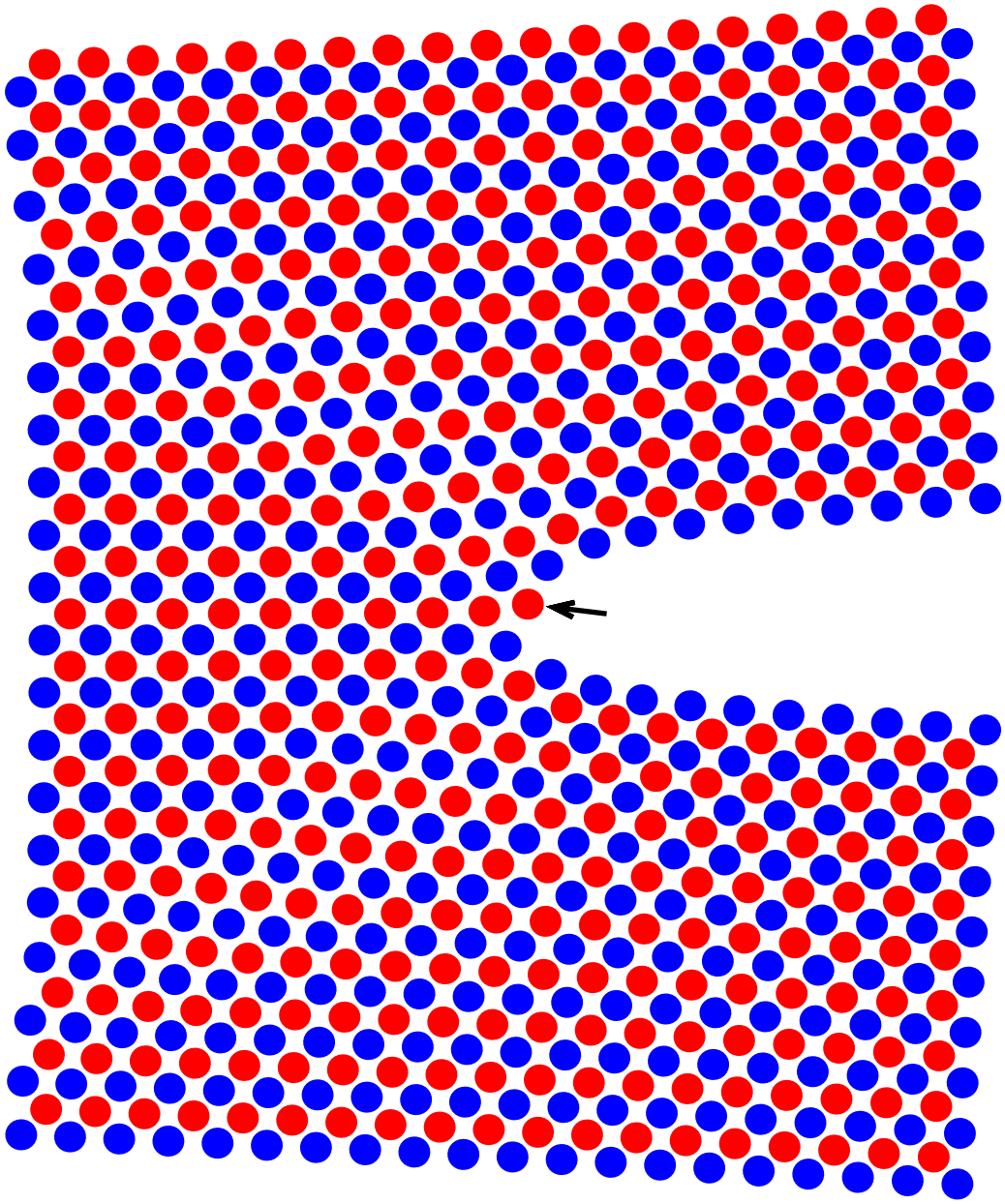

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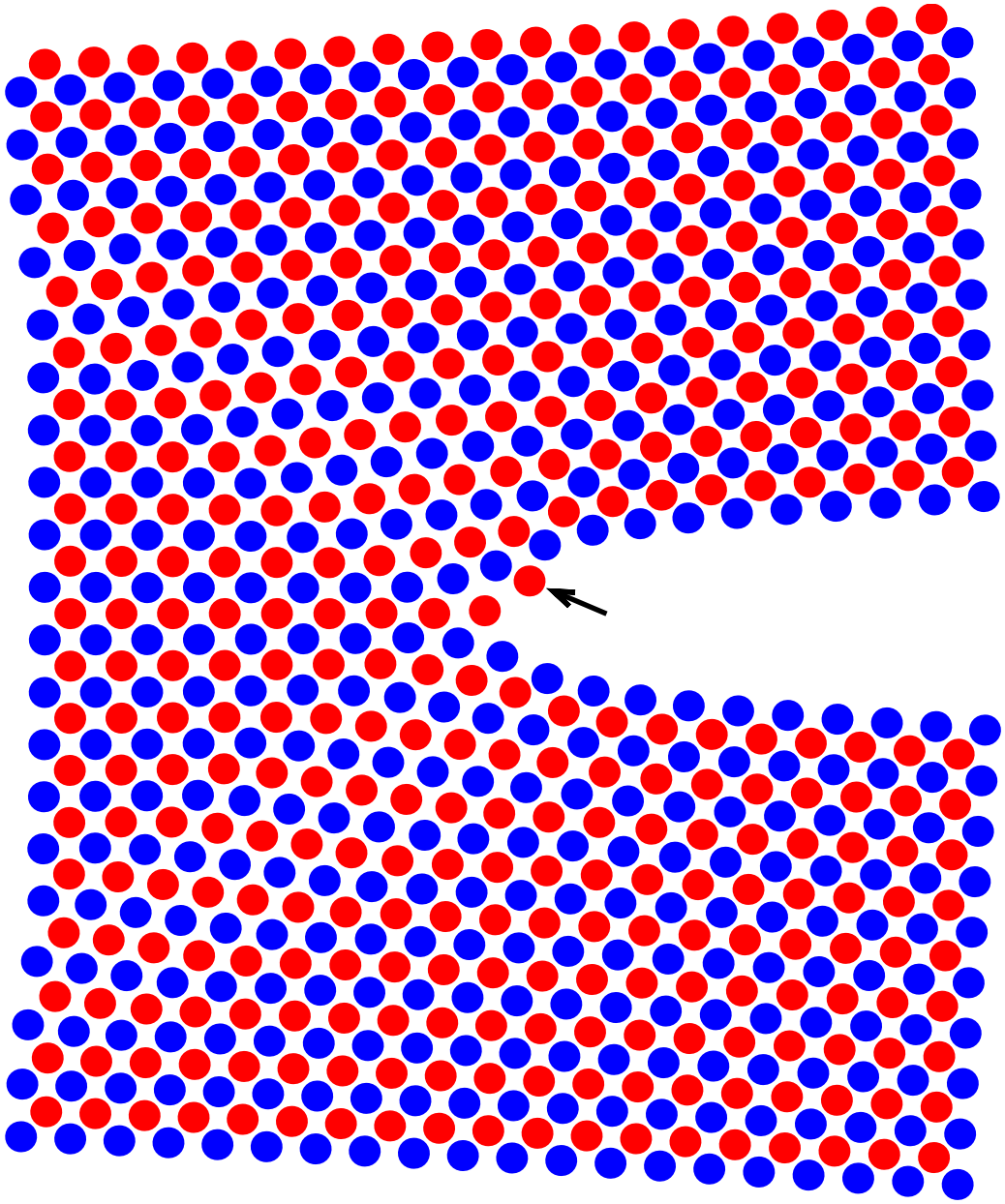

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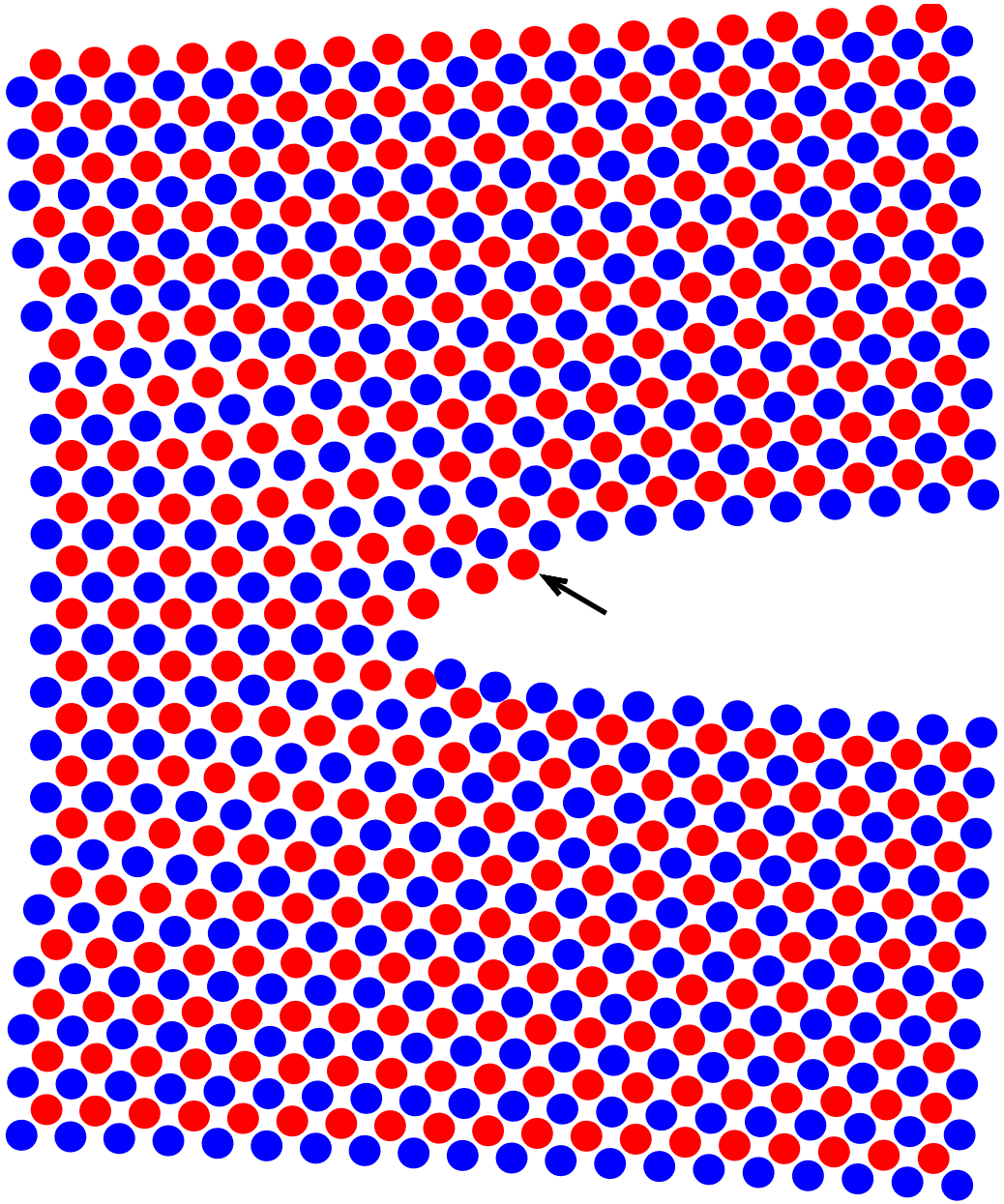

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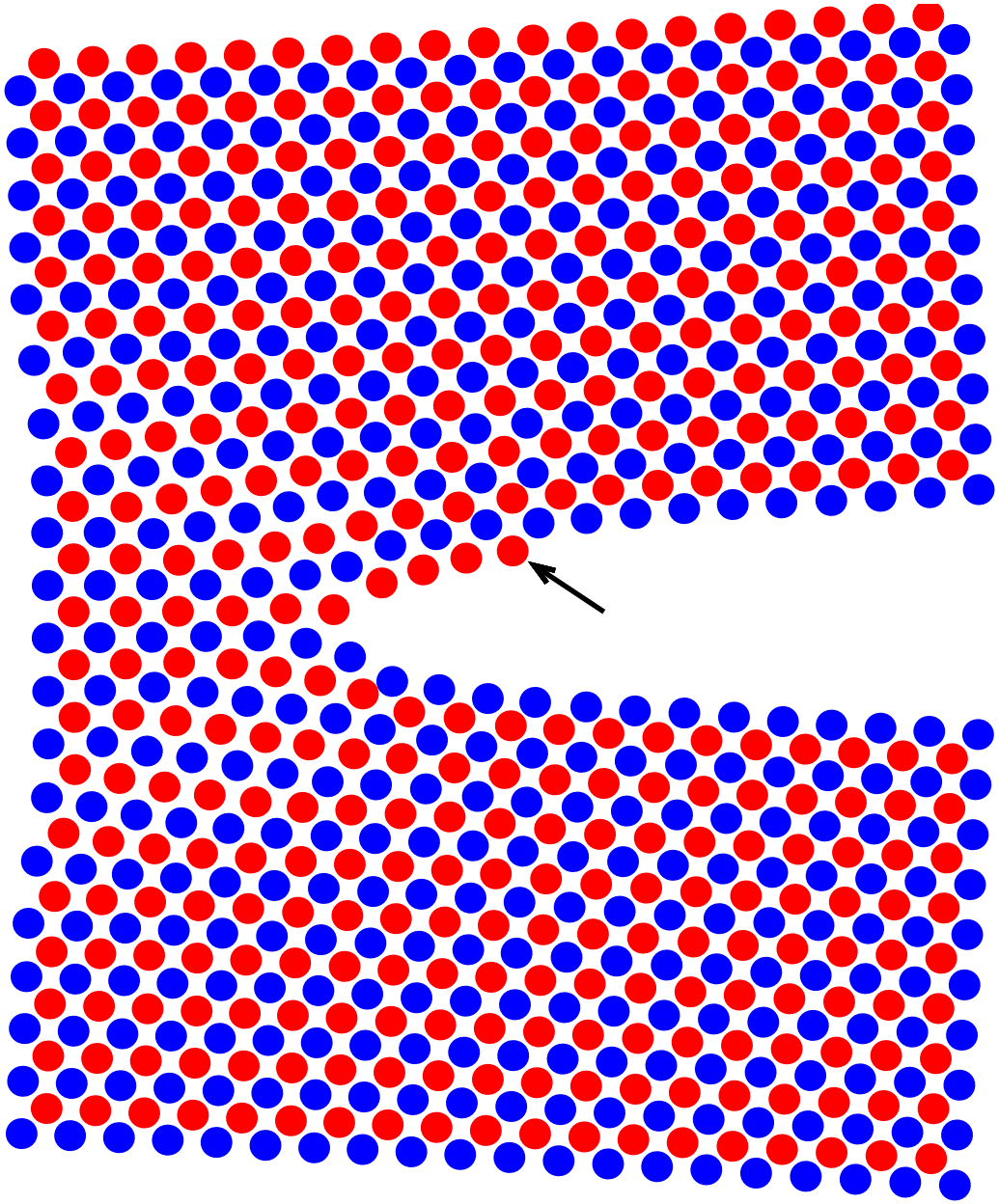

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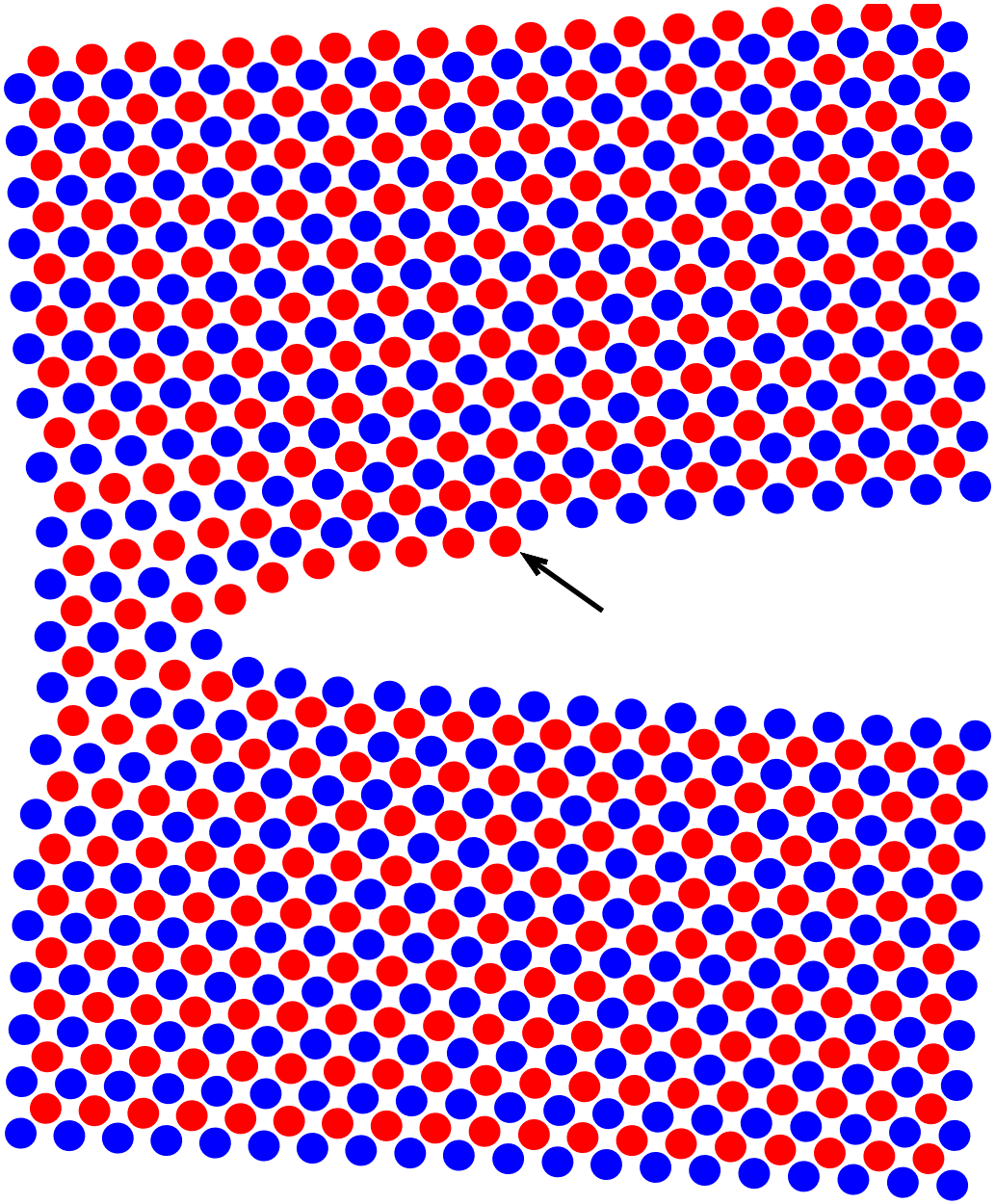

