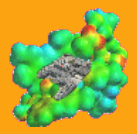
HELSINGIN YLIOPISTO
HELSINGFORS UNIVERSITET
UNIVERSITY OF HELSINKI



CMS

HIP

Dislocation nucleation on near surface void under tensile stress in Cu

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Kai Nordlund

Helsinki Institute of Physics and Department of Physics

University of Helsinki

Finland

Steve Fitzgerald

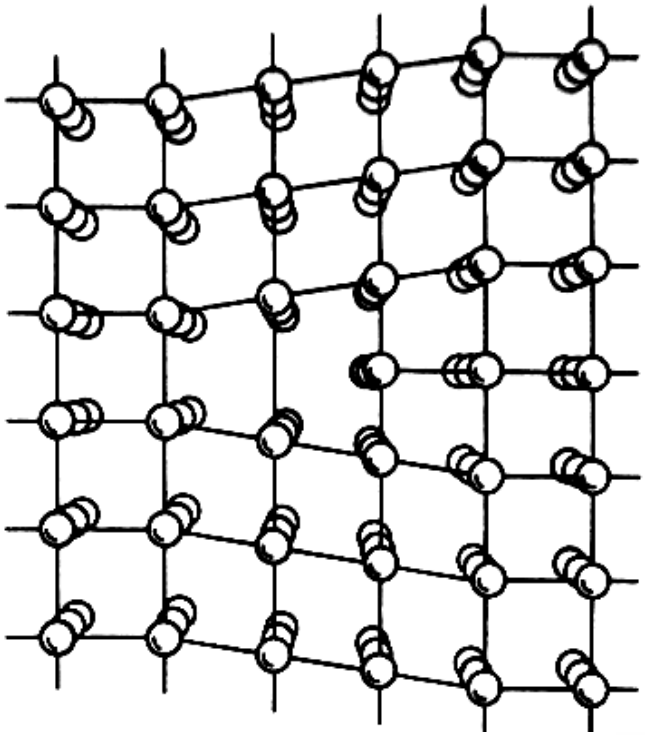
Theory and Modelling

Culham Centre for Fusion Energy

UK

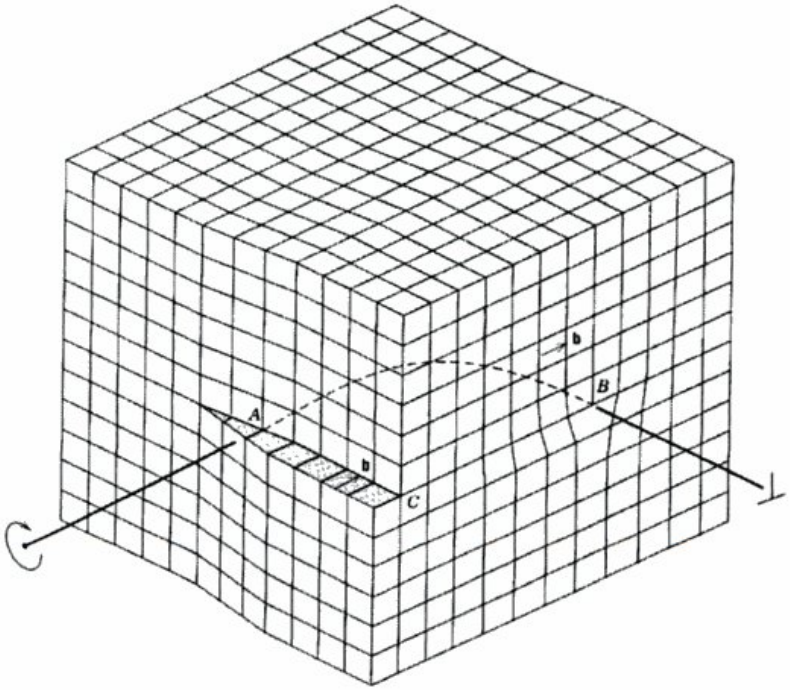
Dislocations

Edge dislocation in simple cubic lattice



Theory of Dislocations, Hirth, Lothe, 1982

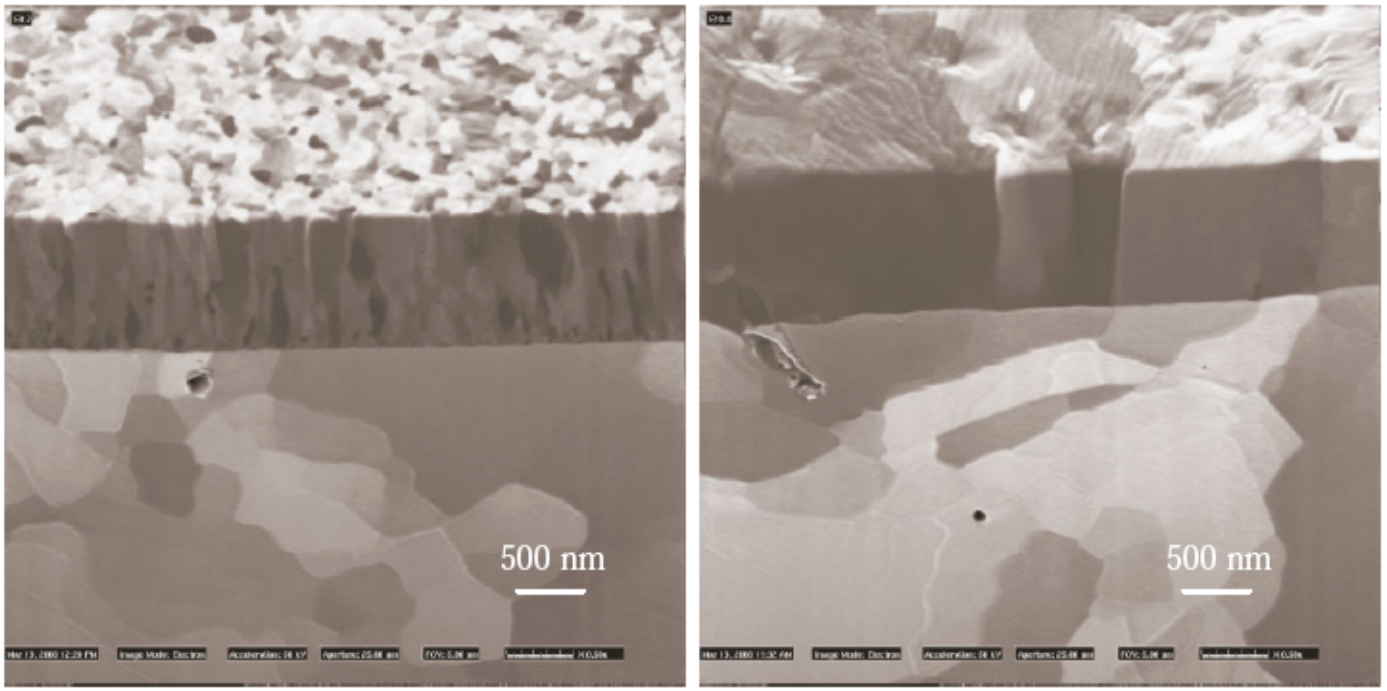
Mixed screw-edge dislocation



Materials Science and Engineering, Callister, 2000

Voids

Voids are observed in cavities

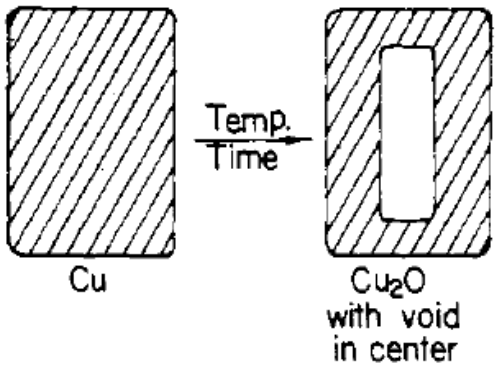


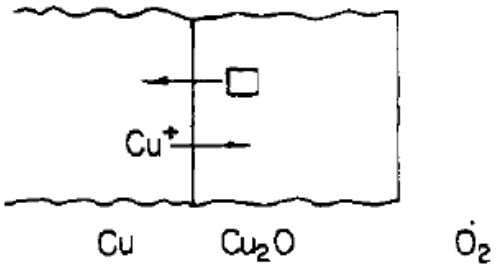
Cross sectional FIB images of niobium films on oxidised (left) and oxide-free (right) copper substrates

CERN Studies on Niobium Coated 1.5 GHz Copper Cavities
Benvenuti, Calatroni, Hakovirta, Neupert, Prada, Valente, 2001

Voids

Possible near surface void formation mechanism: Kirkendall effect



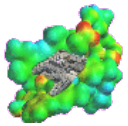


Copper oxidation and void formation.