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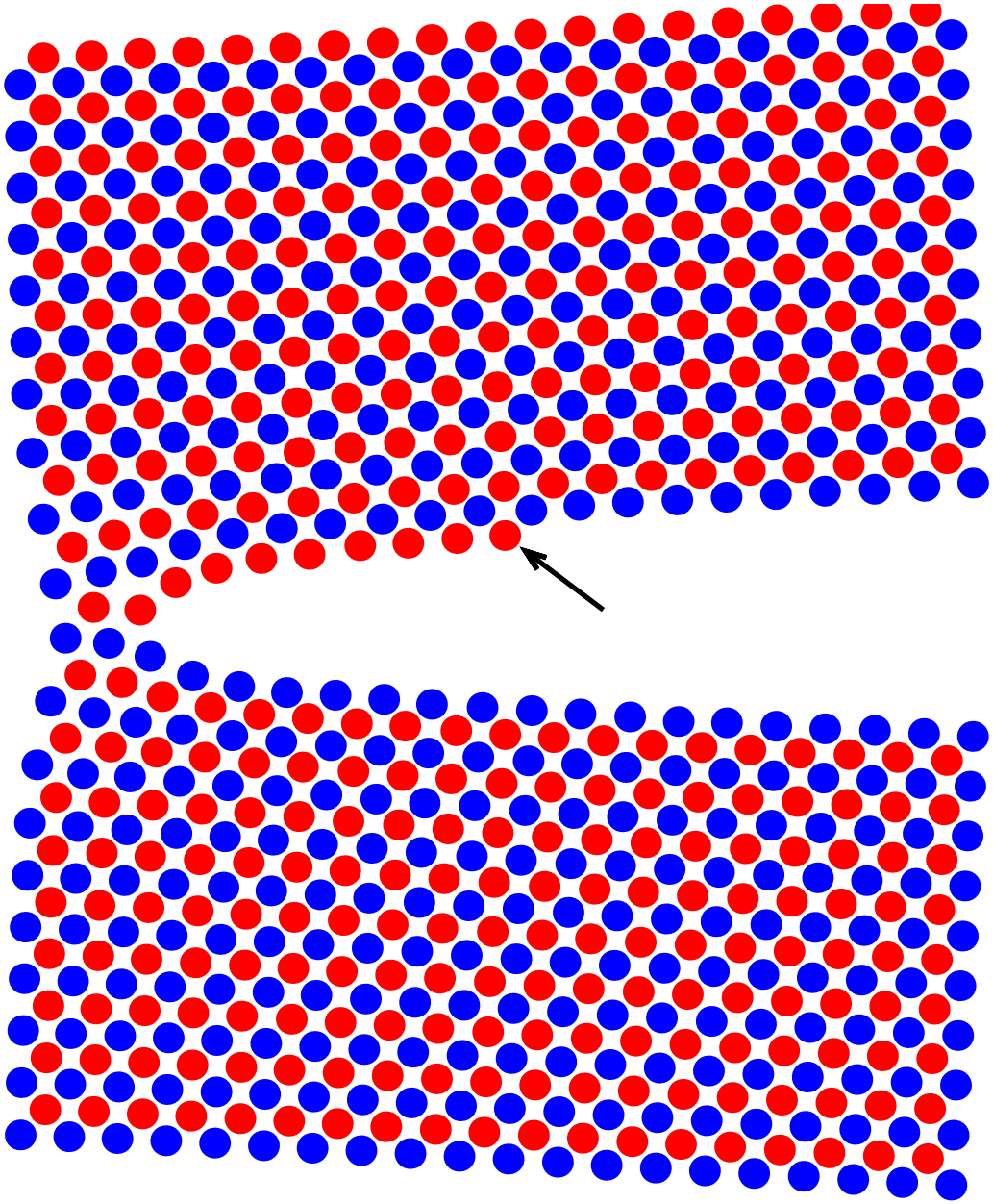

Time step:
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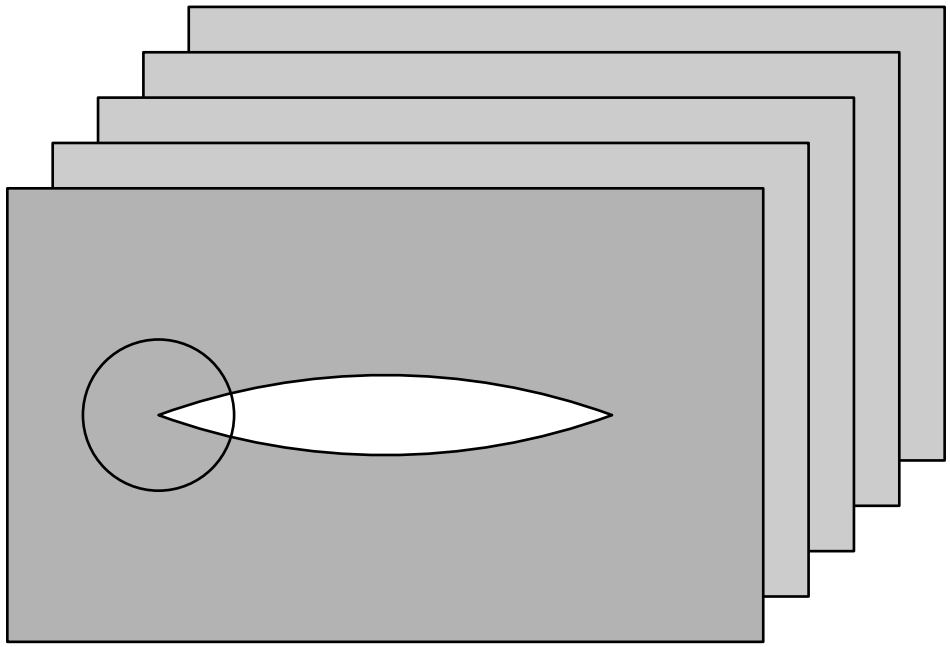
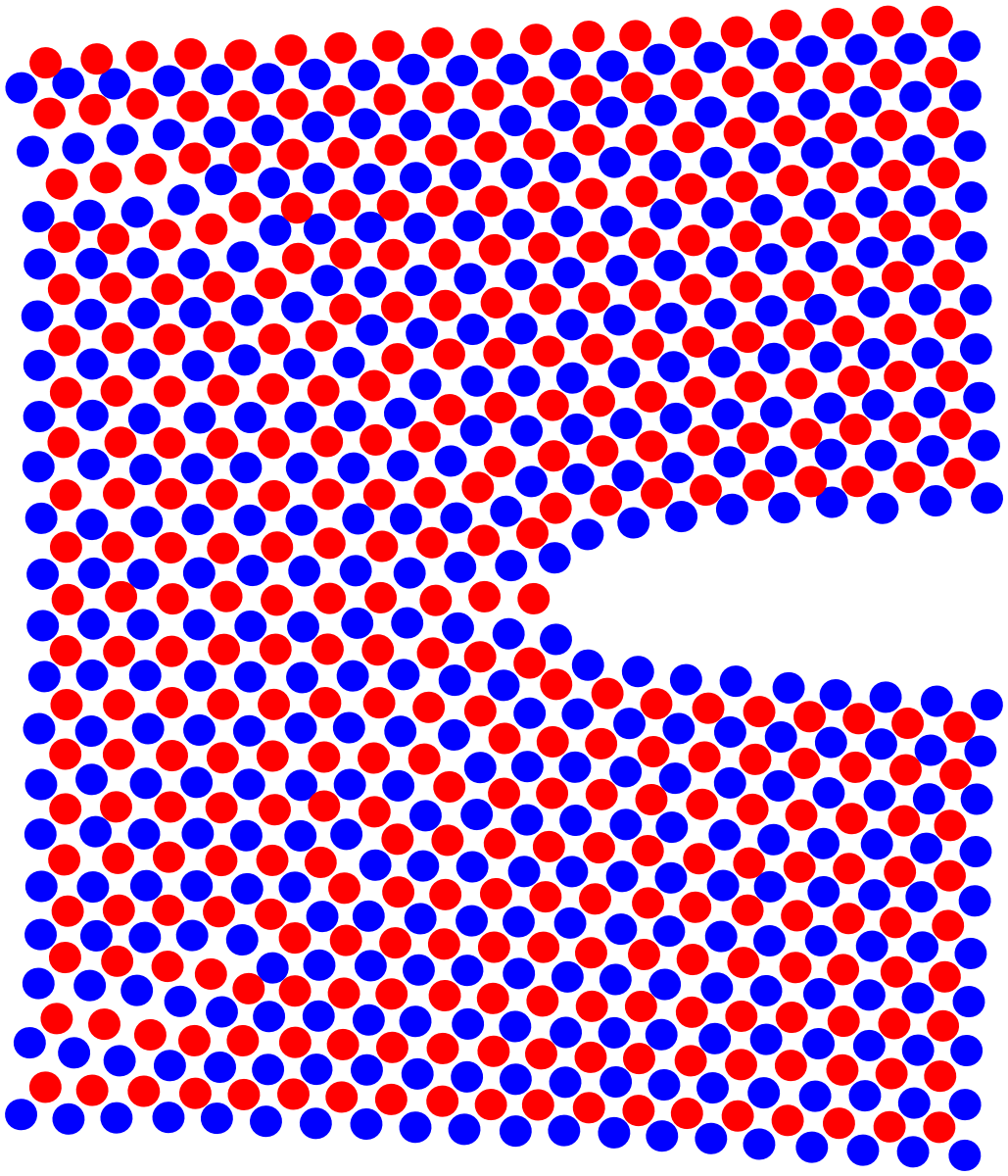
Ductile behavior at 300 K



Slip planes and patterns at the left crack front.
Time step $14\,100$**, view** $(010)[010]$**.**



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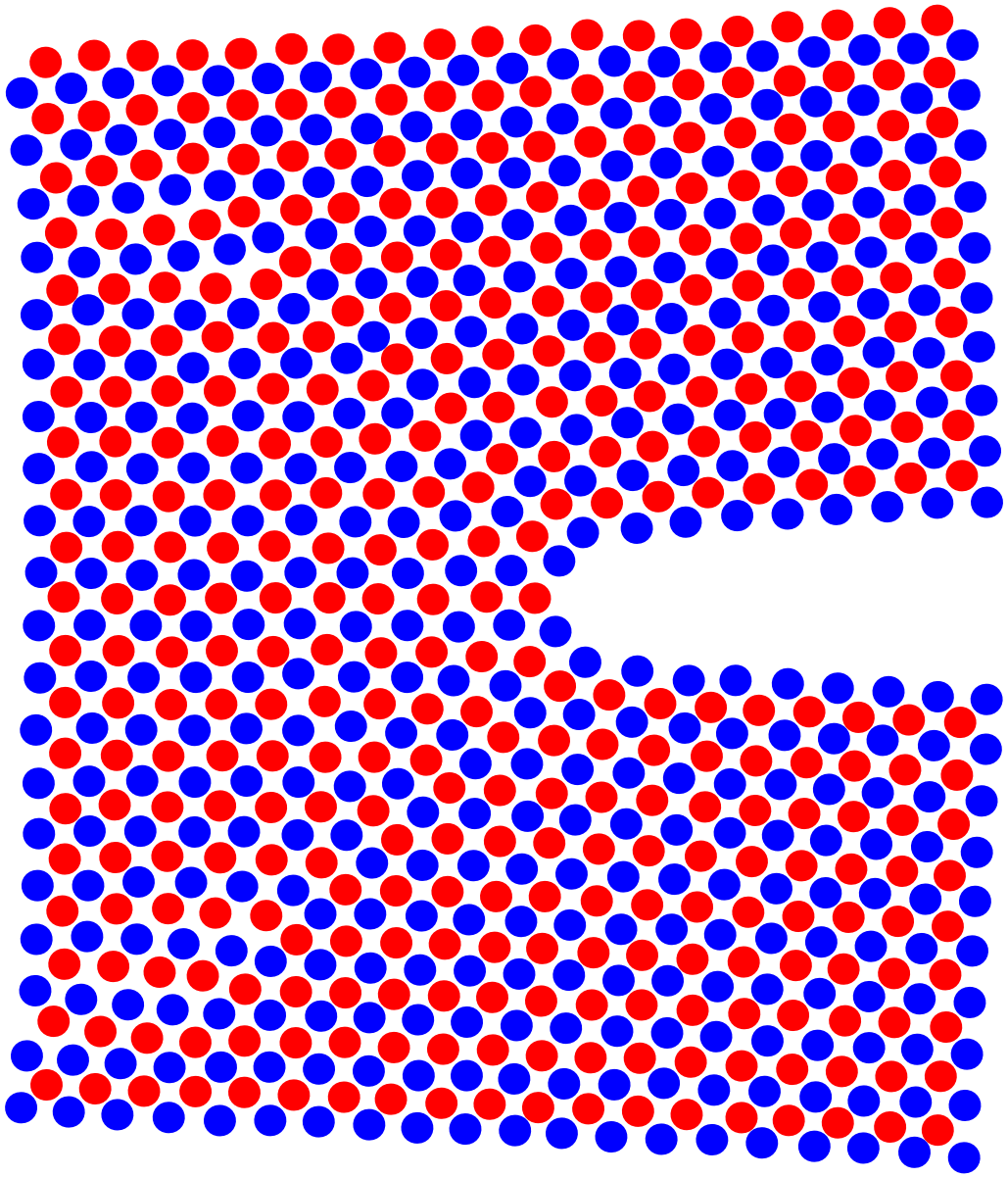

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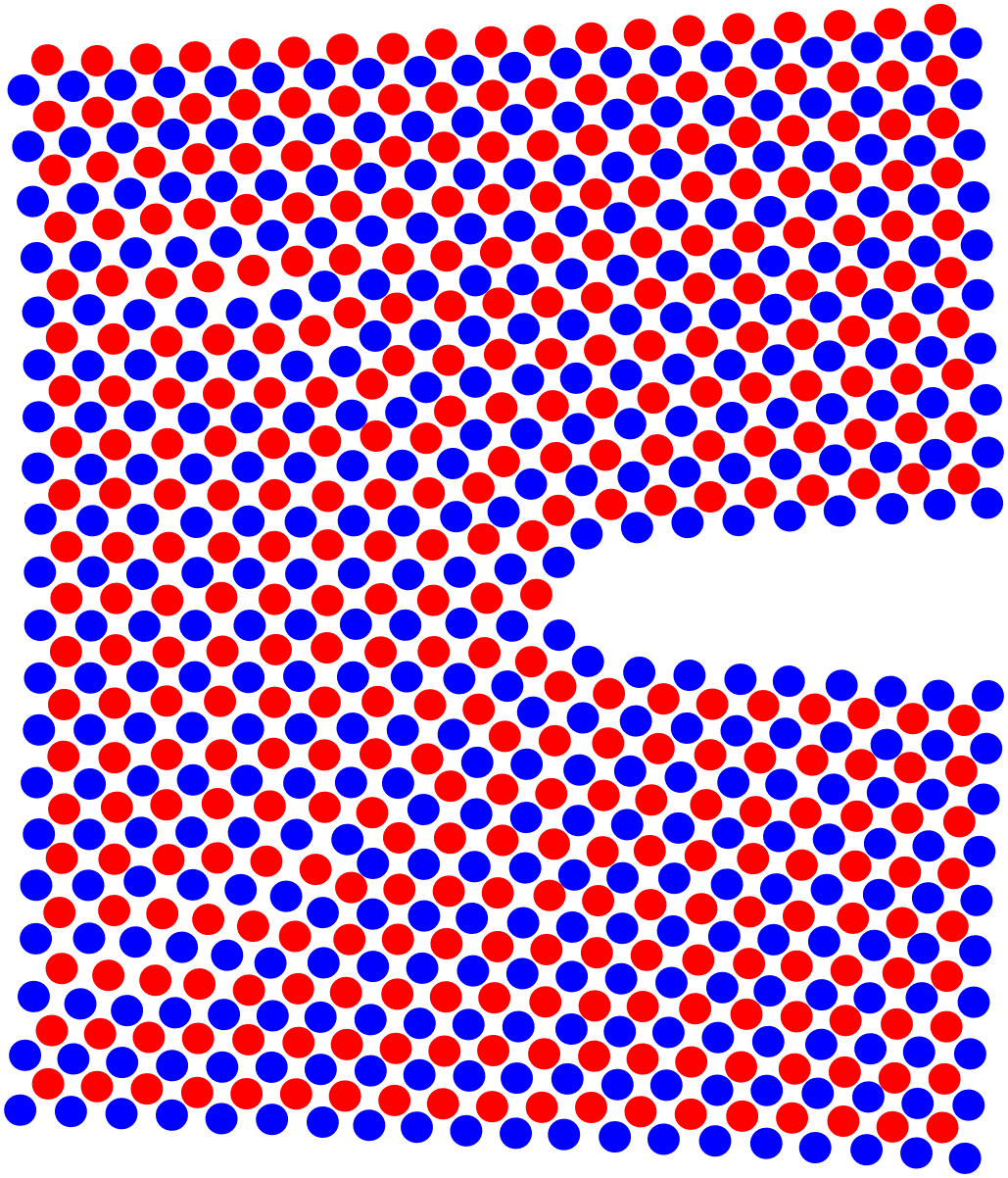

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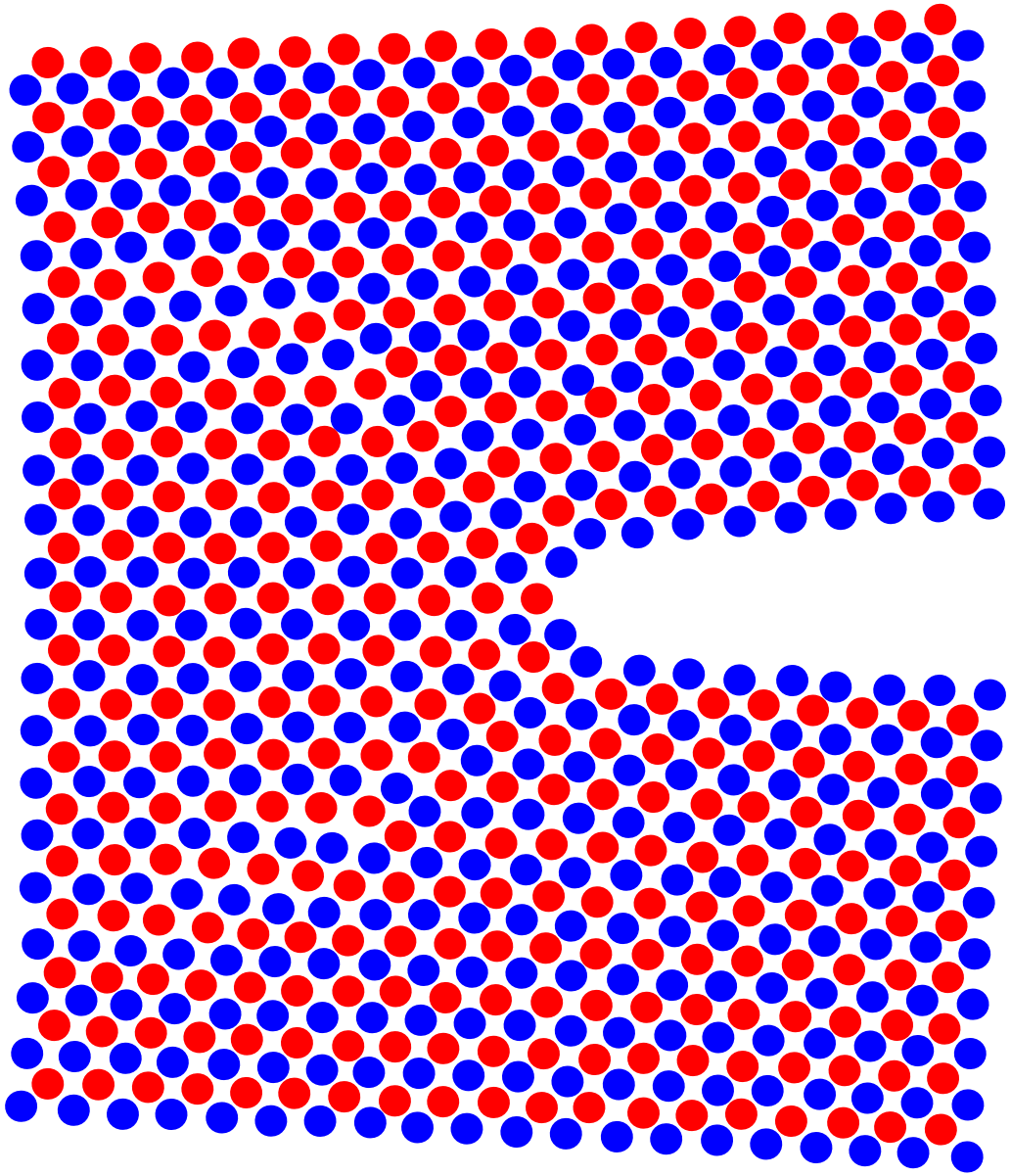