Void Formation Failure Mechanisms in Integrated Circuits, Selikson, 1969

Simulations

1. Relax the system for 20 ps, no force



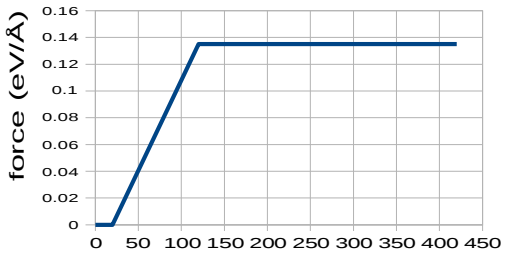
2. ”Ramp up” the force in 20...120 ps

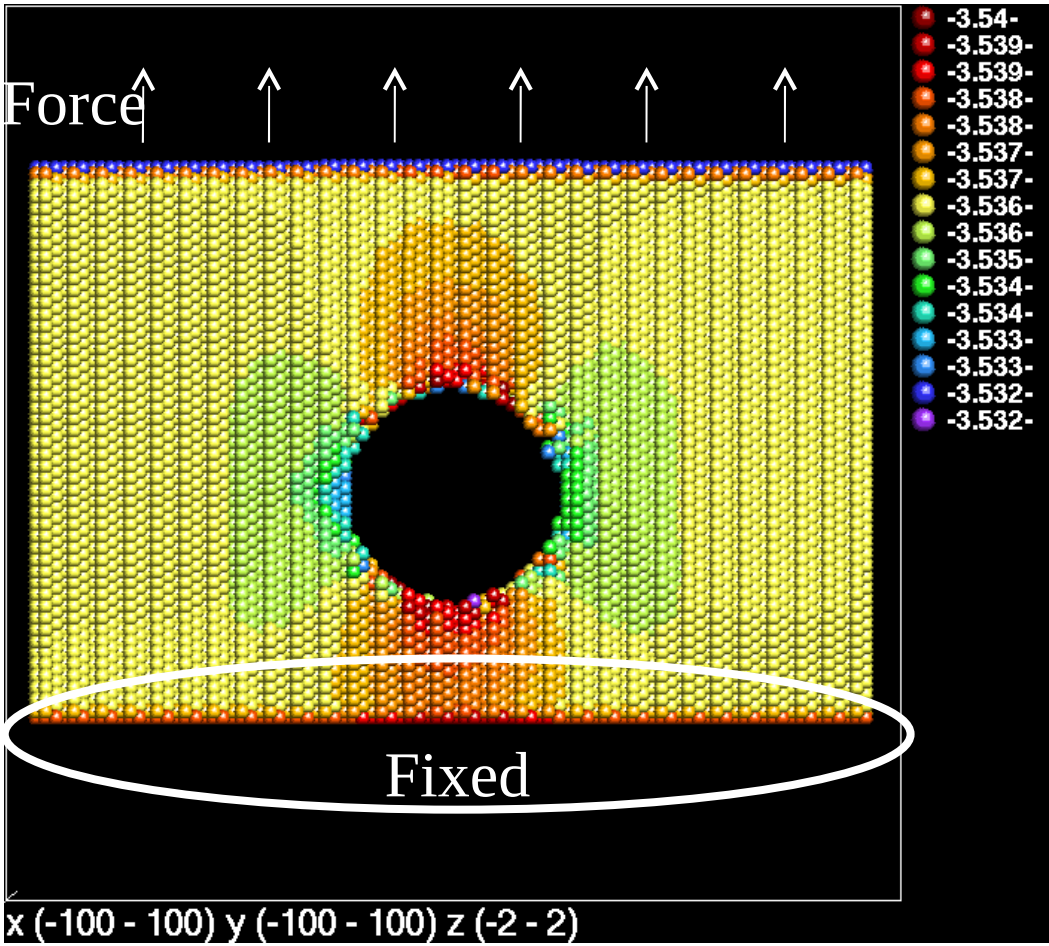
3. Continue with

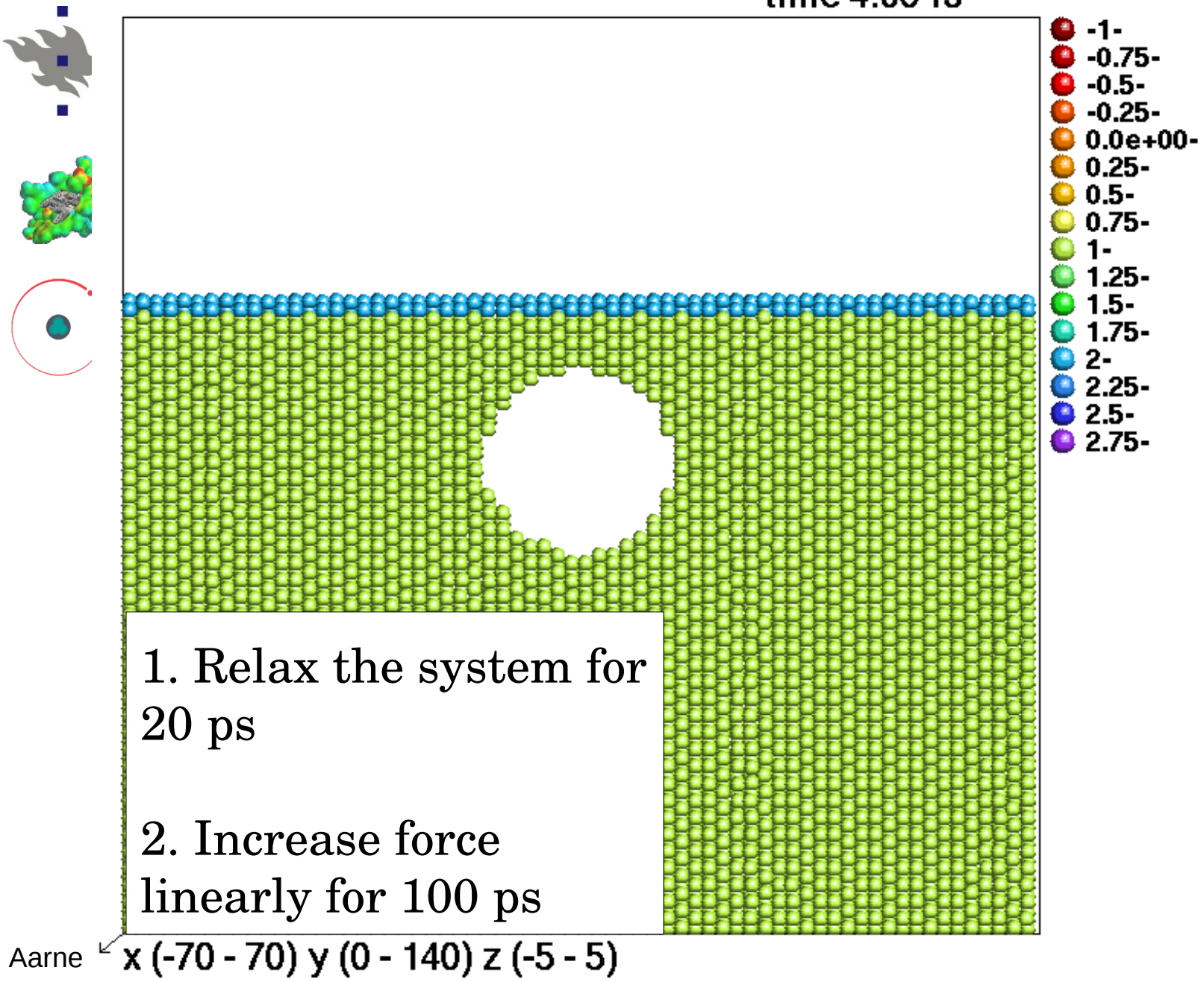
timescale $\Delta t = 300$ ps

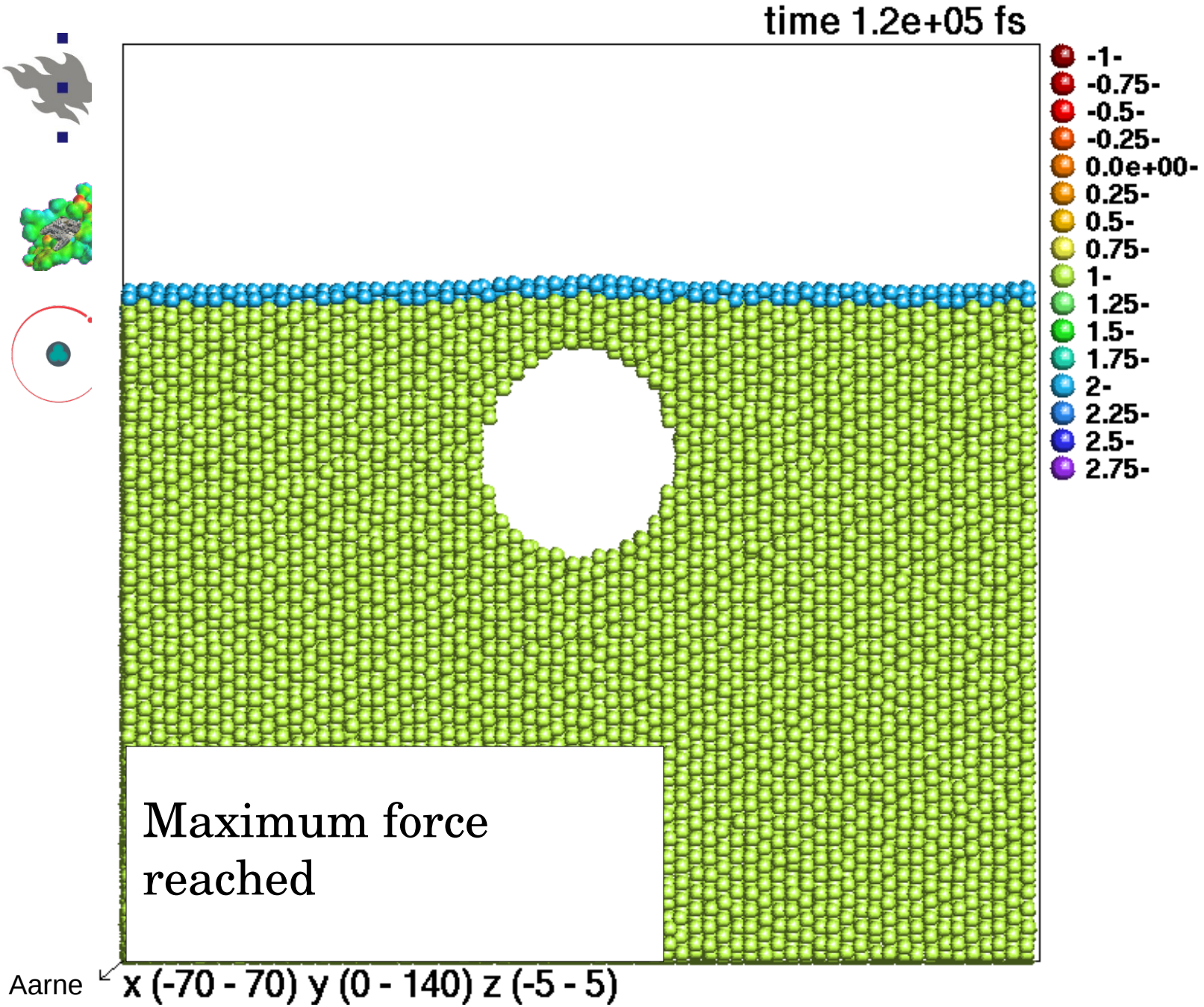
force/atom $F = 0.135$ eV/Å

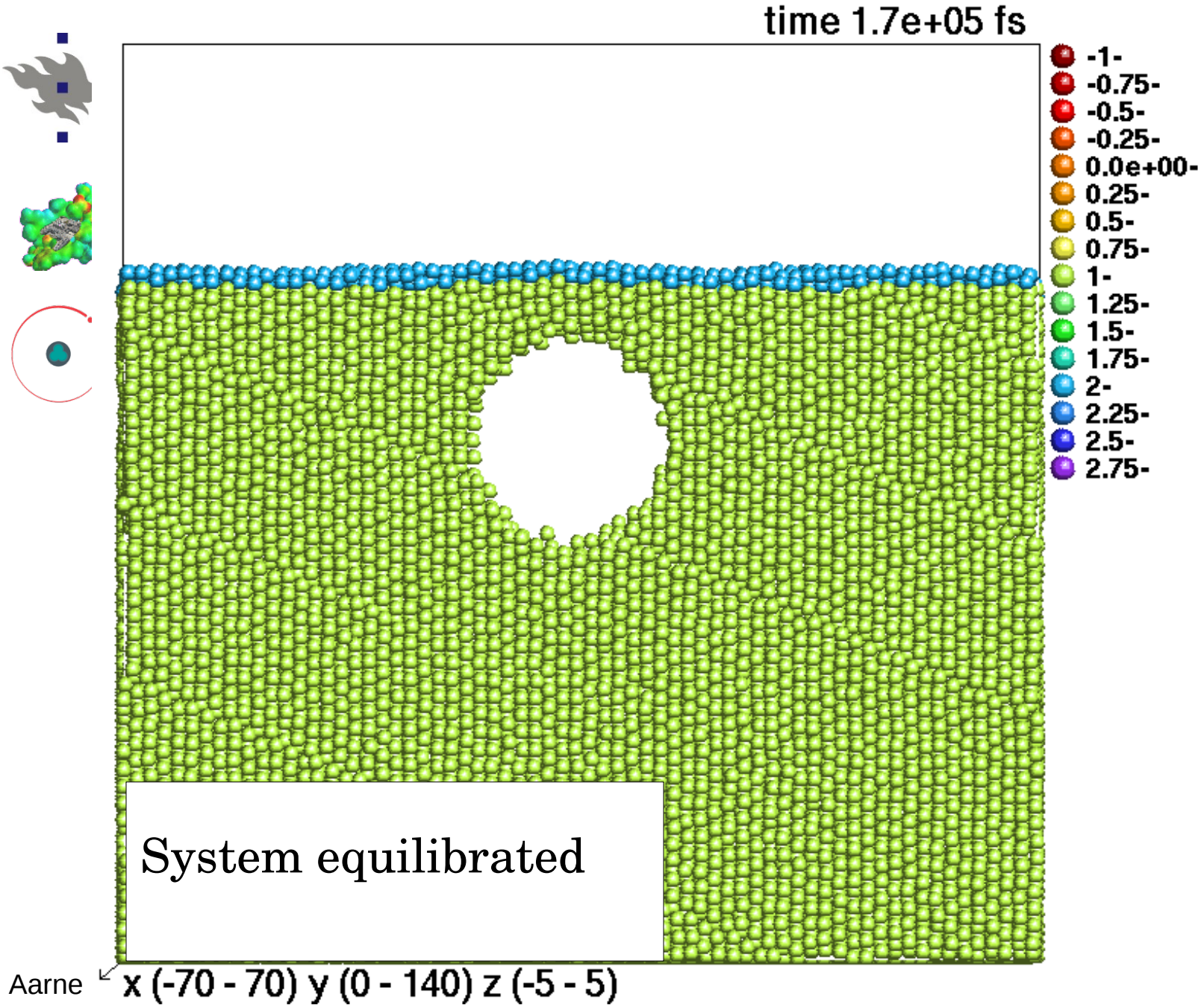
temperature $T = 600$ K

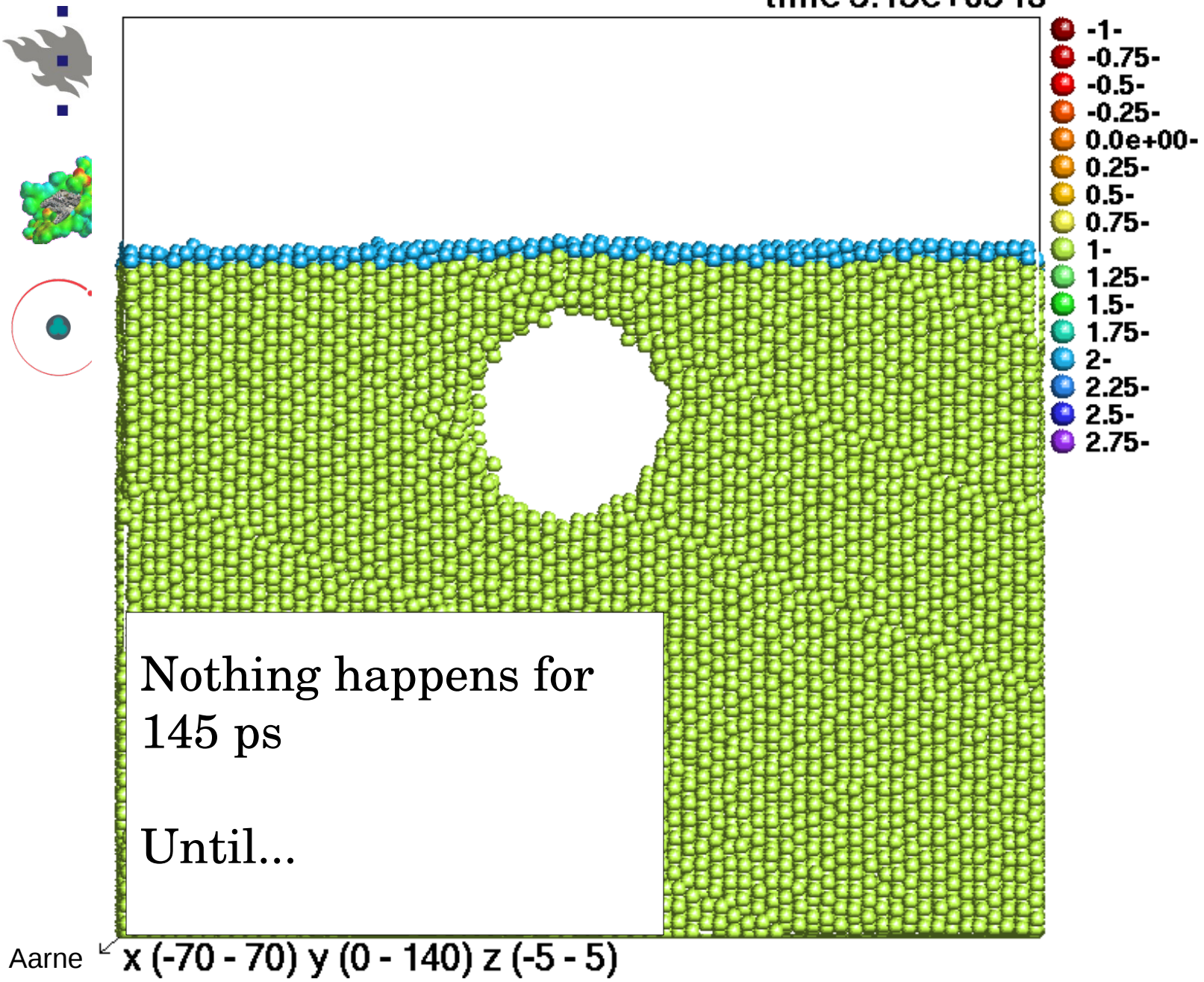


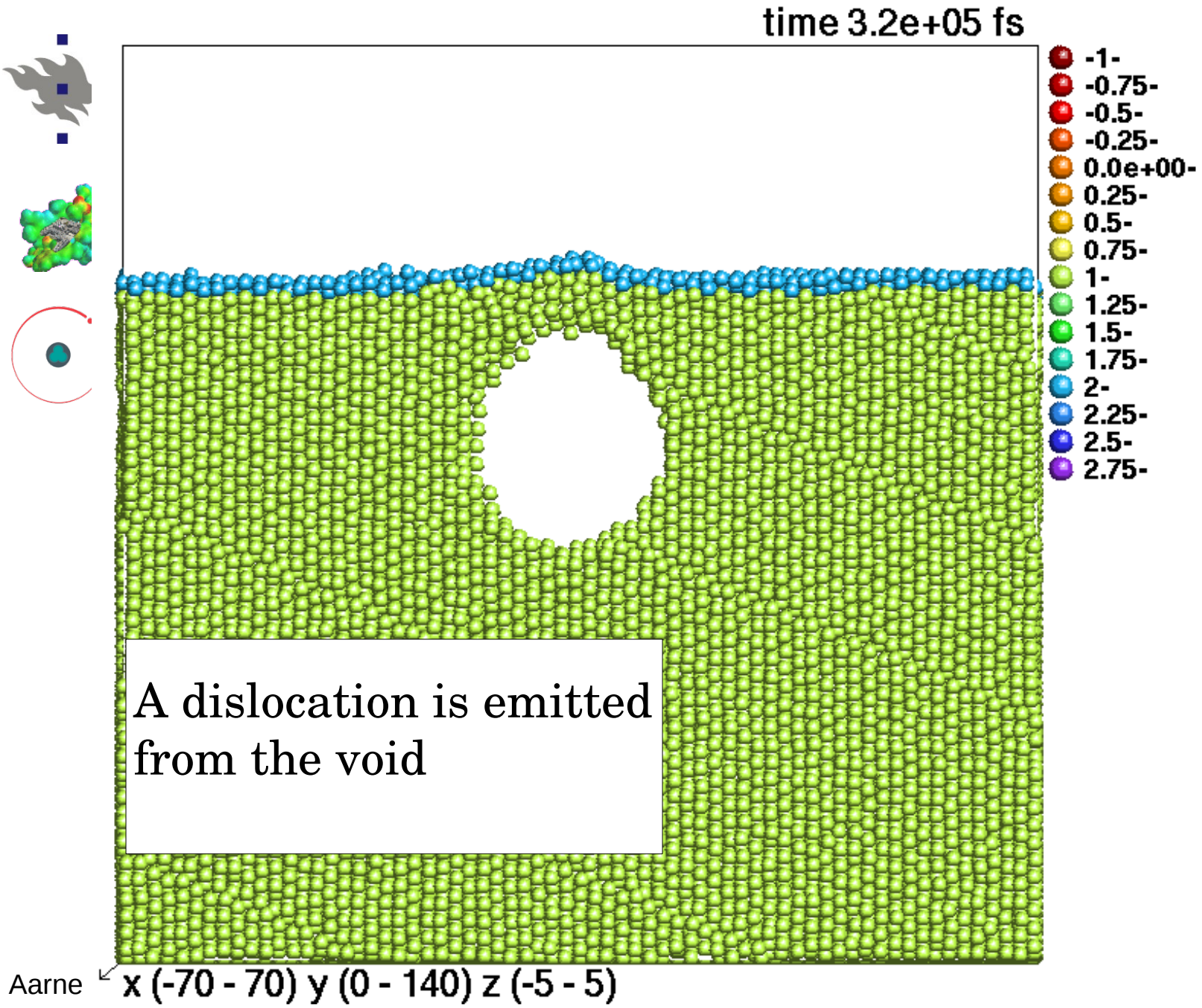


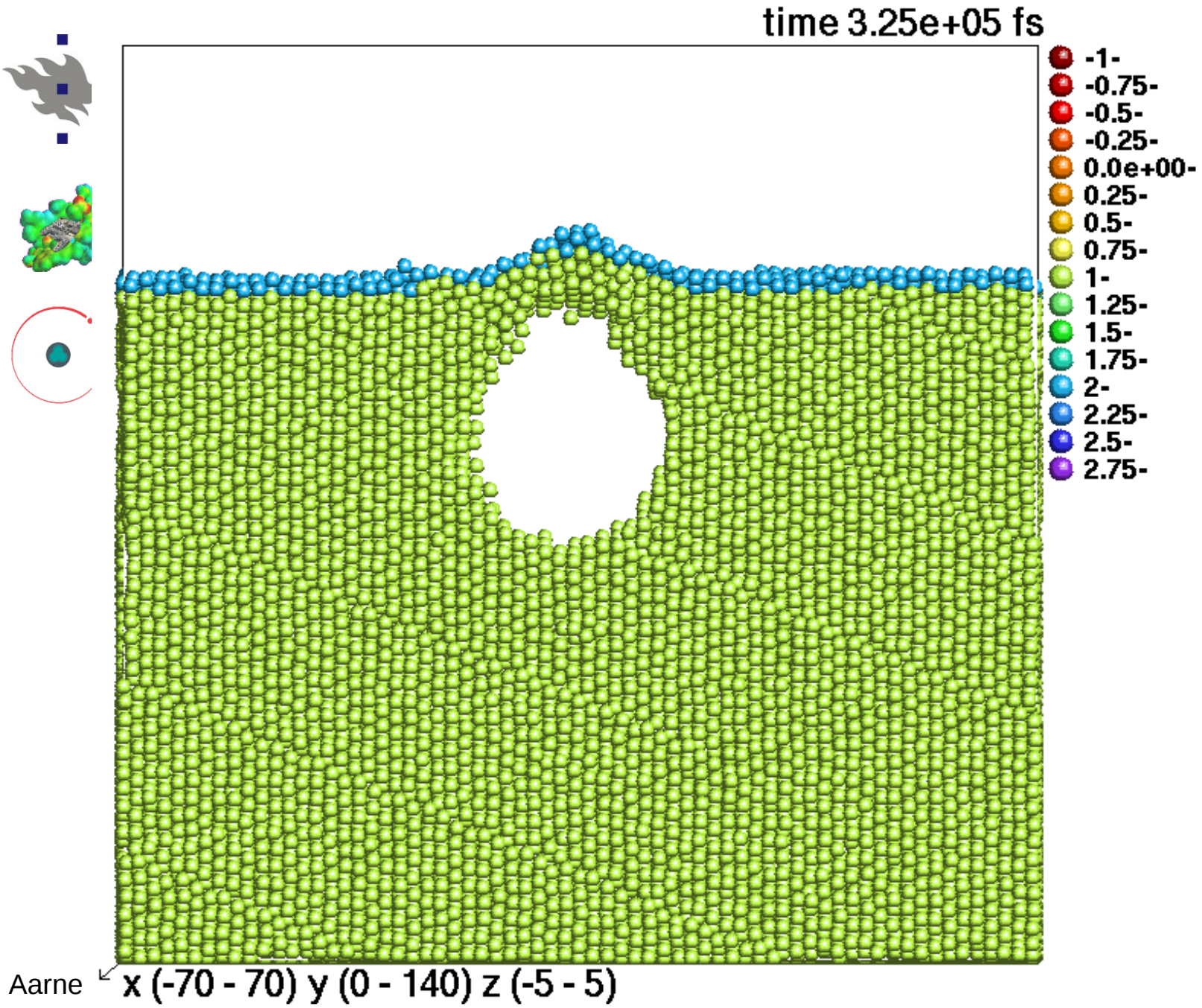

time 4.06 fs
-1-
-0.75-
-0.5-
-0.25-
0.0e+00-
0.25-
0.5-
0.75-
1-
1.25-
1.5-
1.75-
2-
2.25-
2.5-
2.75-
1. Relax the system for 20 ps
2. Increase force linearly for 100 ps
Aarne
x (-70 - 70) y (0 - 140) z (-5 - 5)


time 1.2e+05 fs
-1-
-0.75-
-0.5-
-0.25-
0.0e+00-
0.25-
0.5-
0.75-
1-
1.25-
1.5-
1.75-
2-
2.25-
2.5-
2.75-
Maximum force reached
Aarne
x (-70 - 70) y (0 - 140) z (-5 - 5)