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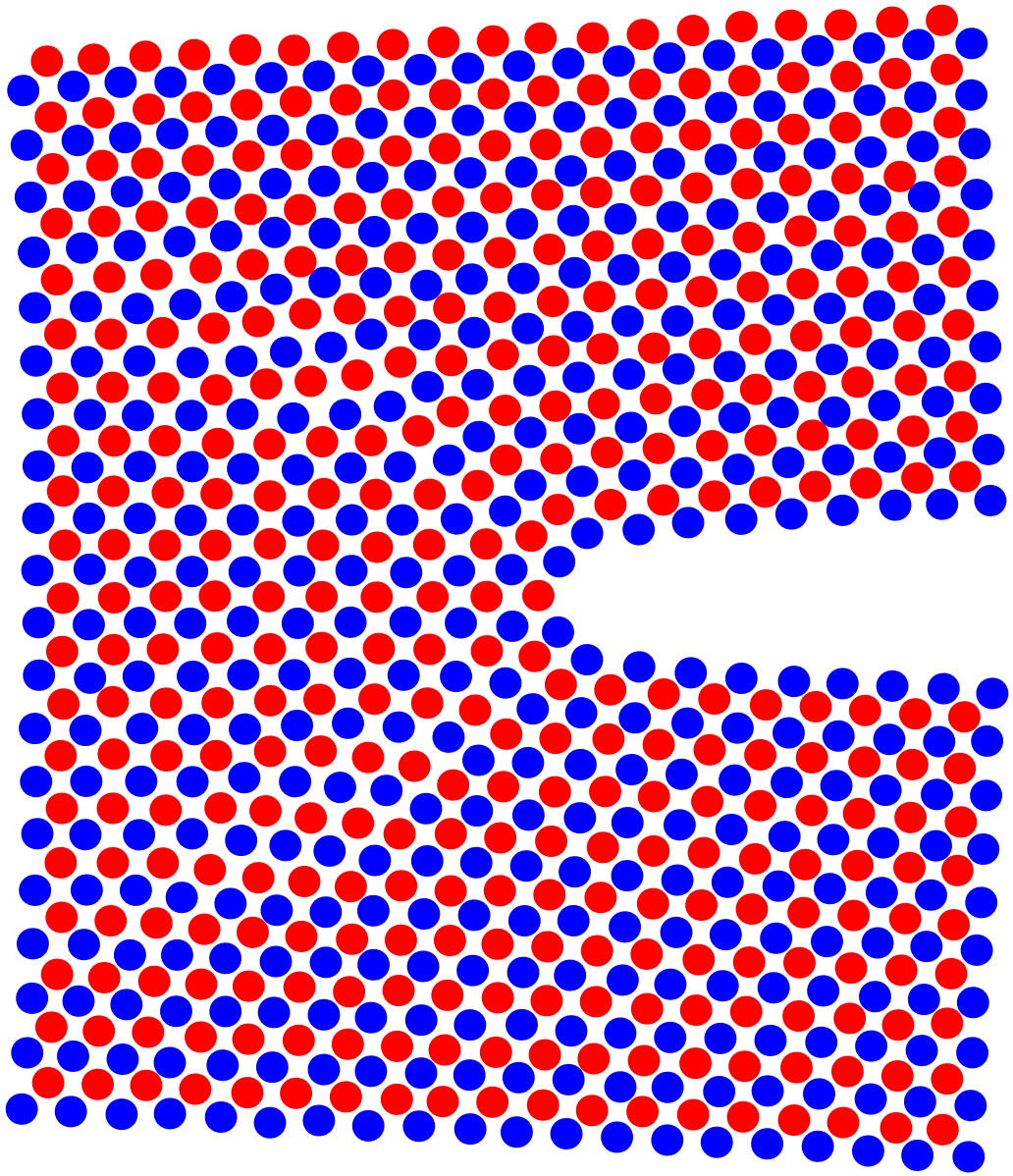

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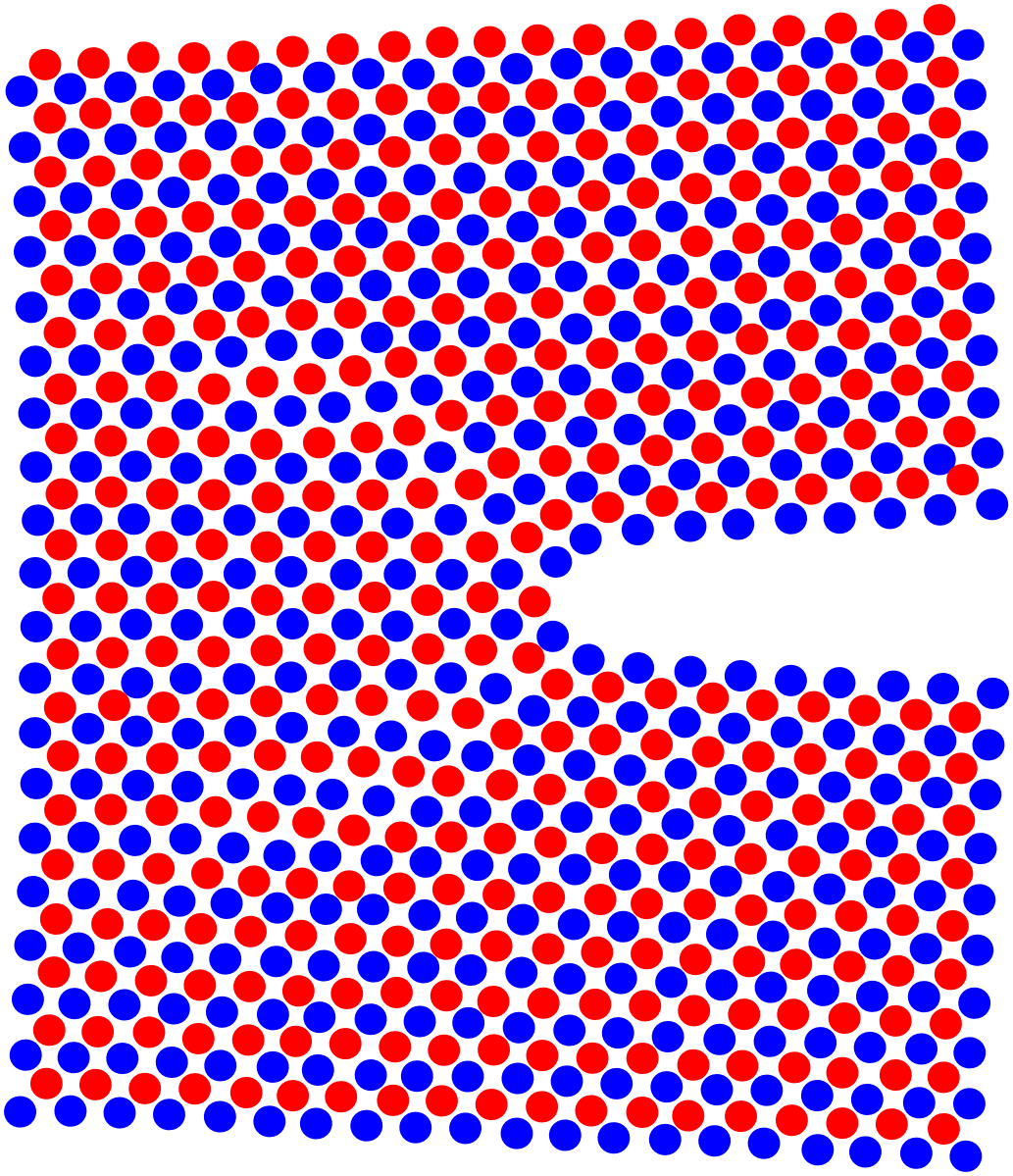

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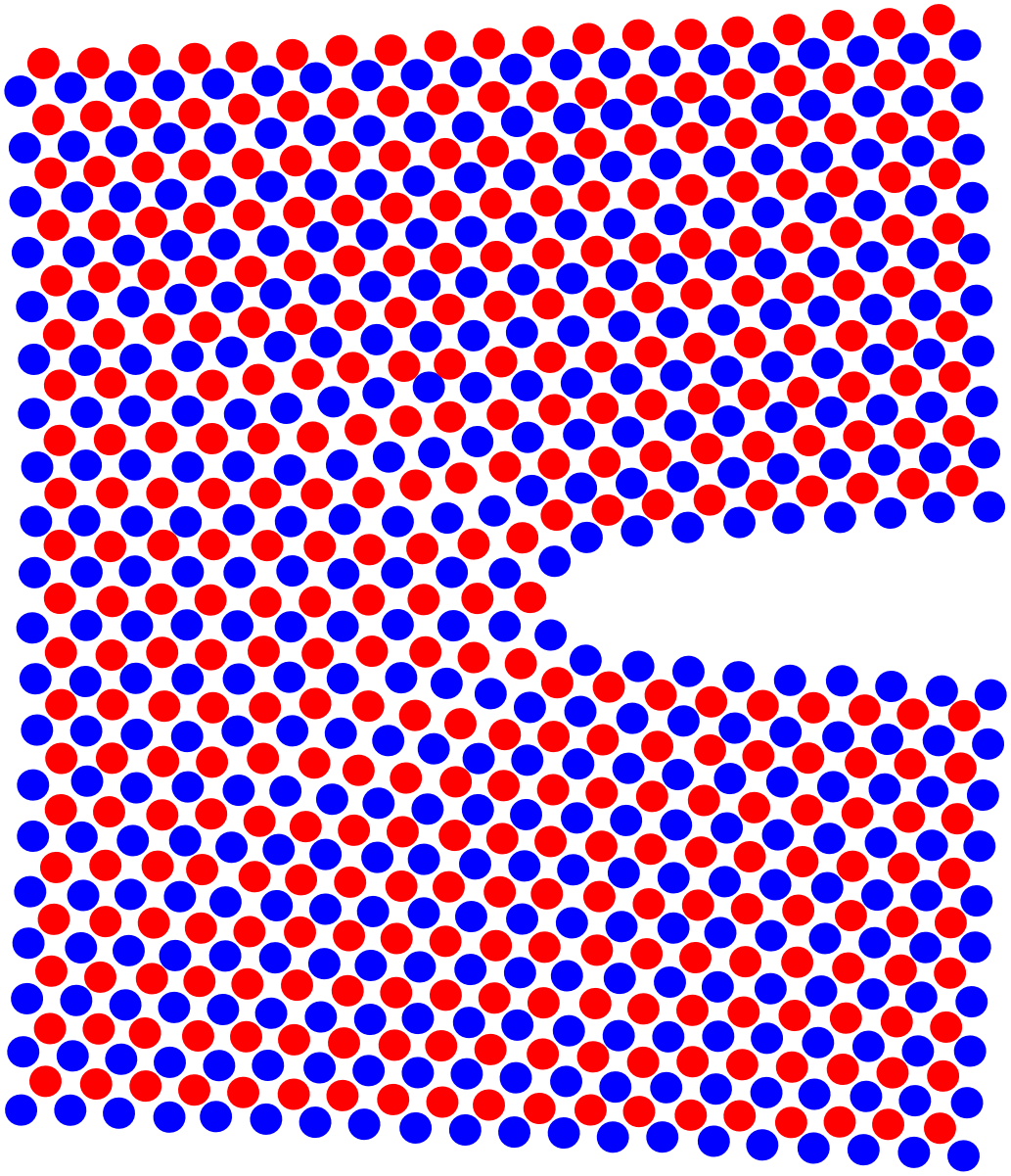

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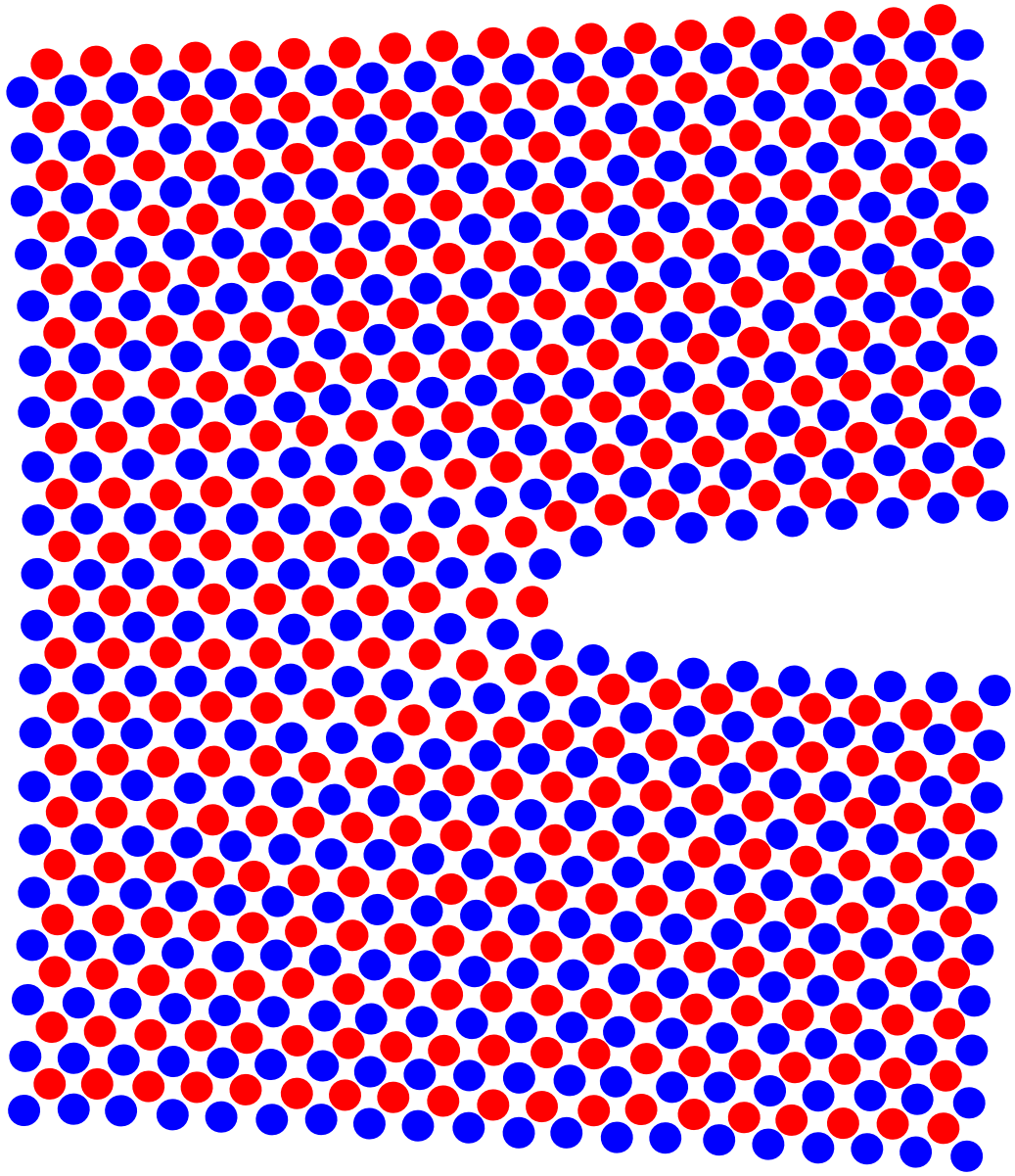

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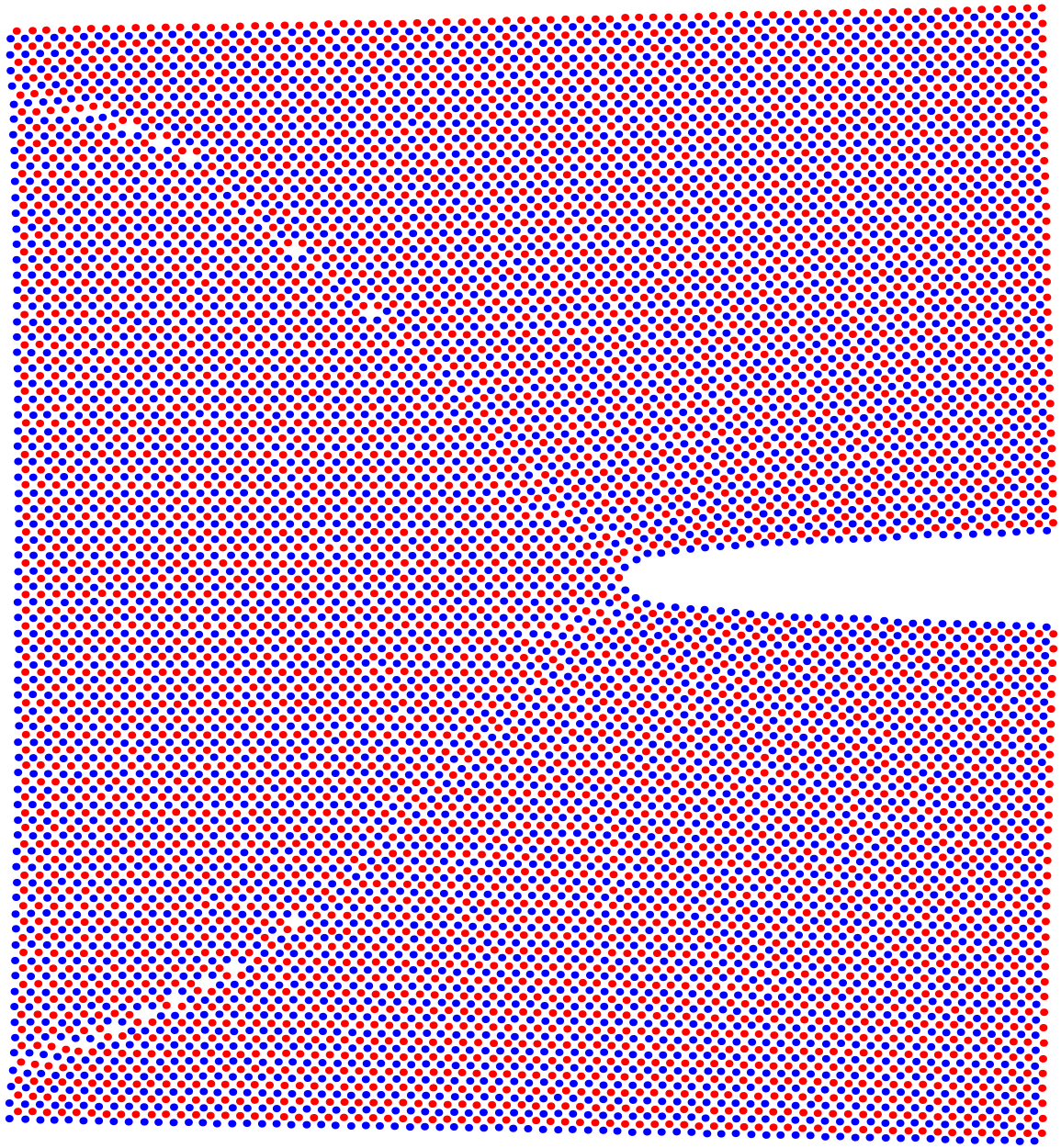
22–23

Time step 15 000

Two different slip patterns:

- BLS $\Rightarrow \{101\}, \theta \approx 45^\circ$
- BLS $\Rightarrow \{112\}, \theta = 26.565^\circ$