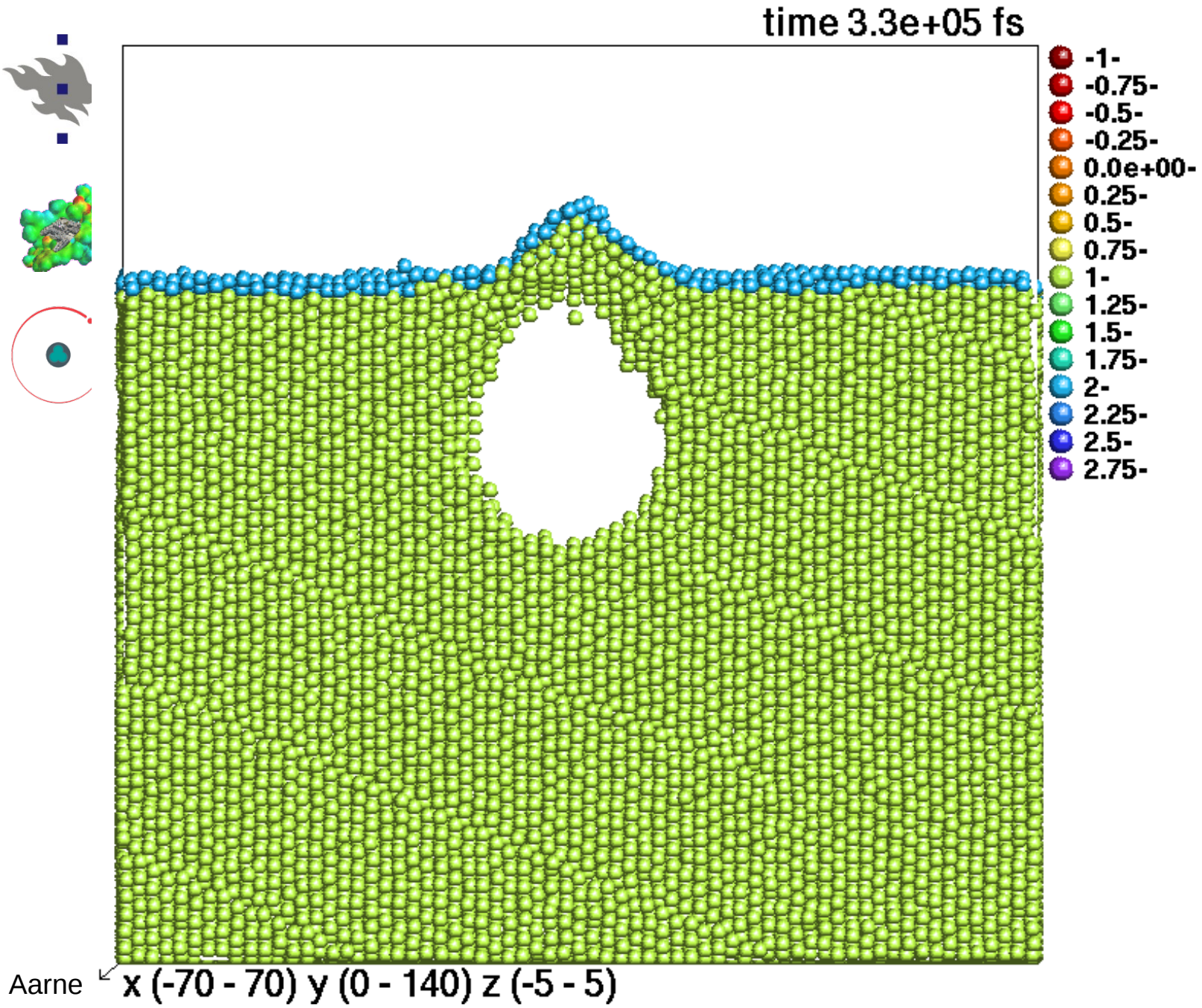

time 1.7e+05 fs
-1-
-0.75-
-0.5-
-0.25-
0.0e+00-
0.25-
0.5-
0.75-
1-
1.25-
1.5-
1.75-
2-
2.25-
2.5-
2.75-
System equilibrated
Aarne
x (-70 - 70) y (0 - 140) z (-5 - 5)


time 3.15e+05 fs
-1-
-0.75-
-0.5-
-0.25-
0.0e+00-
0.25-
0.5-
0.75-
1-
1.25-
1.5-
1.75-
2-
2.25-
2.5-
2.75-
Nothing happens for 145 ps
Until...
Aarne
x (-70 - 70) y (0 - 140) z (-5 - 5)

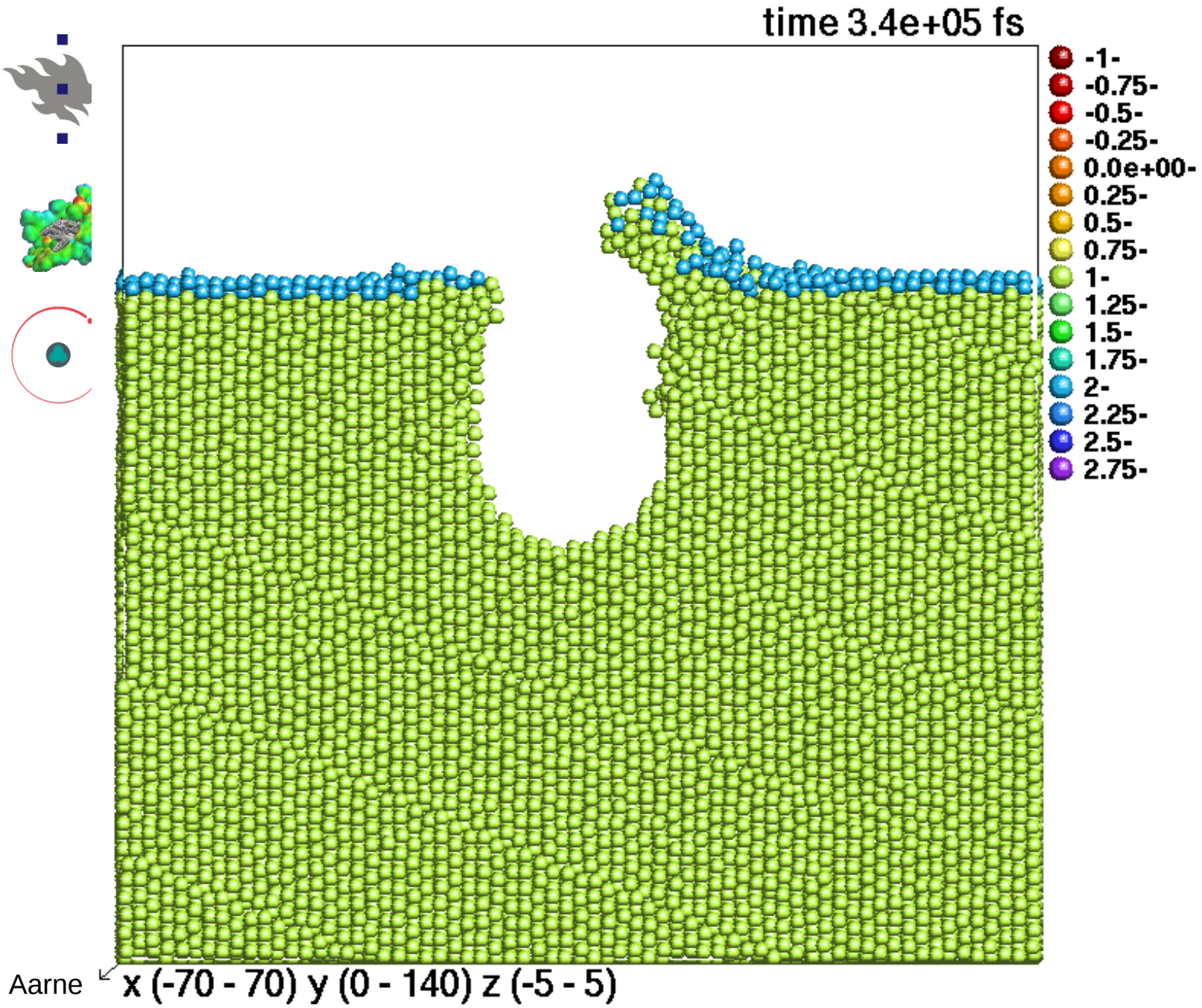

time 3.2e+05 fs
-1-
-0.75-
-0.5-
-0.25-
0.0e+00-
0.25-
0.5-
0.75-
1-
1.25-
1.5-
1.75-
2-
2.25-
2.5-
2.75-
A dislocation is emitted from the void
Aarne
x (-70 - 70) y (0 - 140) z (-5 - 5)

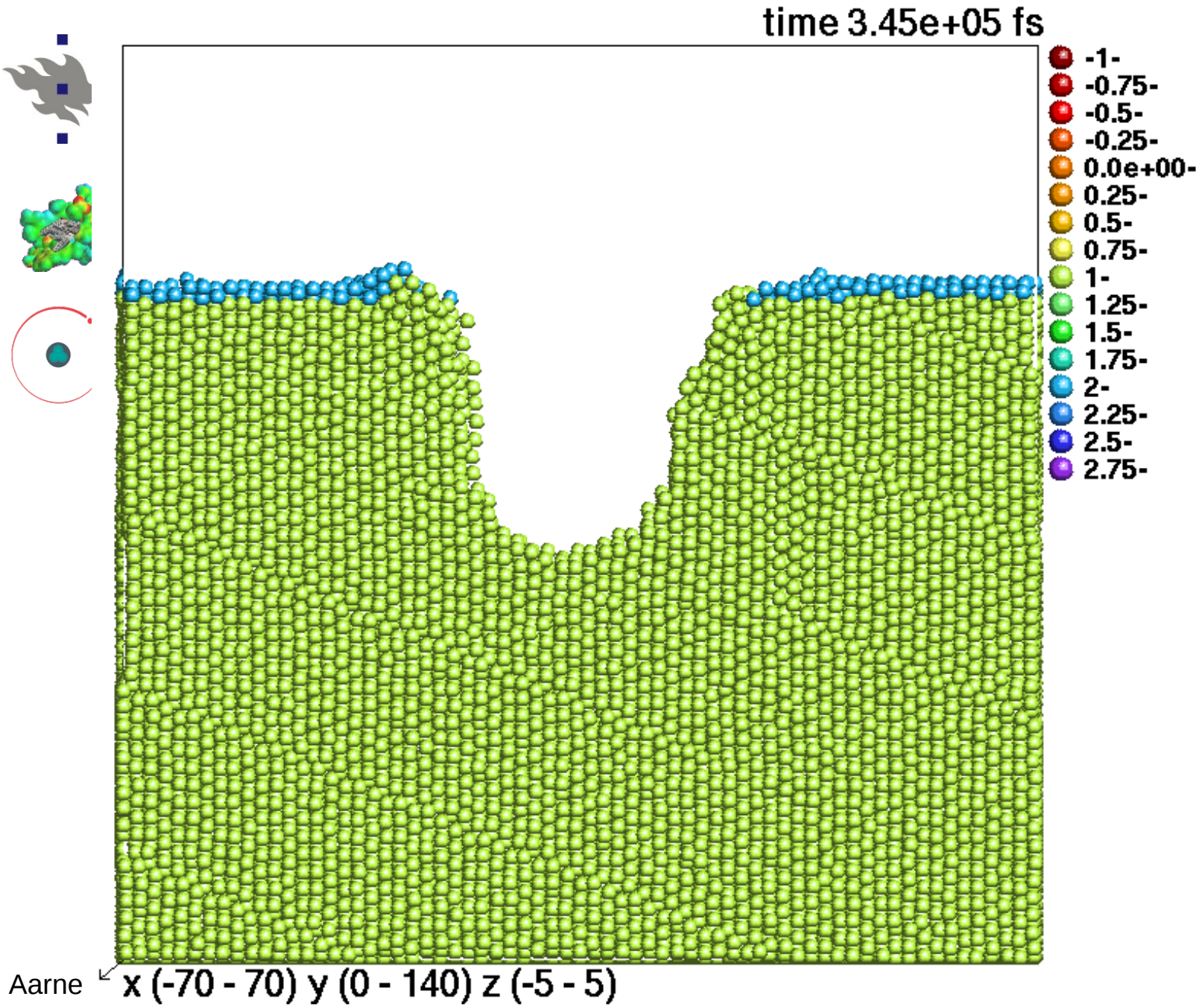

time 3.25e+05 fs
-1-
-0.75-
-0.5-
-0.25-
0.0e+00-
0.25-
0.5-
0.75-
1-
1.25-
1.5-
1.75-
2-
2.25-
2.5-
2.75-
x (-70 - 70) y (0 - 140) z (-5 - 5)