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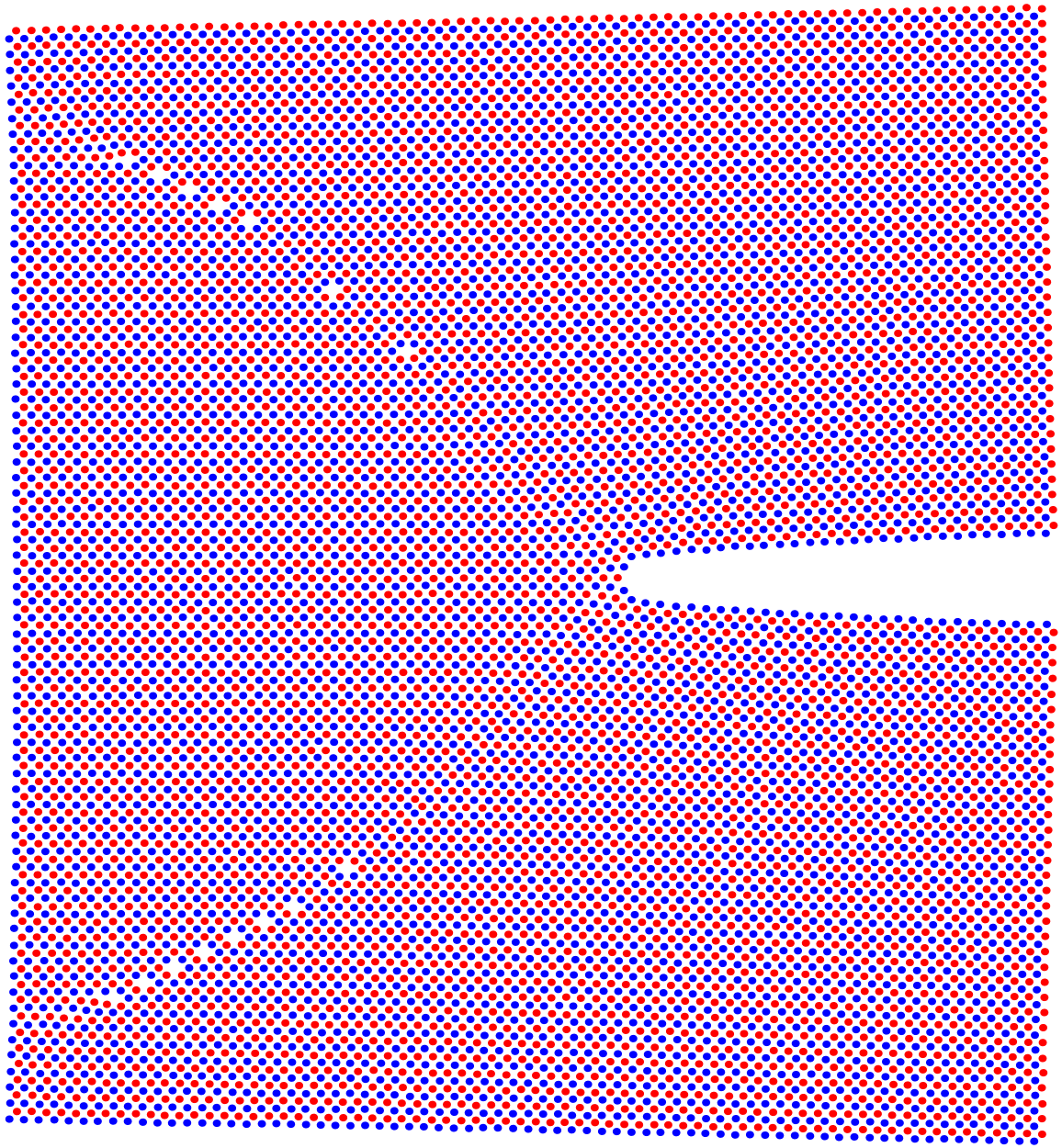

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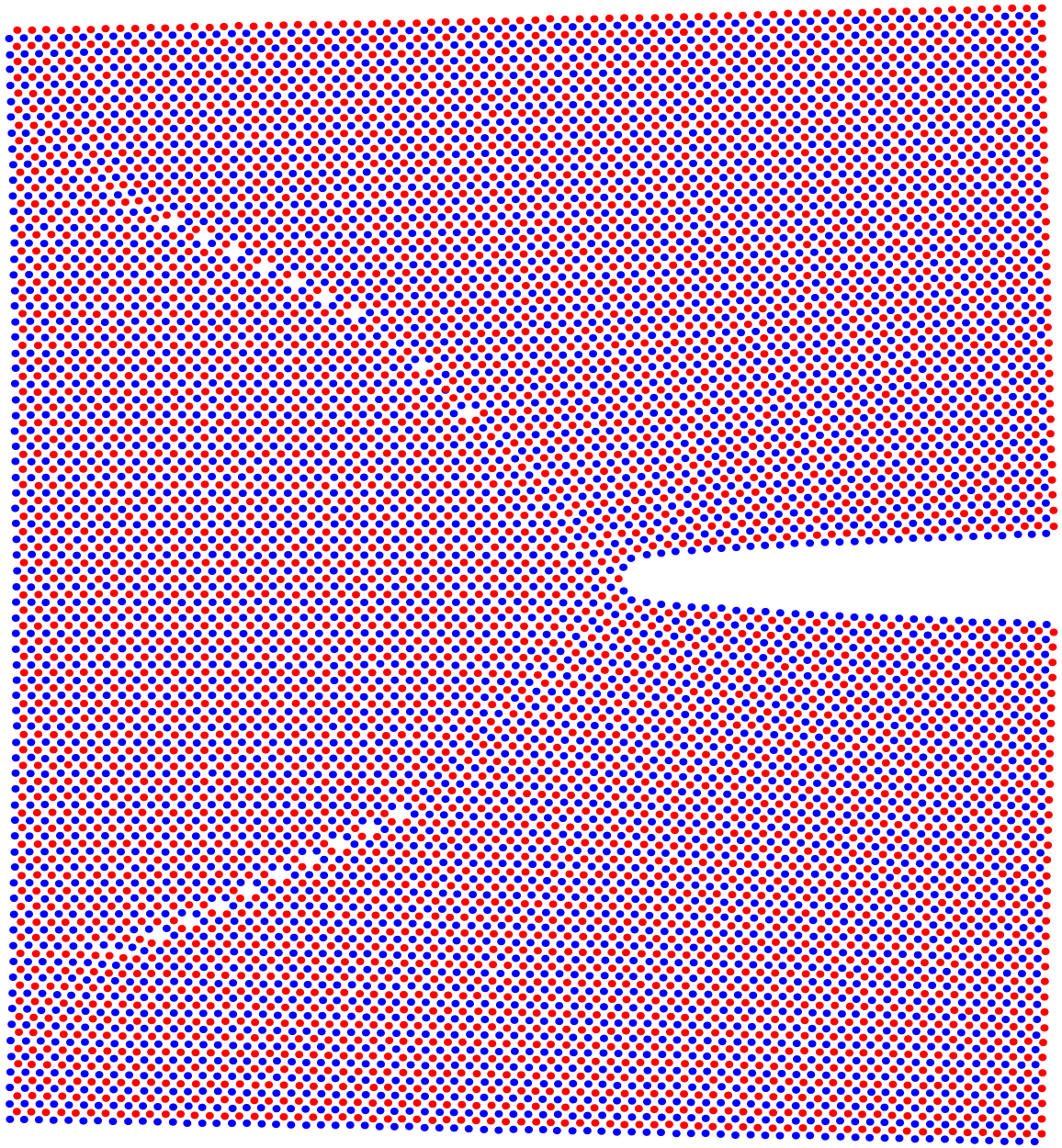

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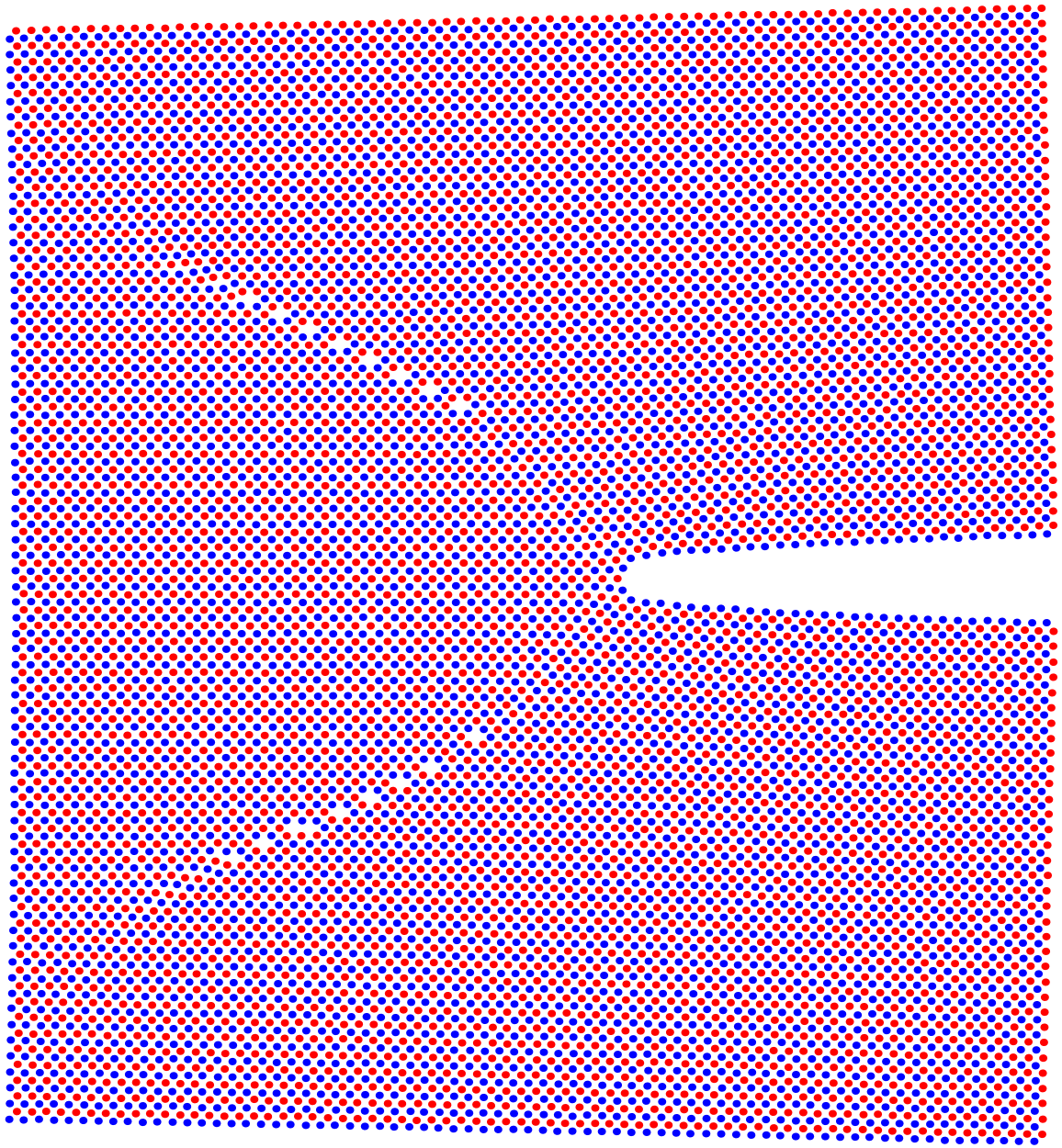

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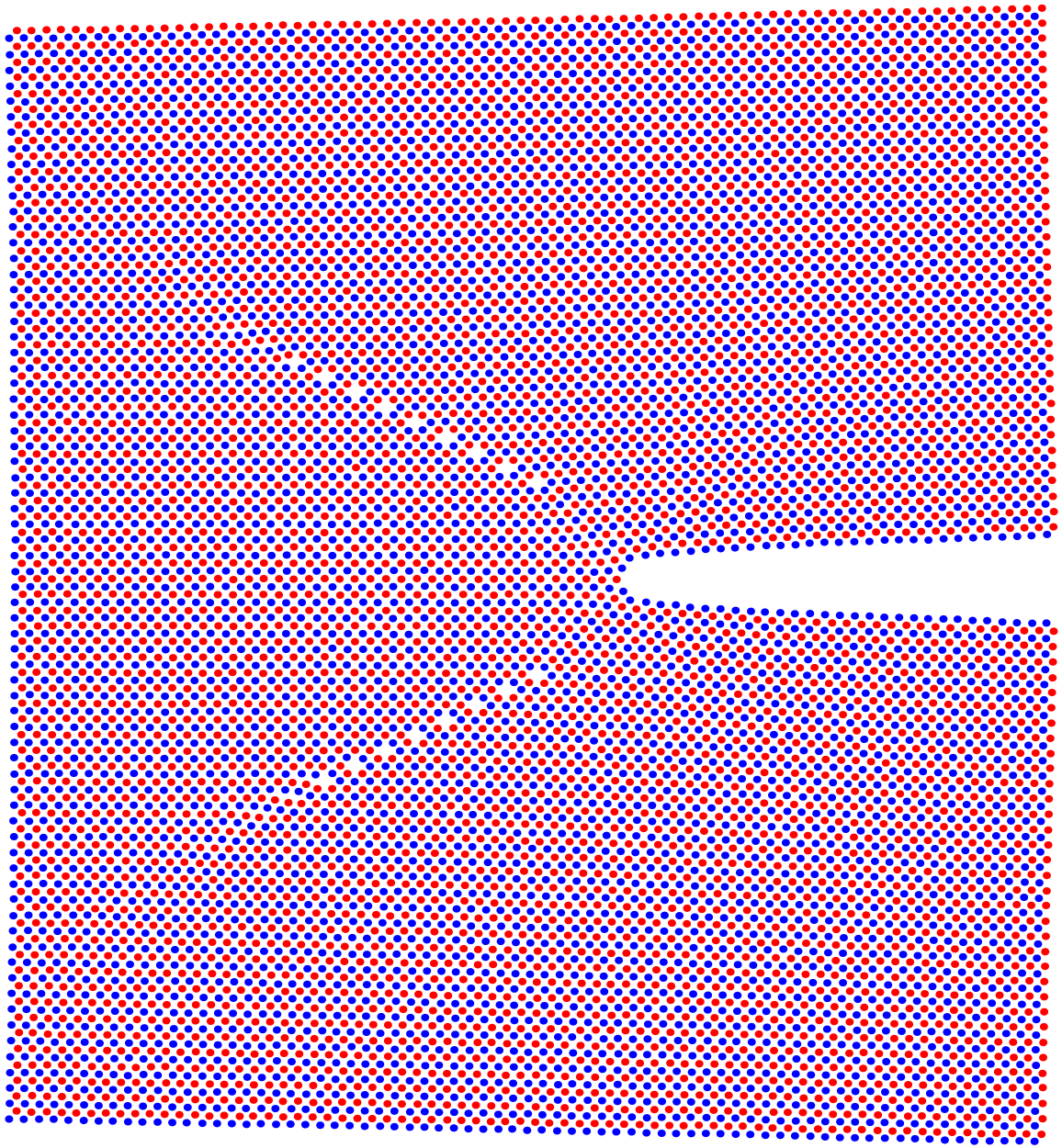

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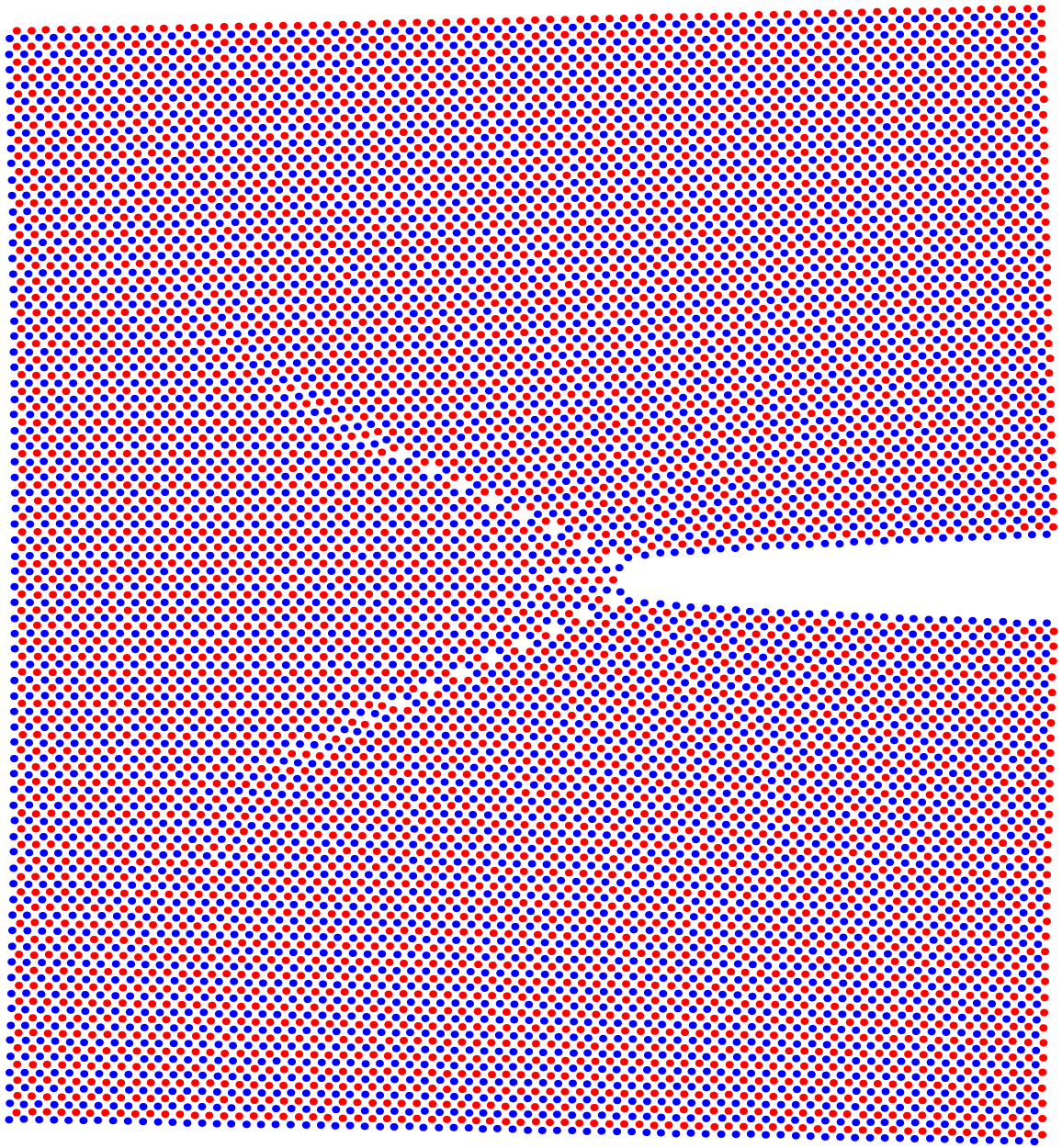

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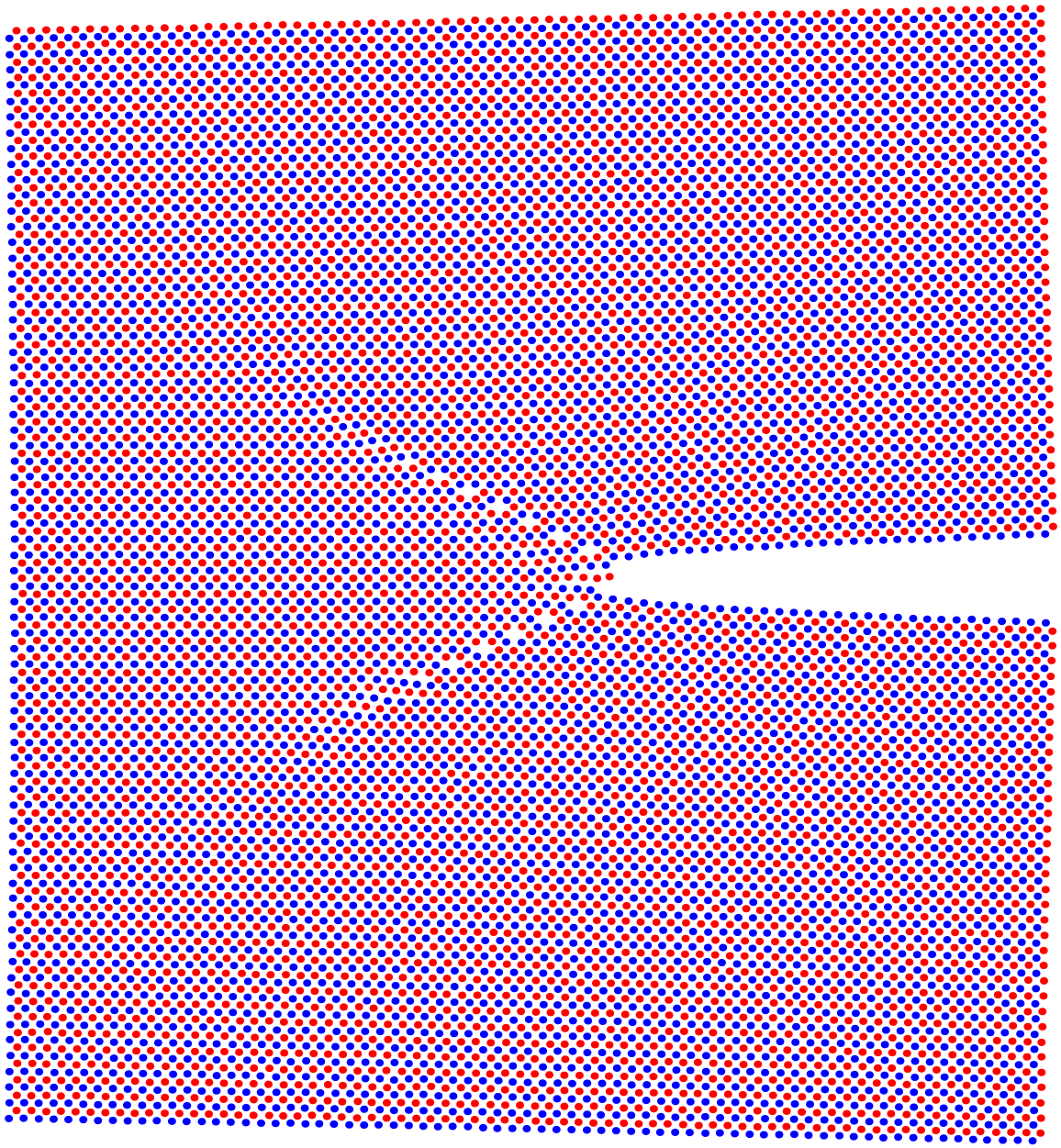

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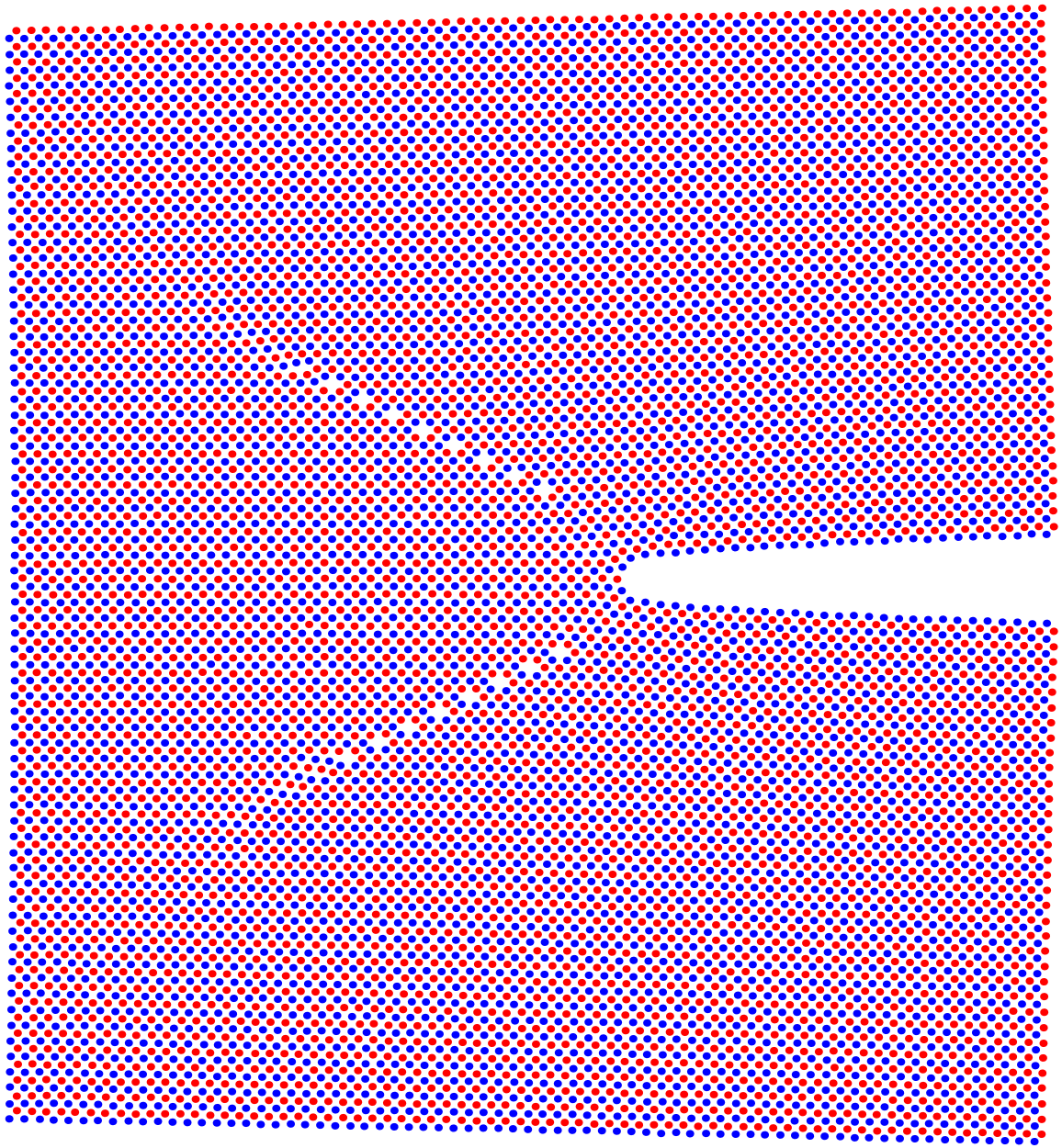

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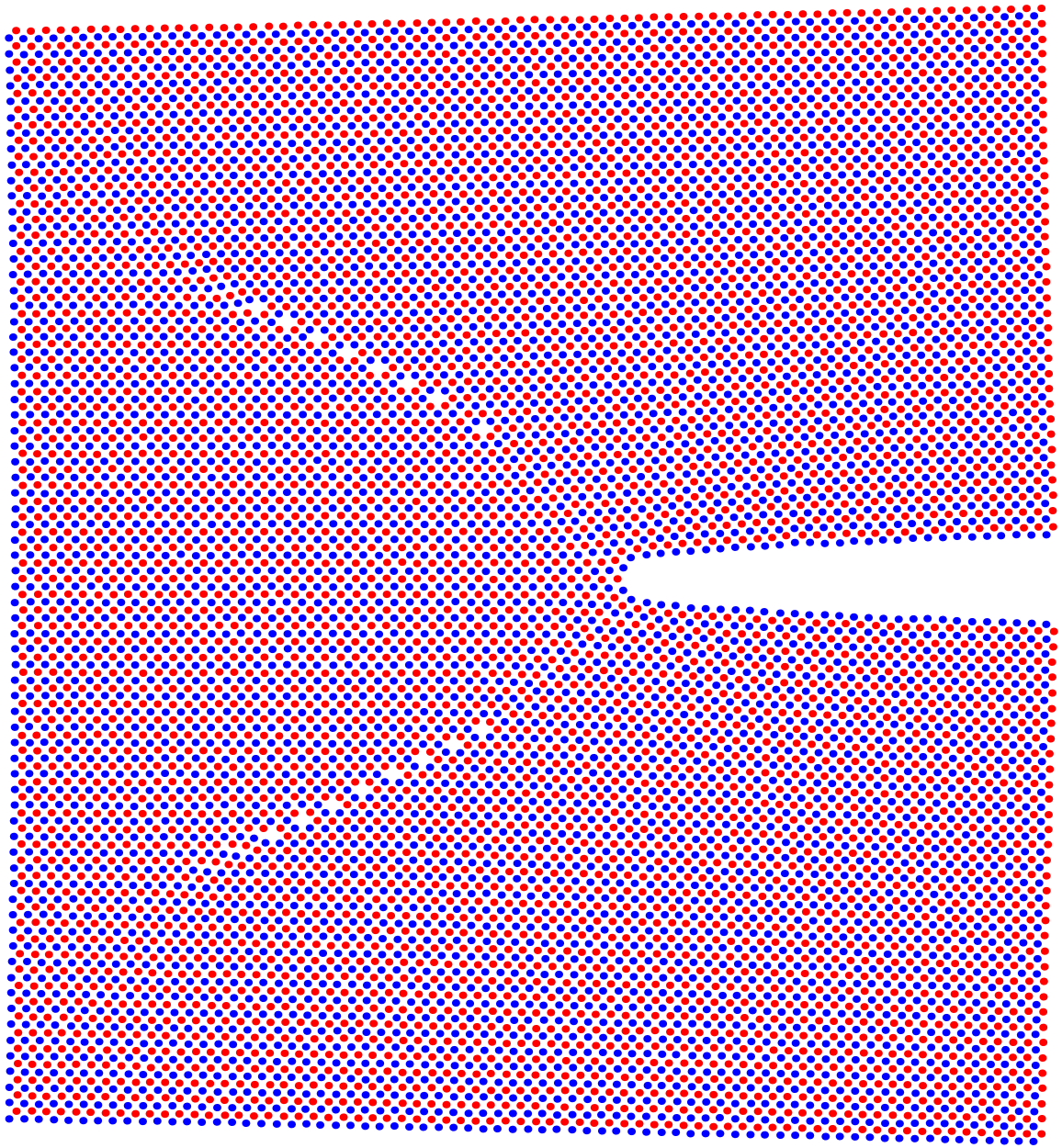

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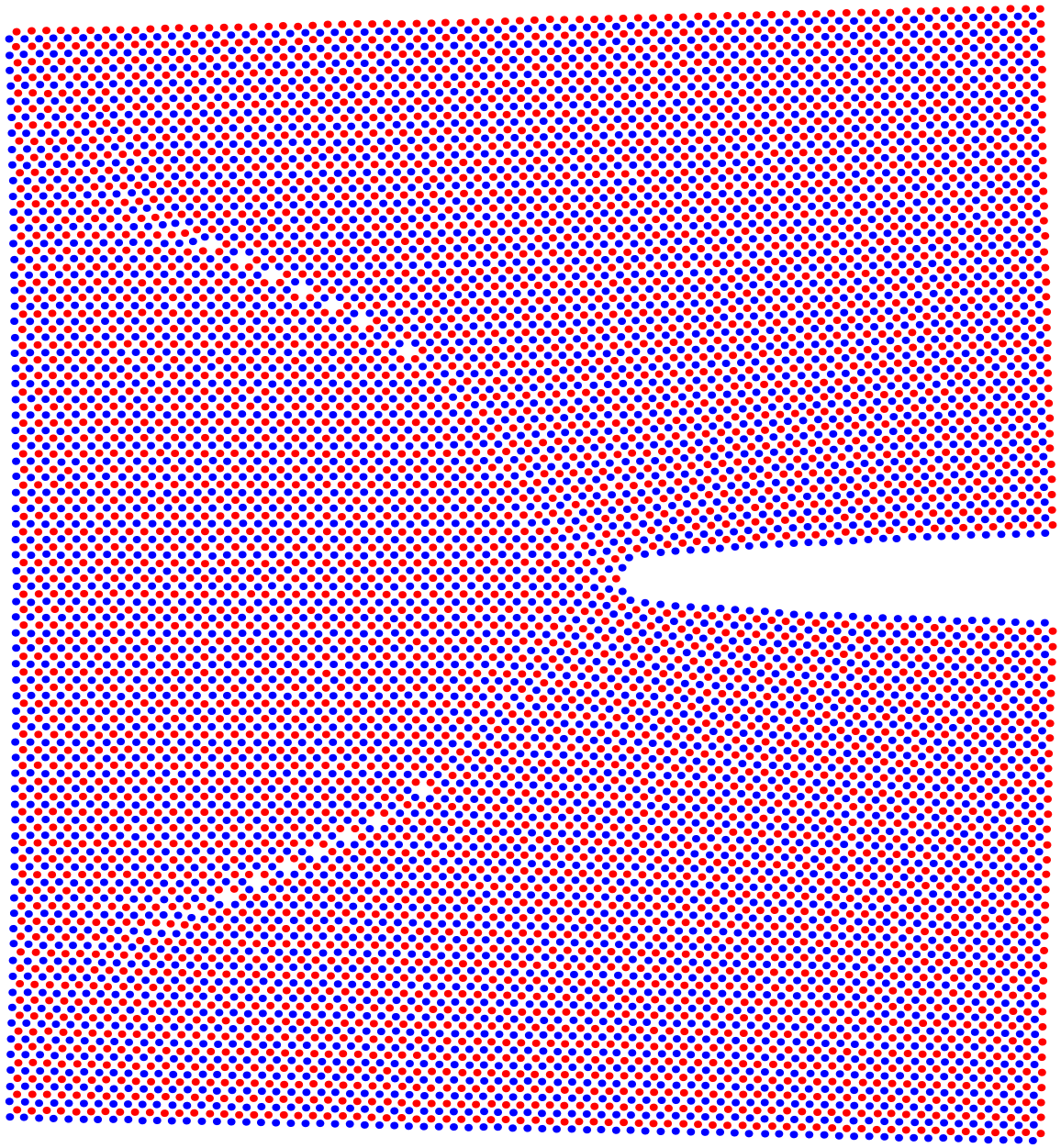

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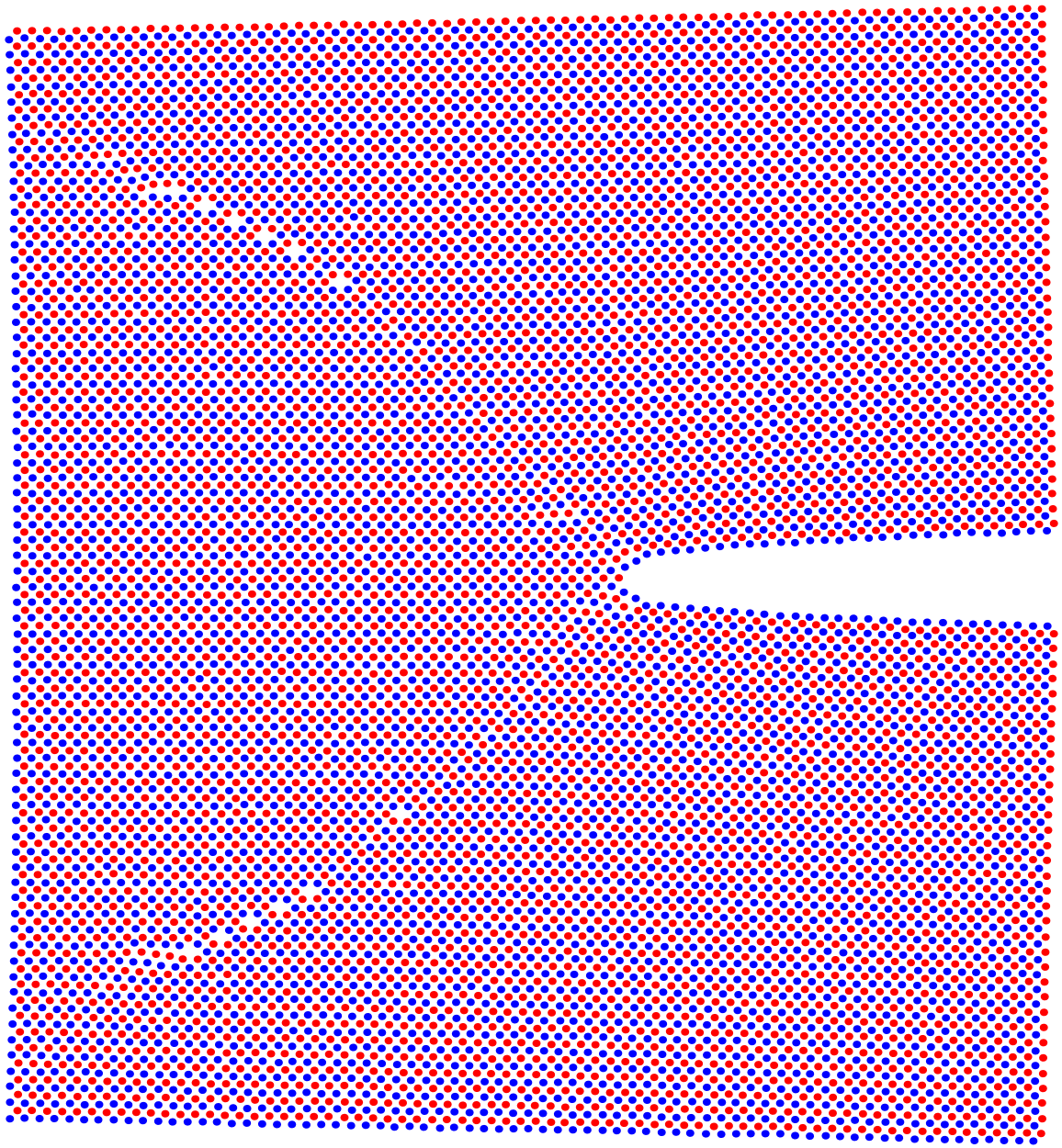
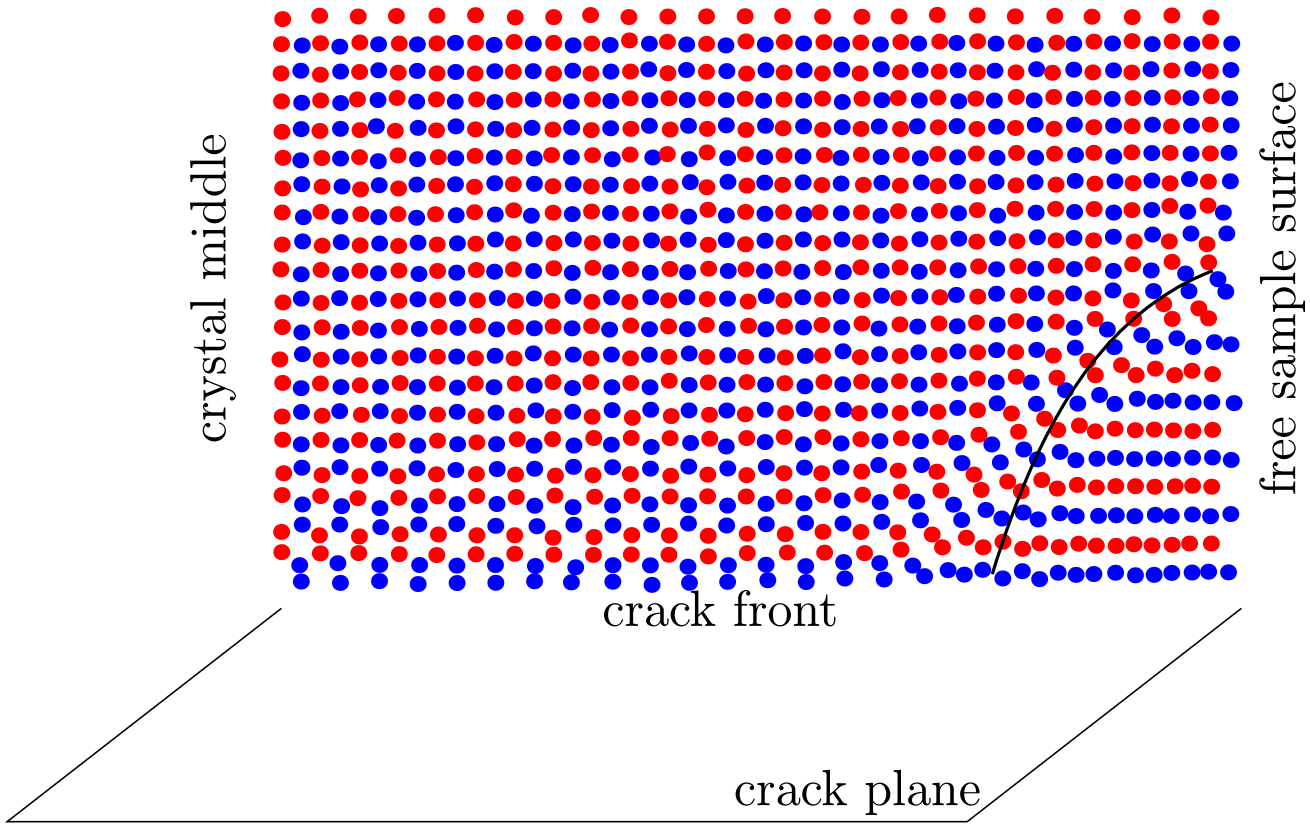
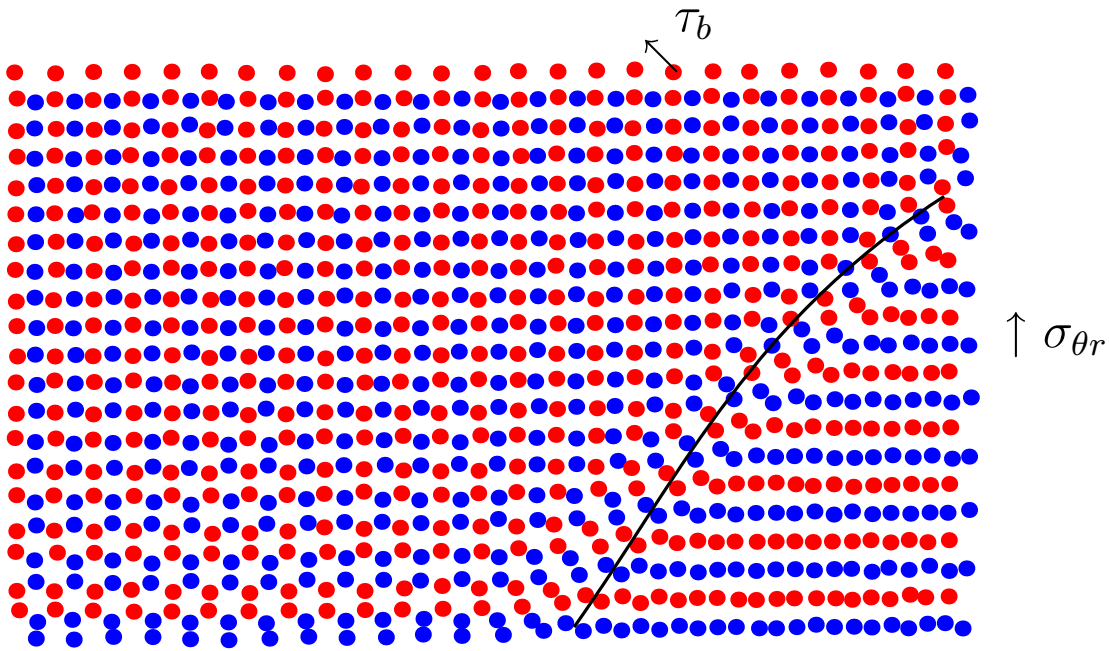