Aarne


time 3.3e+05 fs
-1-
-0.75-
-0.5-
-0.25-
0.0e+00-
0.25-
0.5-
0.75-
1-
1.25-
1.5-
1.75-
2-
2.25-
2.5-
2.75-
x (-70 - 70) y (0 - 140) z (-5 - 5)

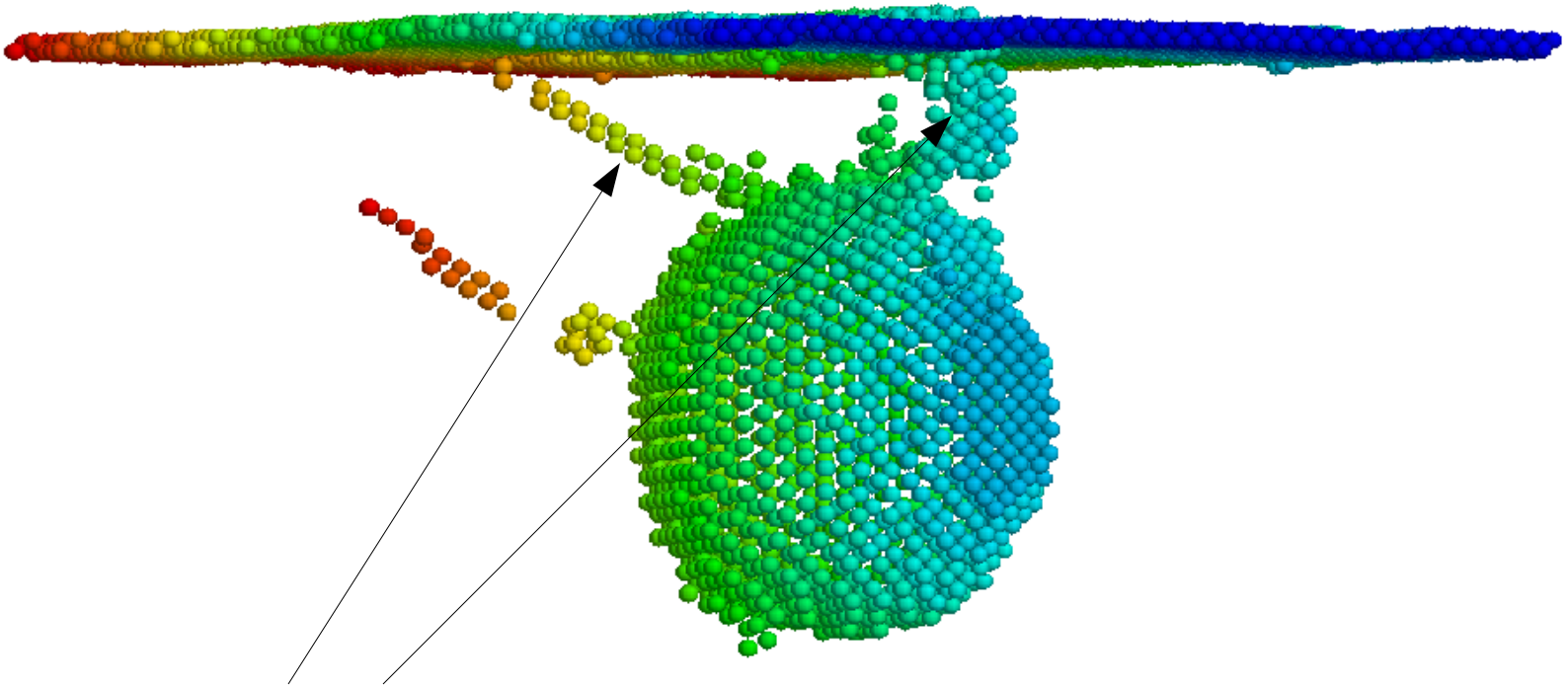
Aarne


time 3.4e+05 fs
-1-
-0.75-
-0.5-
-0.25-
0.0e+00-
0.25-
0.5-
0.75-
1-
1.25-
1.5-
1.75-
2-
2.25-
2.5-
2.75-
Aarne
x (-70 - 70) y (0 - 140) z (-5 - 5)


time 3.45e+05 fs
-1-
-0.75-
-0.5-
-0.25-
0.0e+00-
0.25-
0.5-
0.75-
1-
1.25-
1.5-
1.75-
2-
2.25-
2.5-
2.75-
x (-70 - 70) y (0 - 140) z (-5 - 5)