Layer:
91–99

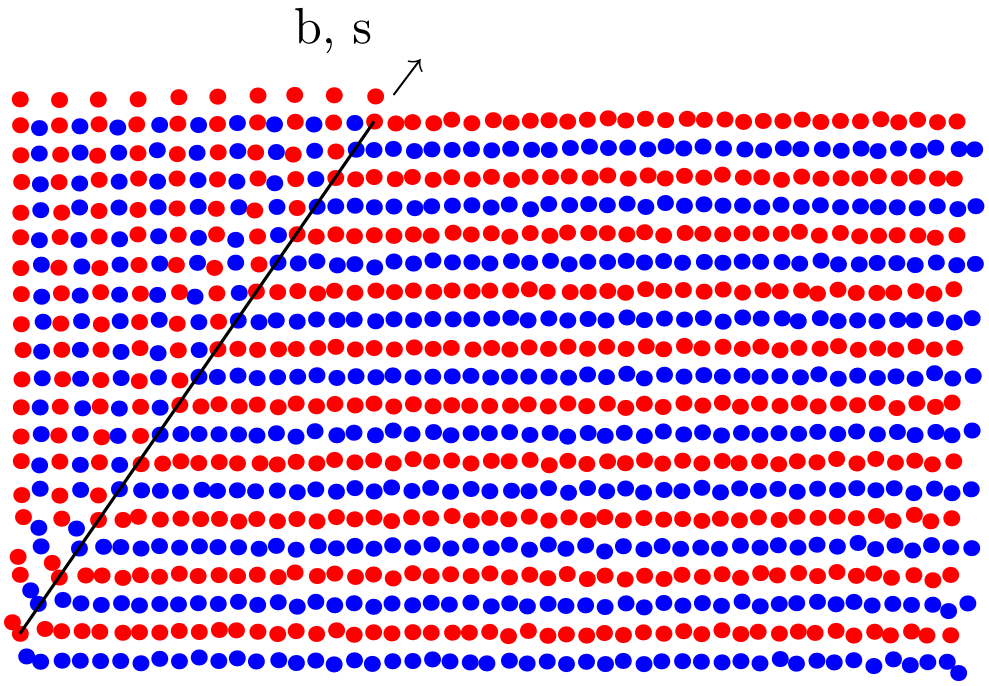
Beginning of plastic deformation: slip patterns on two $\{101\}$ planes for time step $14\,030$, view $(101)[101]$

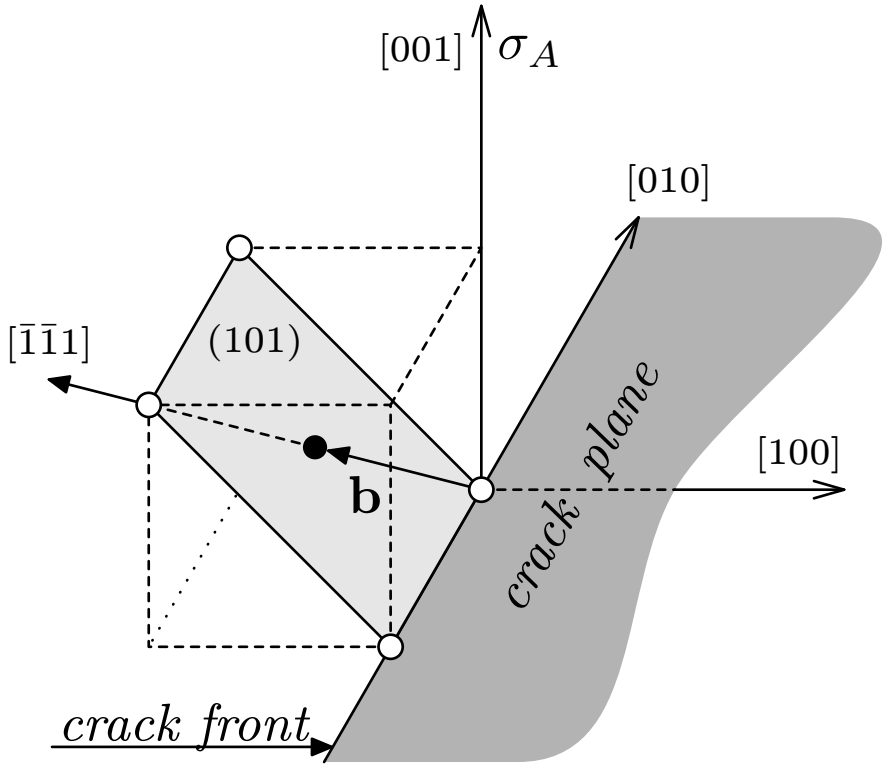


Beginning of plastic deformation: slip patterns on two $\{101\}$ planes for time step $14\,100$, view $(101)[101]$

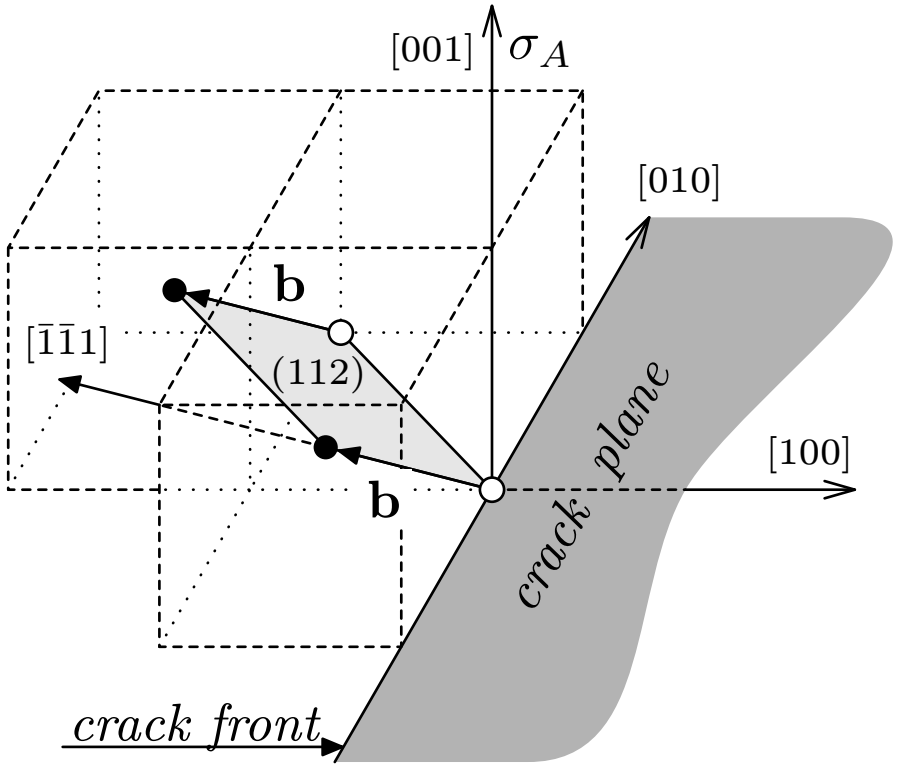


Beginning of plastic deformation: slip patterns on two $\{101\}$ planes for time step $14\,670$, view $(101)[101]$



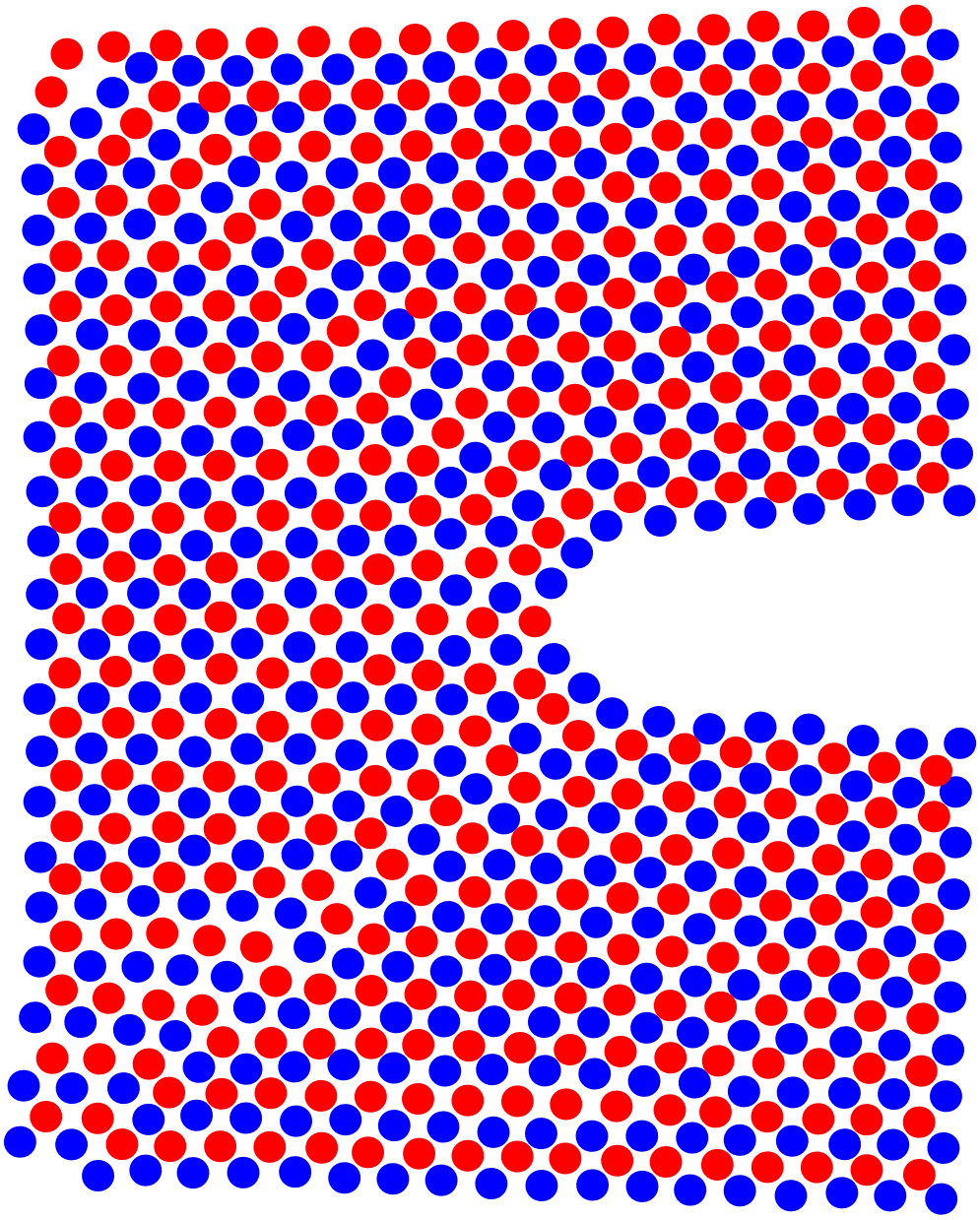


The slip system $(101)[\bar{1}\bar{1}1]$ is inclined to the crack plane and contains the crack front. Dislocation emission in this slip system causes crack tip blunting.



The second slip system $(112)[\bar{1}\bar{1}1]$ is oblique to the crack front and dislocation emission makes a jog in the crack front in the direction of b. It enables (after time step $16\,000$) later a slow plastic crack growth in the middle of the crystal.

Crack stability and slip patterns at the left crack front.
Time step $15\,820$**, view** $(010)[010]$**.**



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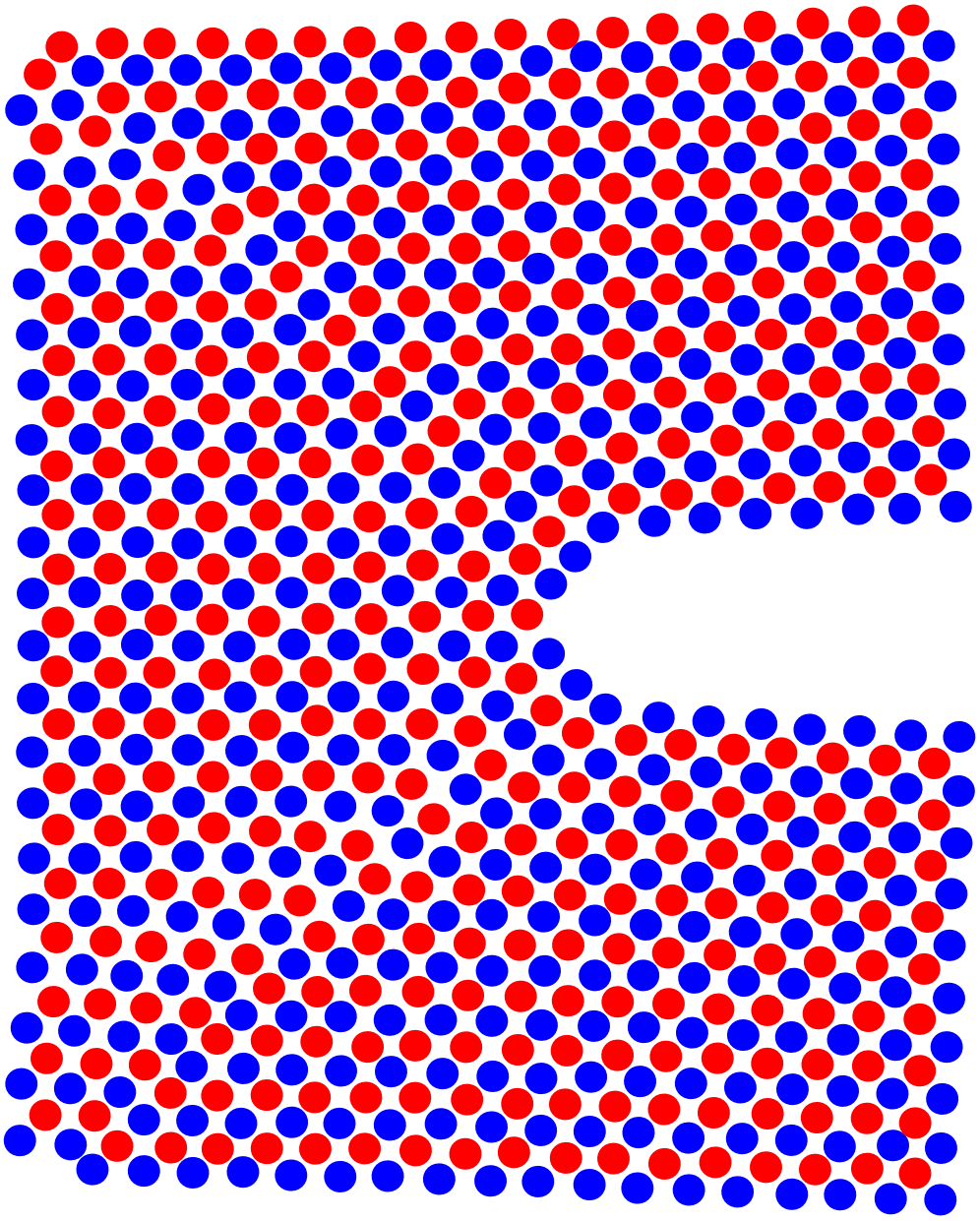

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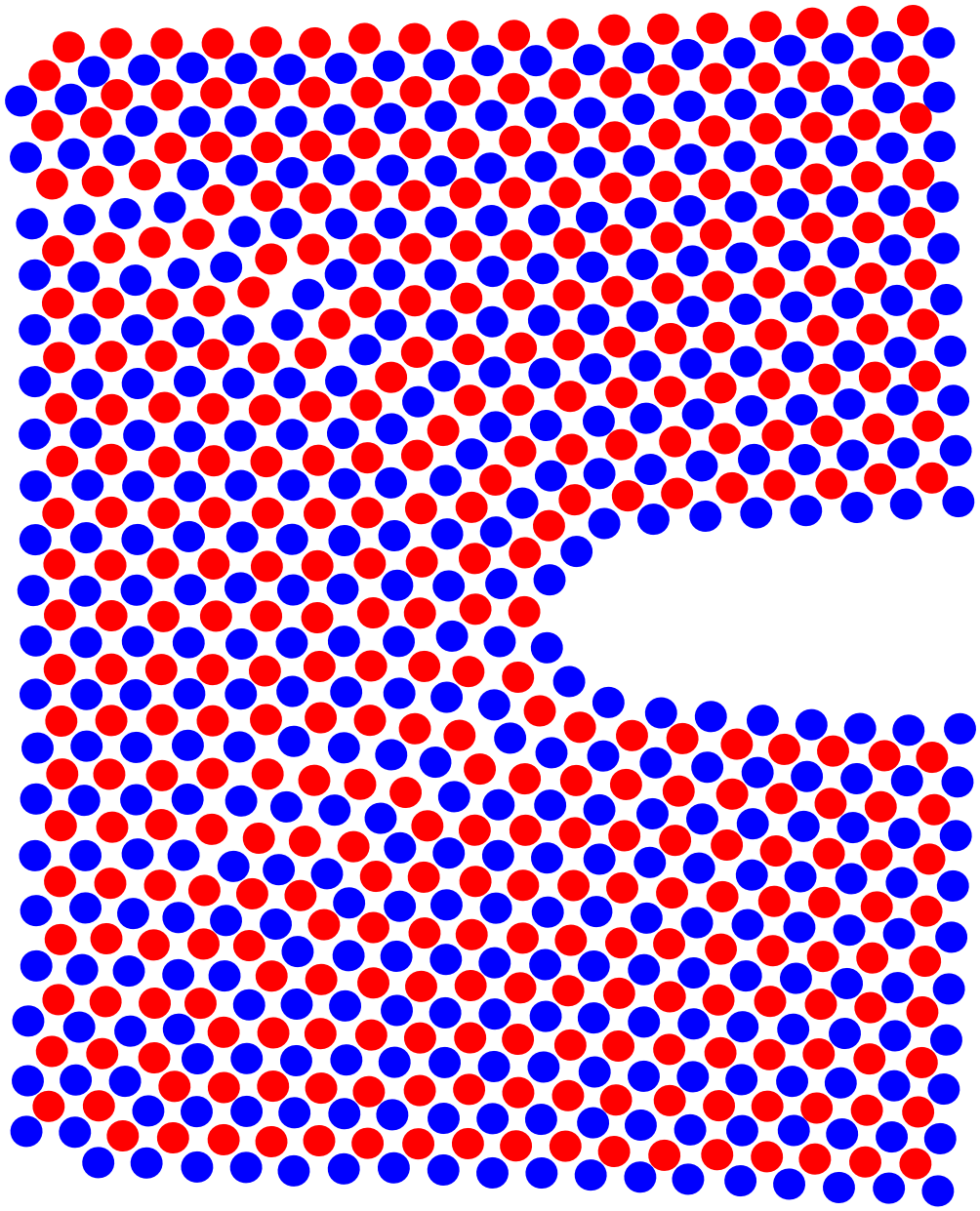

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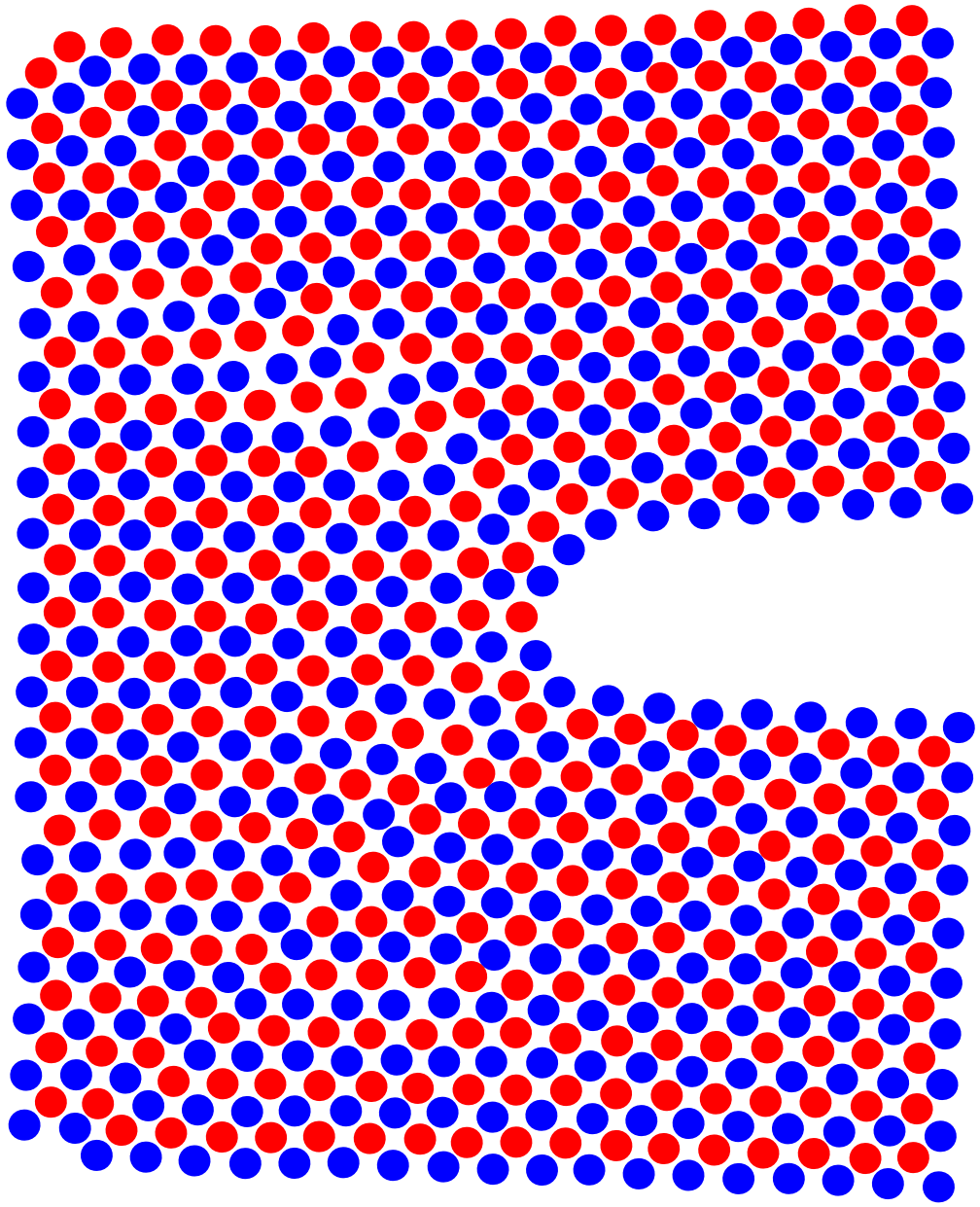

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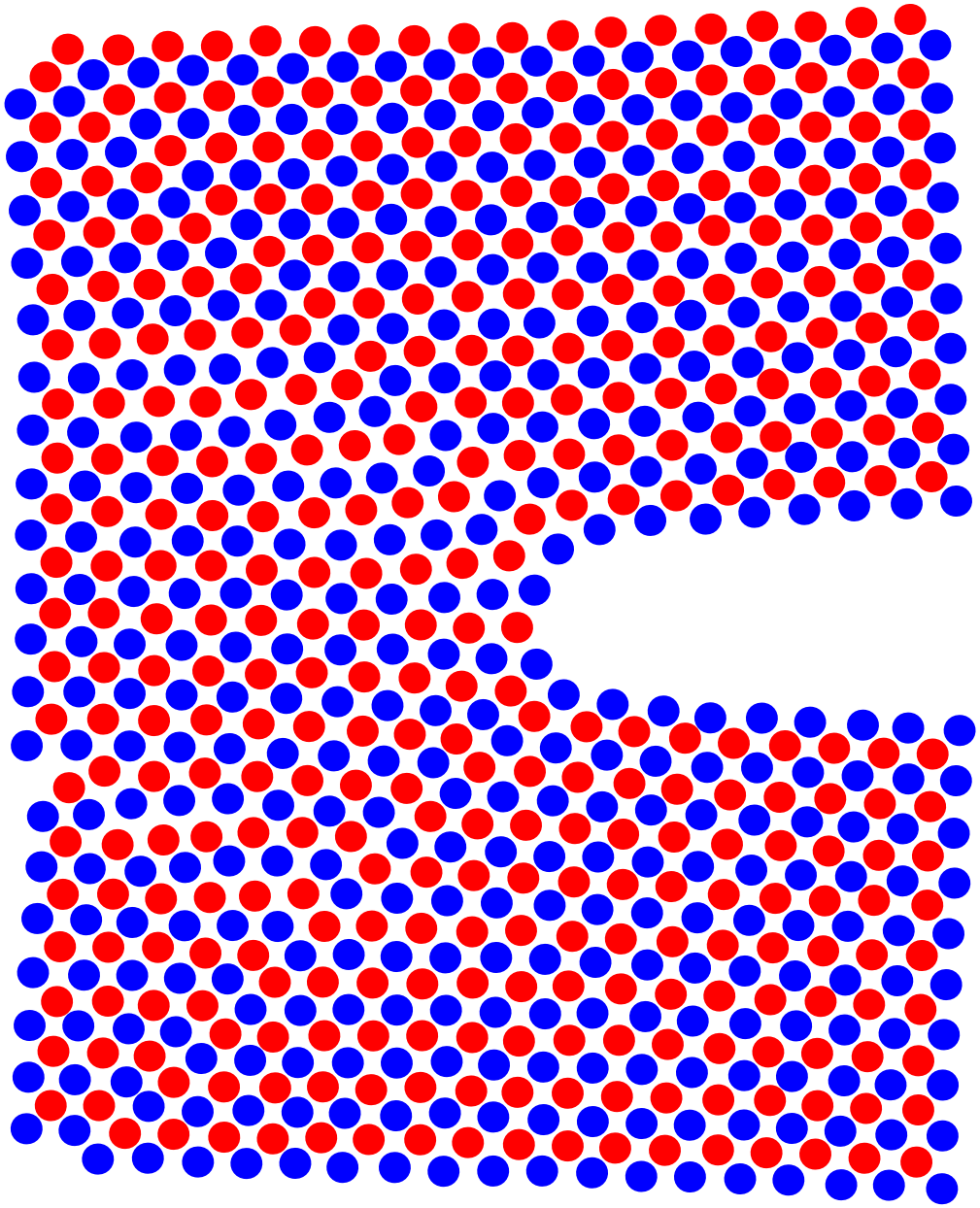

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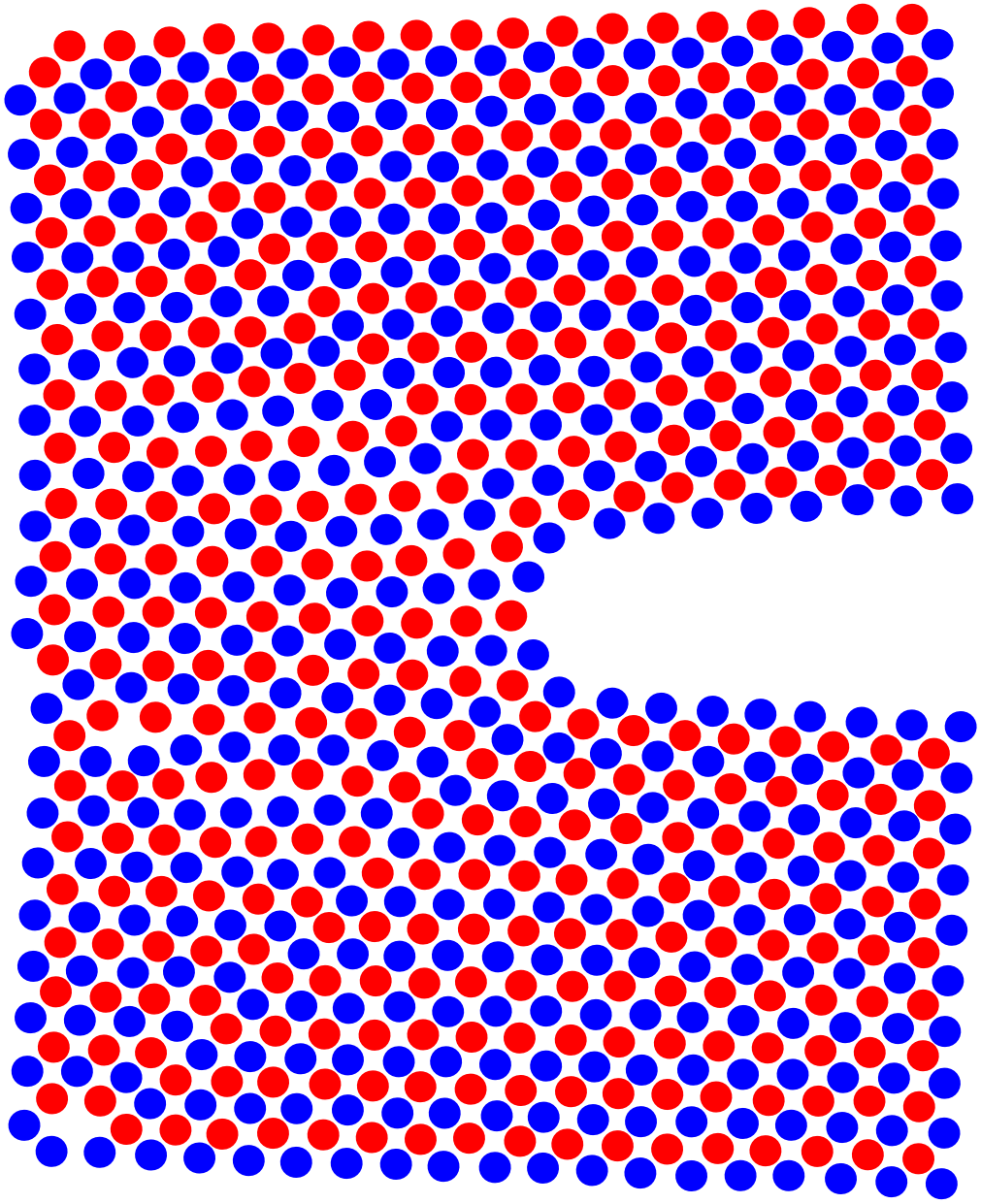

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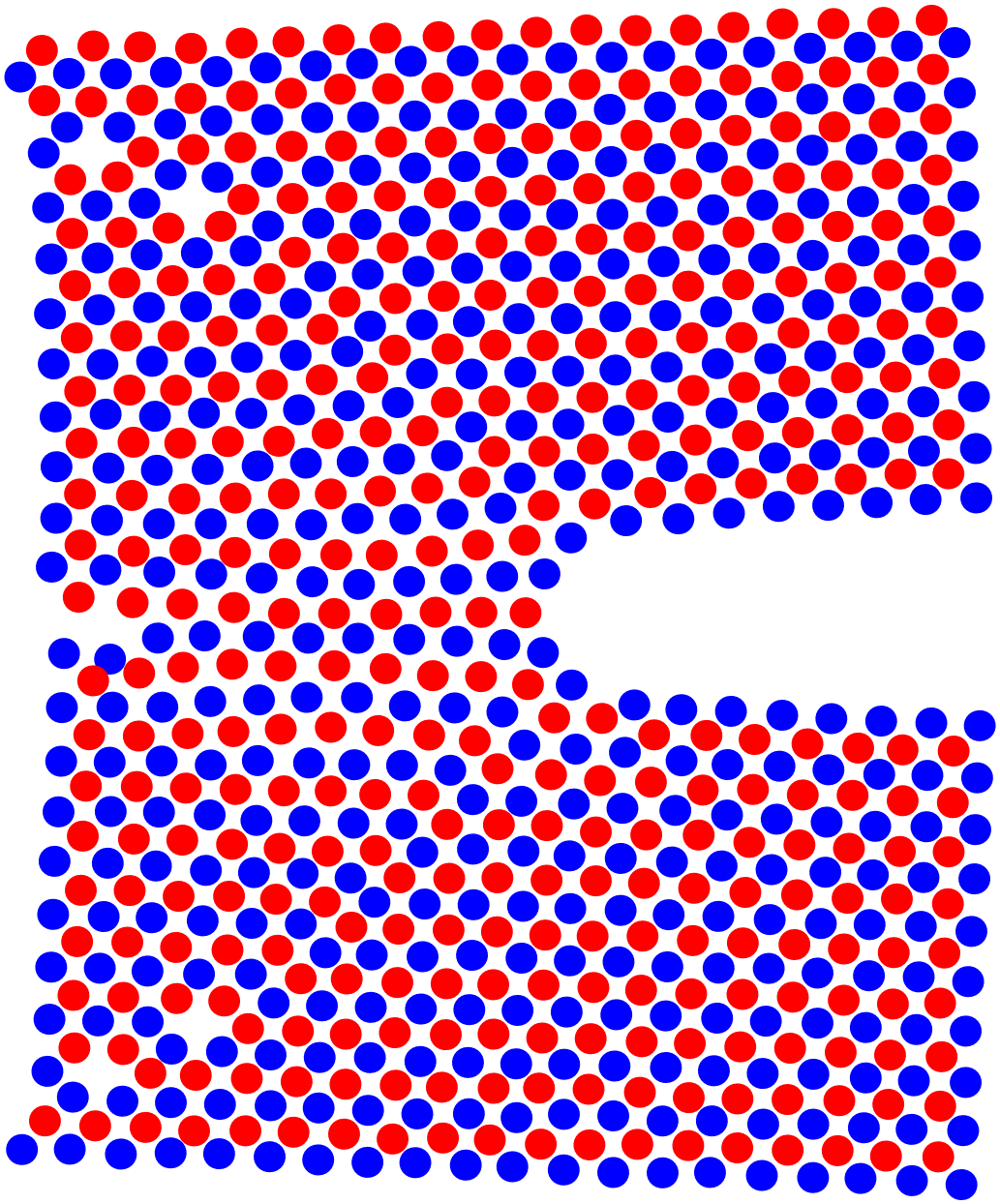

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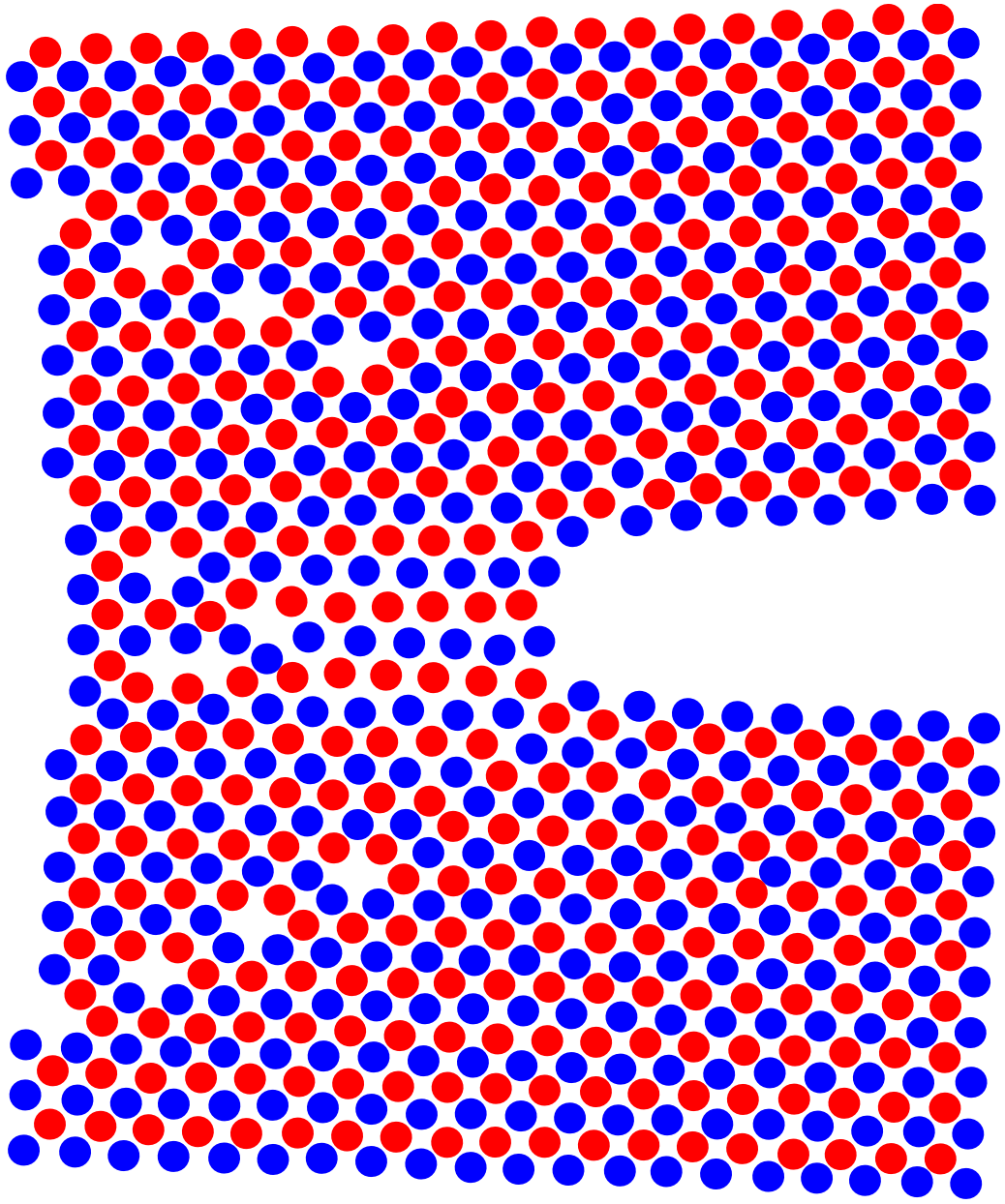