Aarne

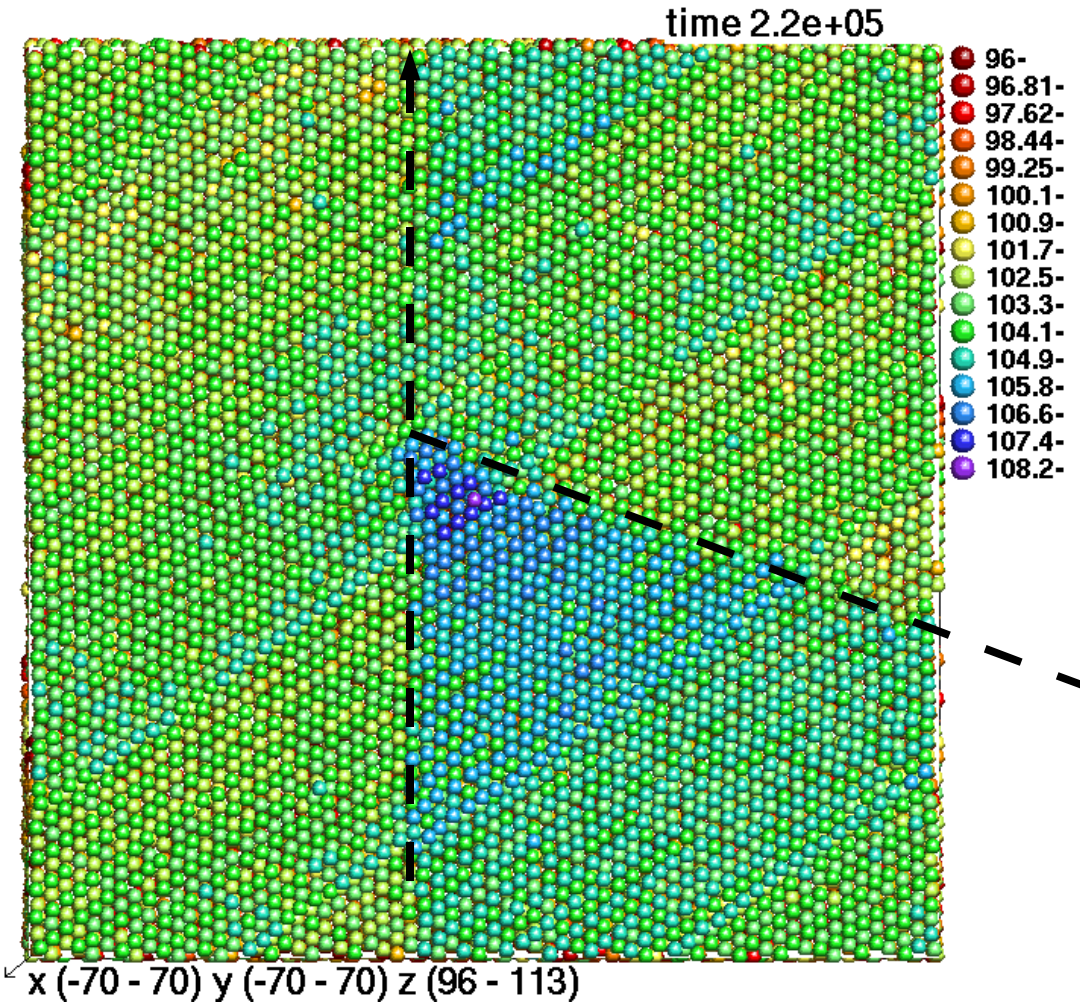
Simulations



Dislocation lines

Simulations

View from top – atoms coloured by height



$\vec{a}=(1,1,-2)$

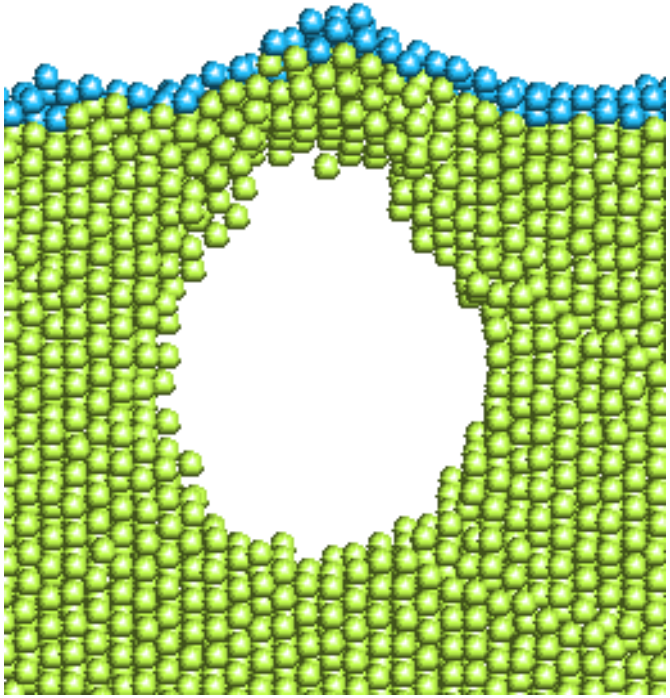
$\vec{b}=(1,1,2)$

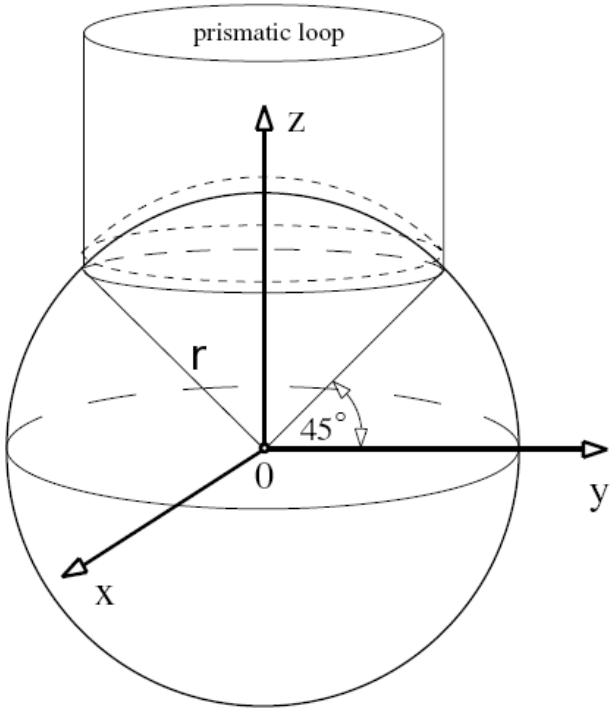
$\cos \sphericalangle(\vec{a},\vec{b})=\frac{\vec{a}\cdot\vec{b}}{|a||b|}$

$\sphericalangle(\vec{a},\vec{b})=109{,}47^{o}$

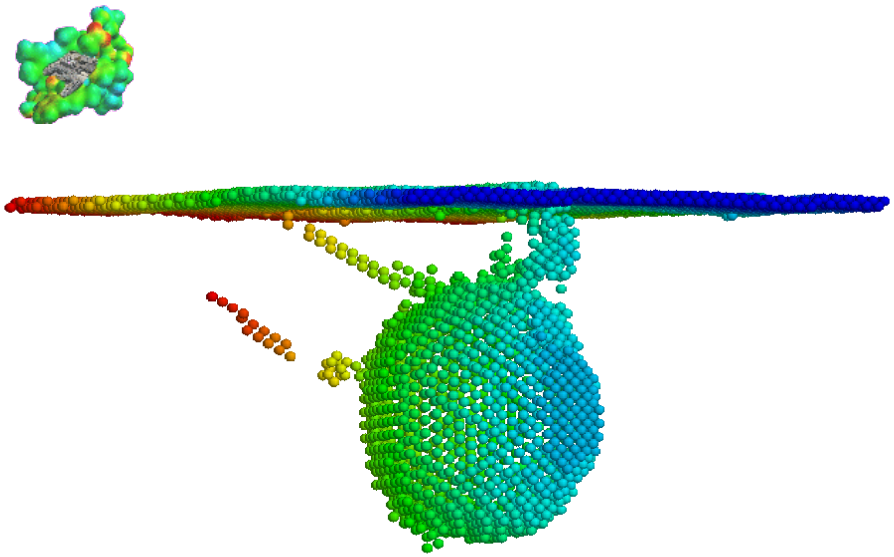
$180^{o}-109{,}27^{o}=70{,}73^{o}$

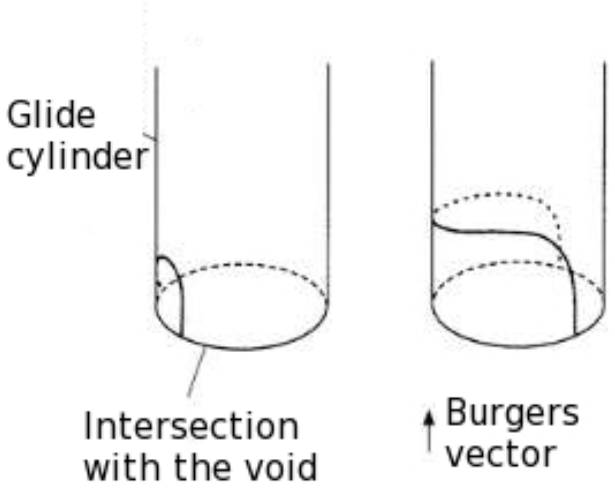
as observed in this image





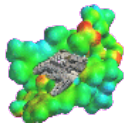
Void Growth by Dislocation Emission, Lubarda, Schneider, Kalantar, Remington, Meyers, 2004