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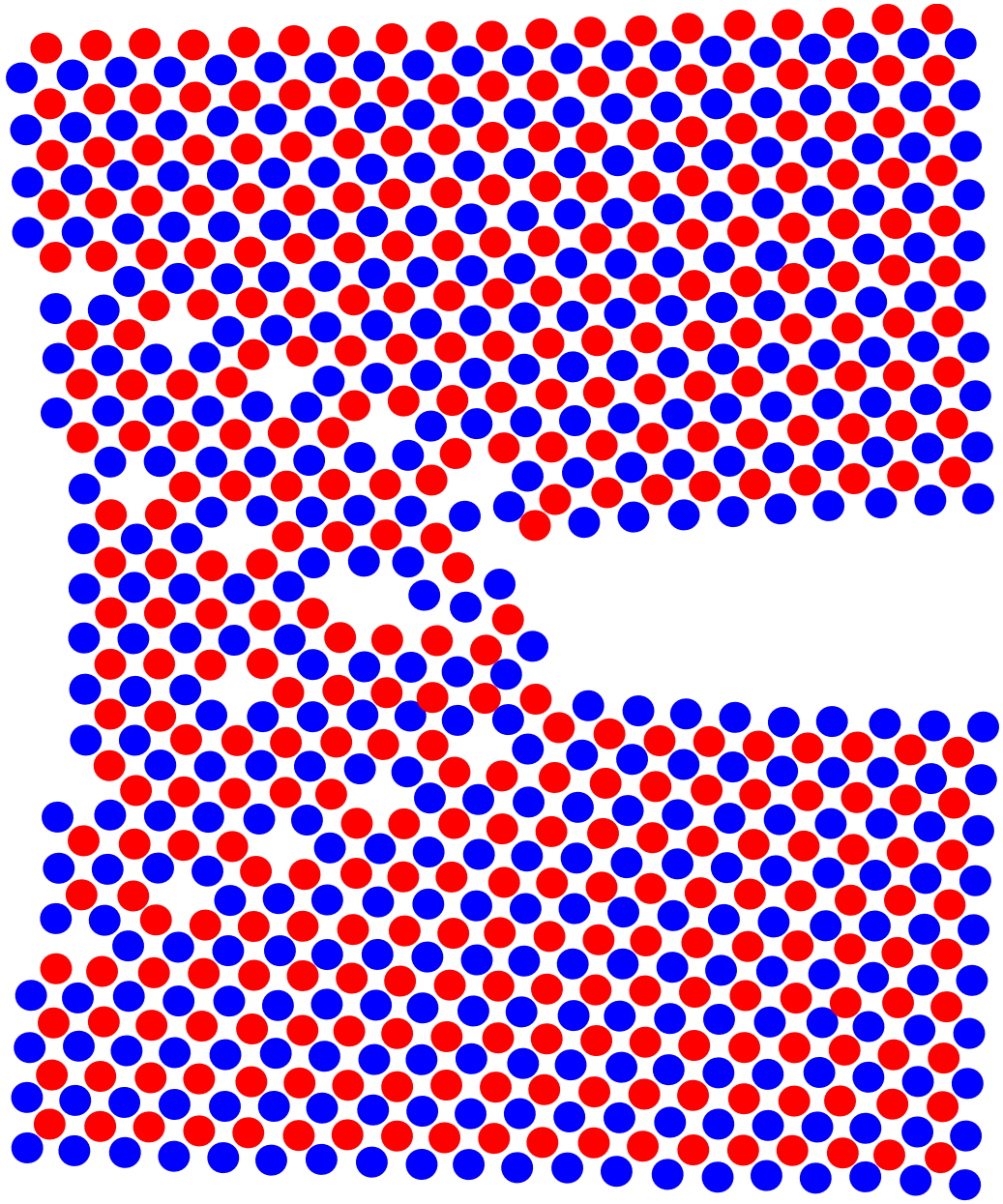

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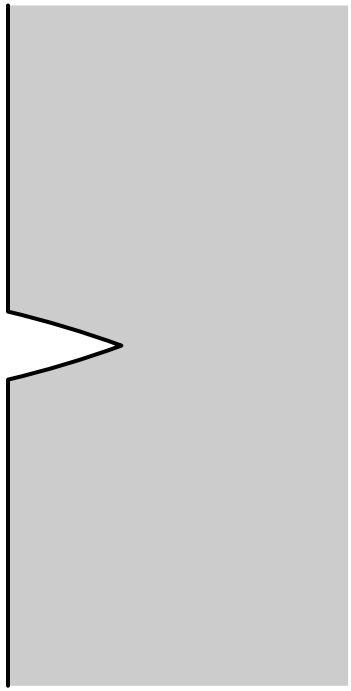
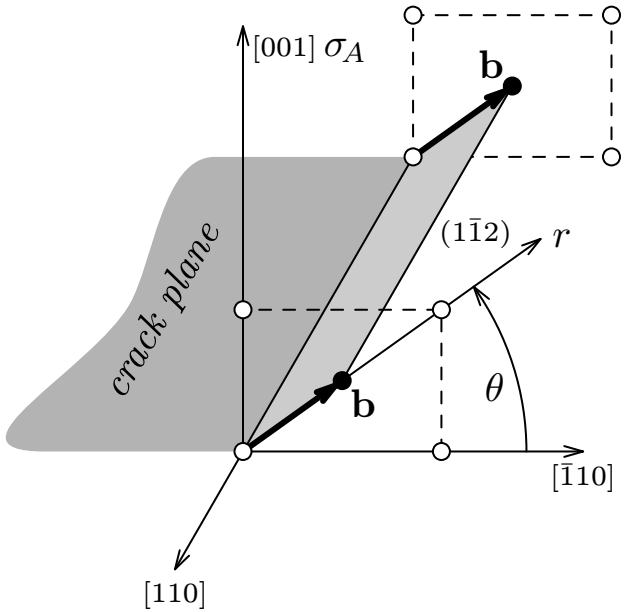
47–48

Results
Edge crack
Temperature of 300 K



The slip systems $\langle 111\rangle\{112\}$ are inclined to the crack plane under the angle $\theta = 35.26°$, contain the crack front and they are oriented in the easy twinning direction, similar to our former plane strain simulations. In this case the stress barrier for twin formation in the $\langle 111\rangle\langle 112\rangle$ slip systems at temperature of 0 K is much lower ($\tau_{twin} = 9.3$ GPa) than for dislocation generation (16.3 GPa) with the used N-body potential.

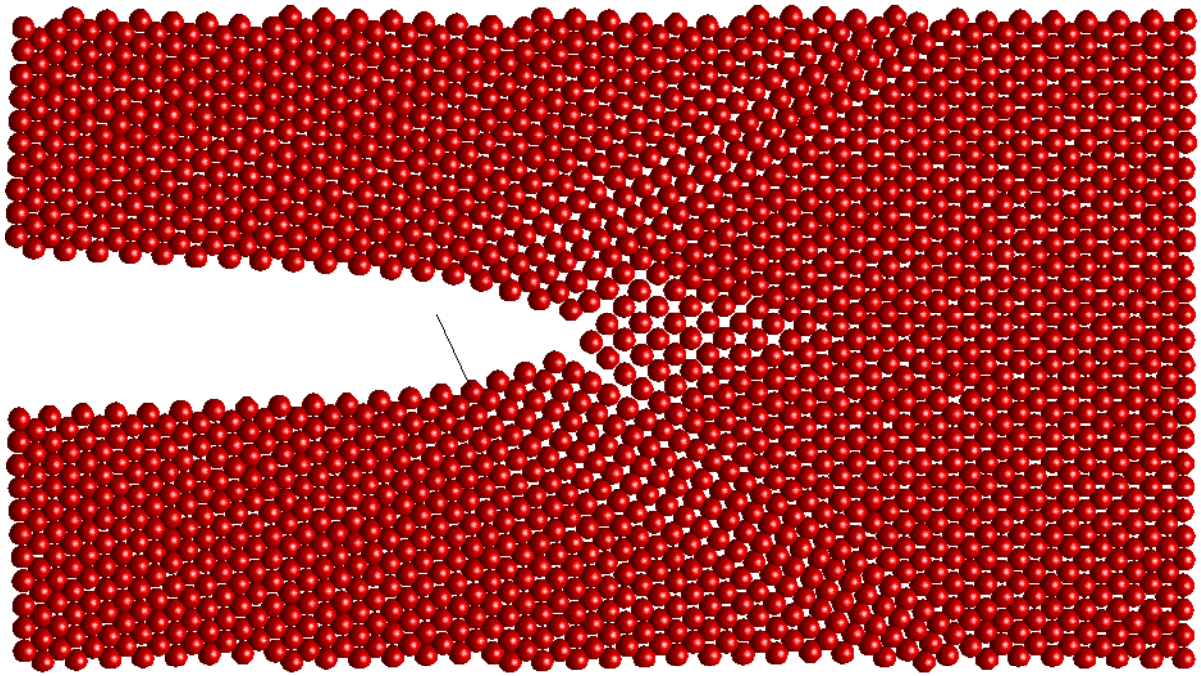


Crack initiation

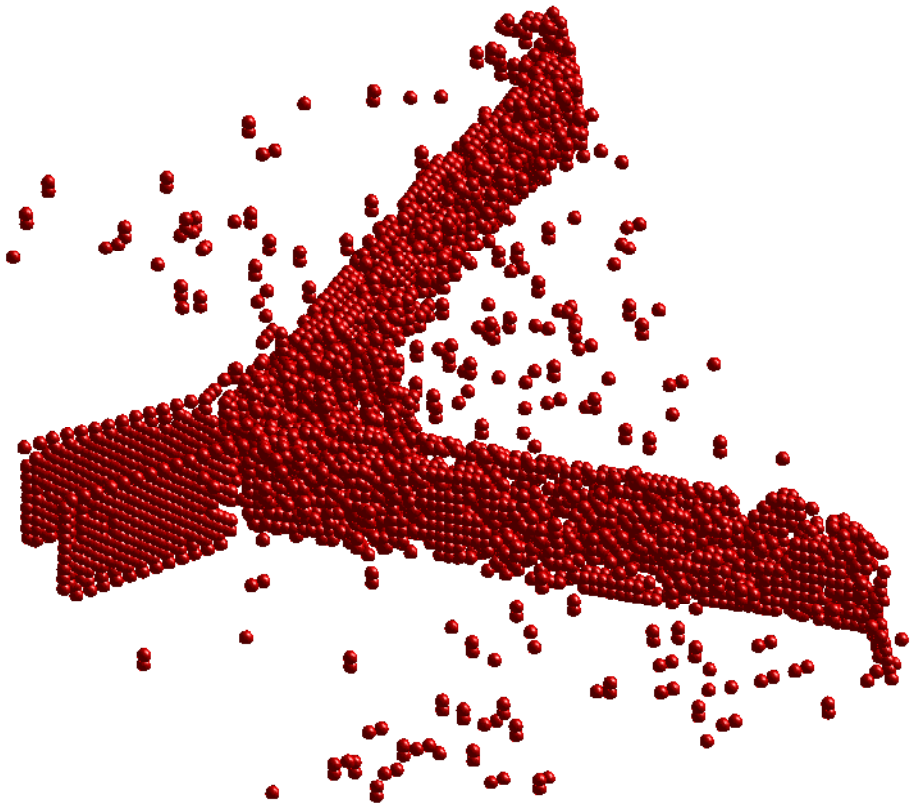
has been monitored first in the middle of the sample, the stress intensity at the crack front was $K_{MD} = 0.749$ MPam$^{1/2}$. It is close to $K_c = 0.835$ MPam$^{1/2}$ expected according to anisotropic LFM for plane stress and the used potential with the surface formation energy $2\gamma_{001} = 3.624$ J/m^2.

Similar to plane strain simulations, crack initiation was accompanied by generation of unstable stacking faults that **later** transform to **twins in the** $\langle 111 \rangle \{112\}$ **slip systems** - see the next slide.

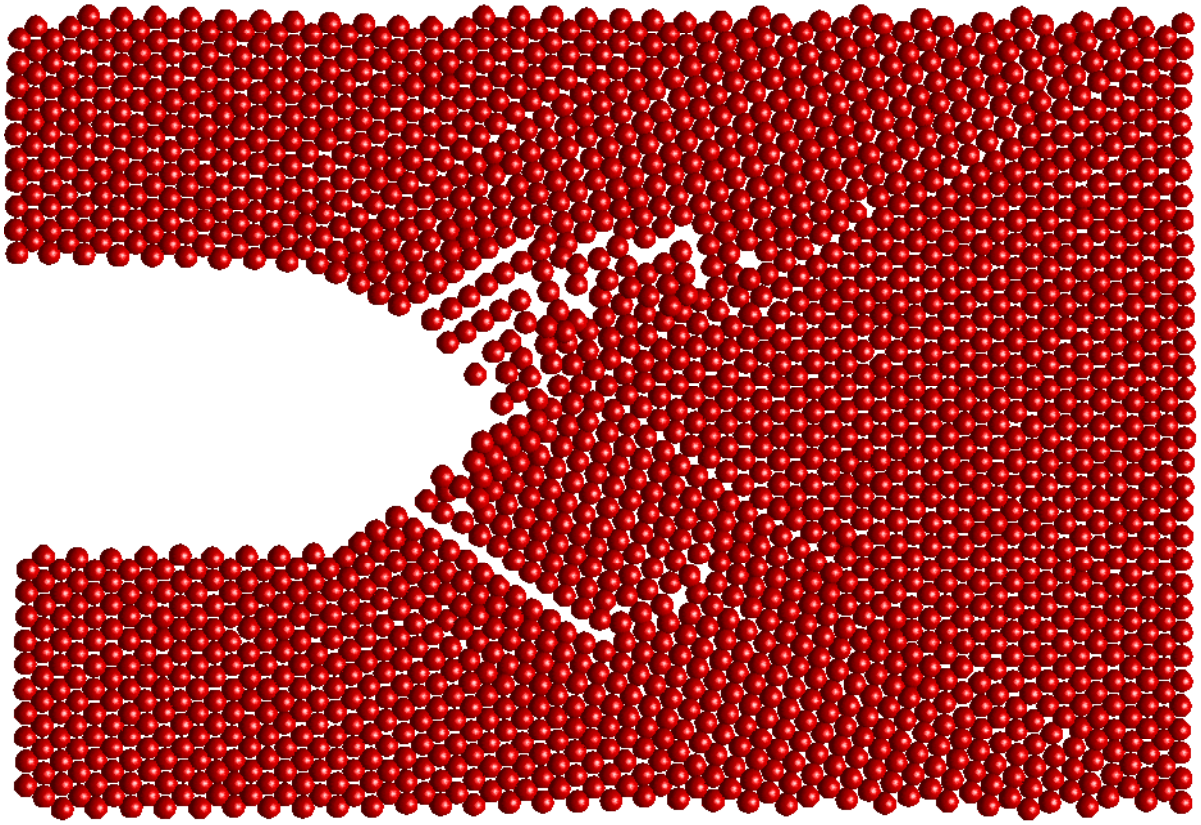
Crack initiation and twinning
in the middle plane (110) of the crystal,
time step $3\,600$,
the original crack tip point is denoted by the line.



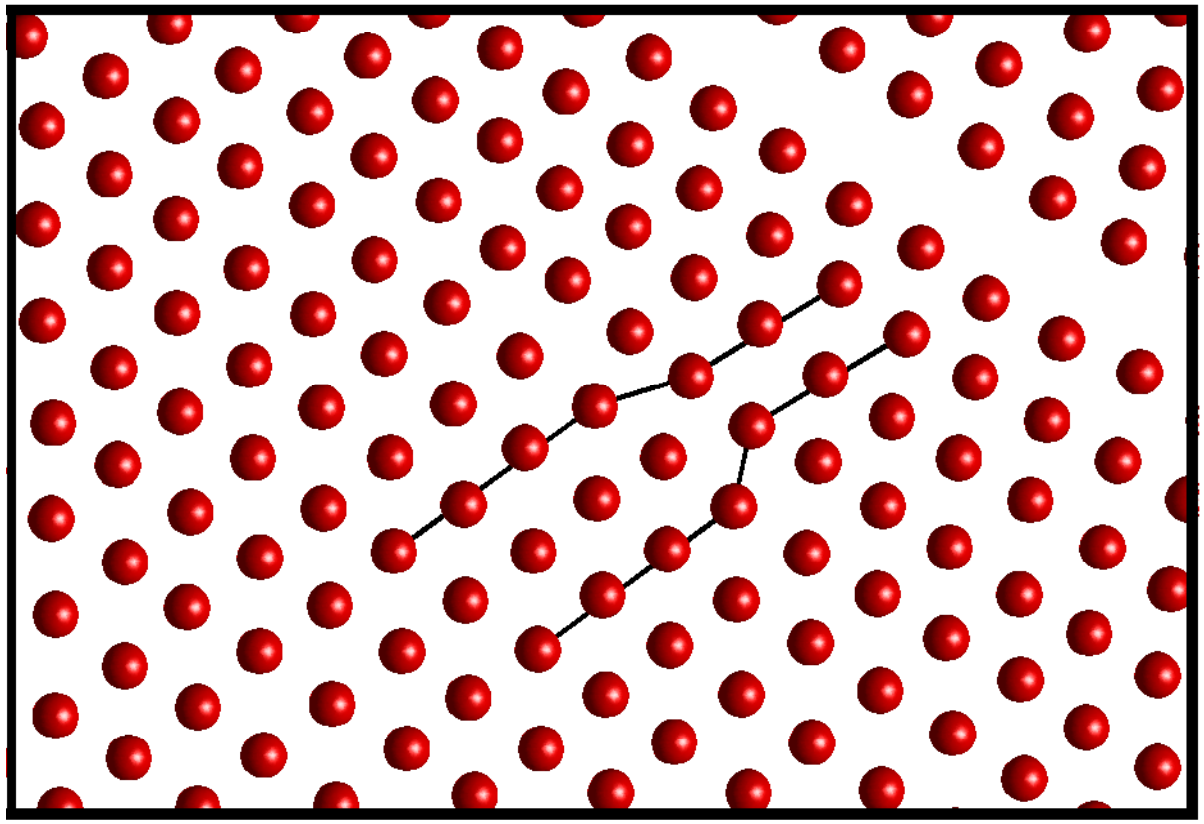
Crack and twin surfaces in 3D, time step $3\,600$.



Dislocation generation in a $\langle 111 \rangle \{ 112 \}$ slip system below the lower twin band, time step $4\,100$, (110) surface.



Detail from the atomic configuration at the dislocation nucleus.



Conclusions

- The results indicate that brittle initiation of the crack (001) is possible at low temperature or under fast loading.
- At temperature of 300 K slip processes are detected.
- Dislocation emission on the inclined slip planes hinder crack growth, while on oblique plane creates jogs in the crack front, which enables a slow plastic crack growth.
- The crack (001) may produce also twins, if the inclined $\{112\}$ slip systems are oriented in the easy twinning direction.
- The results are in agreement with continuum models and experimental observation in bcc iron.

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Time 14100
14030 14100 14670
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