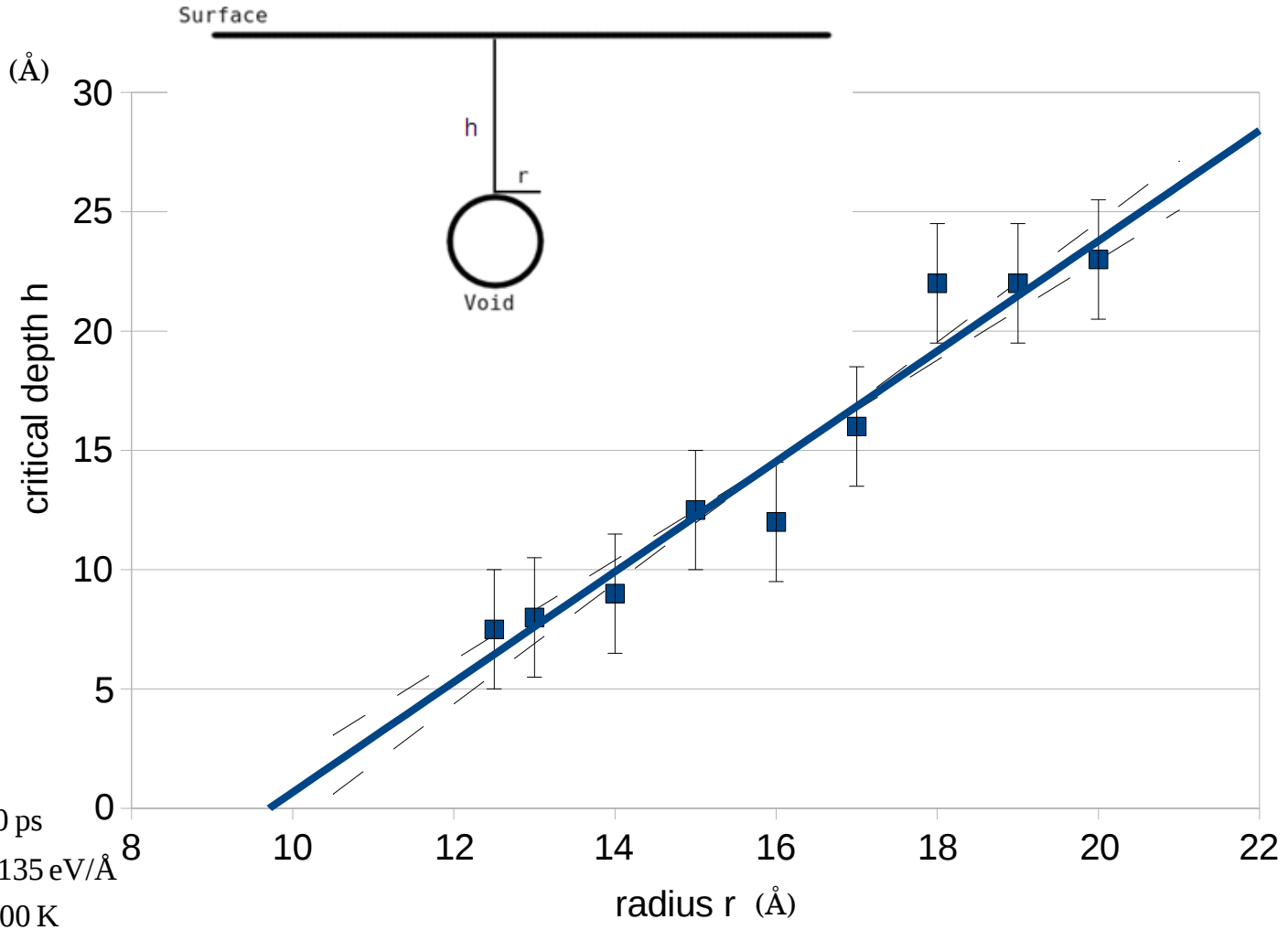




Introduction to Dislocations, Hull, Bacon, 2001

Simulations





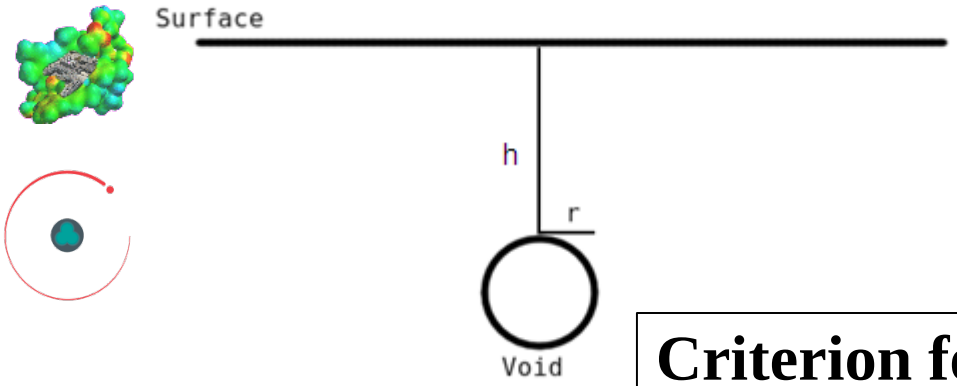
timescale $\Delta t = 300$ ps

force/atom $F = 0.135$ eV/Å

temperature $T = 600$ K

Aarne Pohjonen, HIP, University of Helsinki

Criterion for growth



timescale $\Delta t = 300$ ps

force/atom $F = 0.135$ eV/Å

temperature $T = 600$ K

$a = 2.31 \pm 0.22$

$r_{min} = (9.71 \pm 3.5)\,Å$

Criterion for growth

Growth will occur during timescale Δt if

$$h < a(r - r_{\min})$$

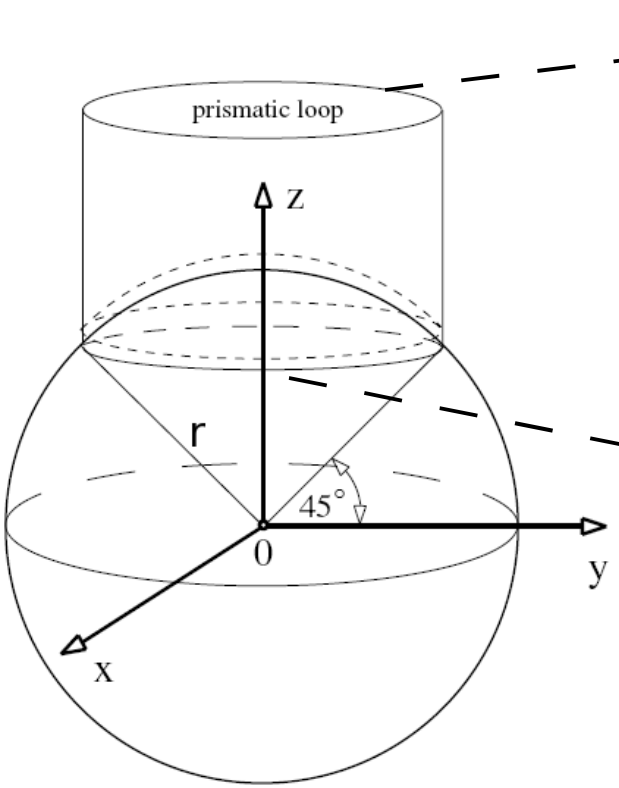
where

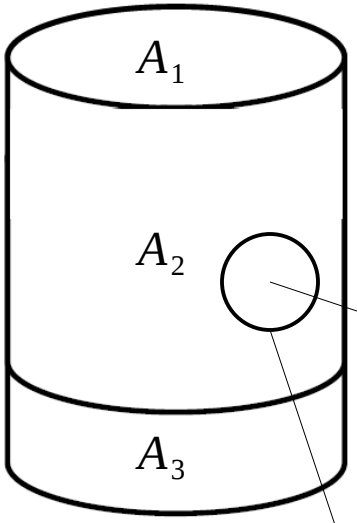
h is the depth of the void

r is the radius of the void

$r_{\min}$ is the minimum radius for the growth to occur

Criterion for growth





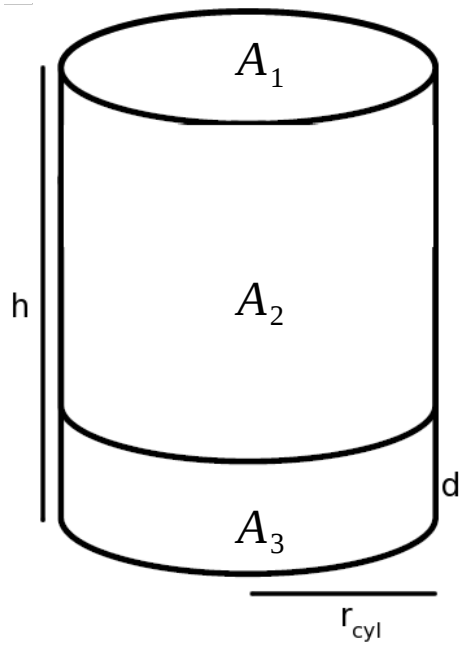
Force on surface element $\vec{F}$

Surface element with area $\Delta\sigma$ and direction $\vec{\nu}$

Void Growth by Dislocation Emission, Lubarda, Schneider, Kalantar, Remington, Meyers, 2004

Stress vector $\vec{T}^{\vec{\nu}} := \lim_{\Delta\sigma \to 0} \frac{\vec{F}}{\Delta\sigma}$

Mathematical Theory of Elasticity, Sokolnikoff, 1956



In equilibrium

$$\int_{surface} \vec{T}^{\vec{\nu}}_y = 0$$

$$\int_{A_1} \vec{T}^{\vec{\nu}}_y + \int_{A_2} \vec{T}^{\vec{\nu}}_y + \int_{A_3} \vec{T}^{\vec{\nu}}_y = 0$$

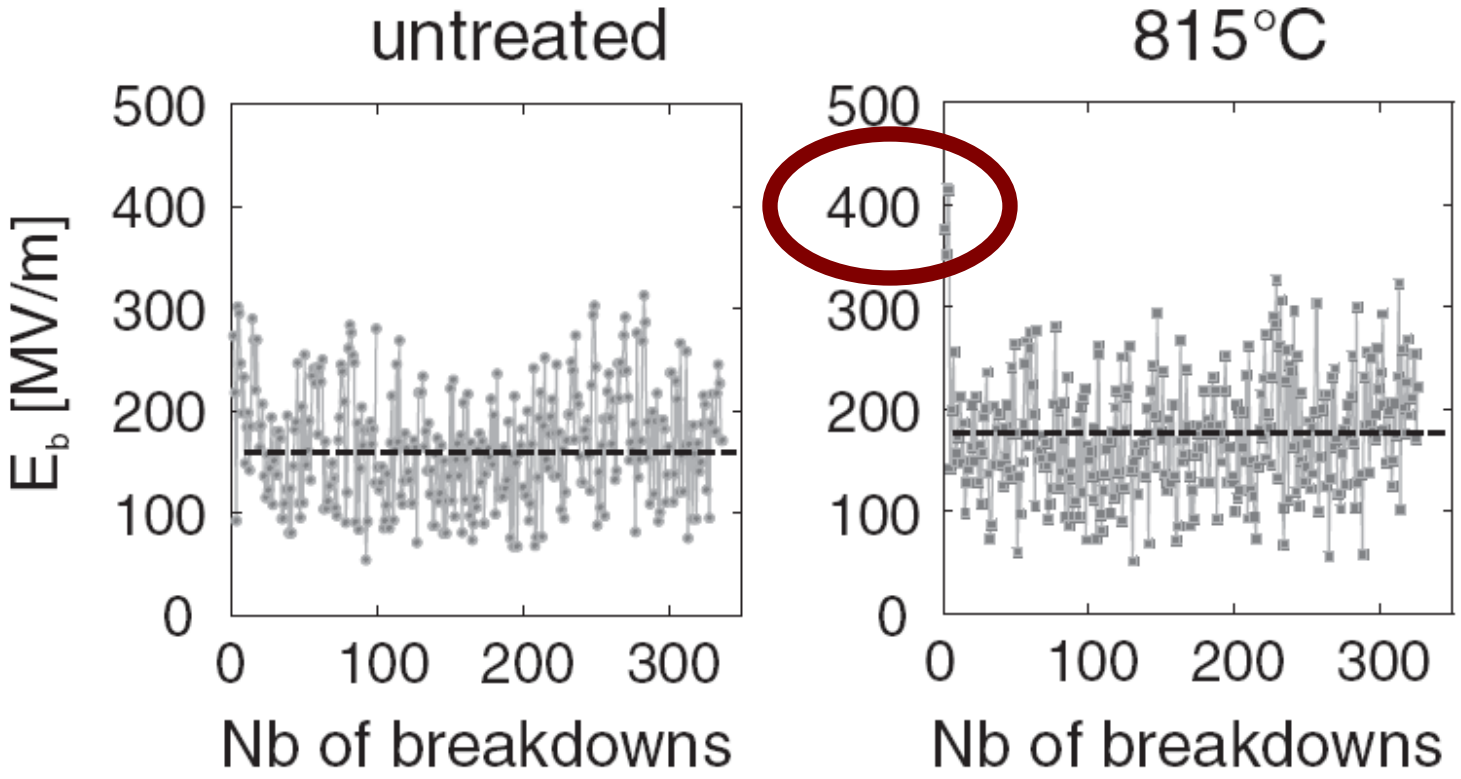
$$<\vec{T}^{\vec{\nu}}_y>_{A_1} \pi r_{cyl}^2 + \underbrace{<\vec{T}^{\vec{\nu}}_y>_{A_2}}_{B_{T,2}} 2\pi r_{cyl}(h-d) + \underbrace{<\vec{T}^{\vec{\nu}}_y>_{A_2}}_{B_{T,3}} 2\pi r_{cyl} d = 0$$

$$h < h_{max} = -\frac{<\vec{T}^{\vec{\nu}}_y>_{A_1}}{2^{3/2} B_{T,2}} \left(r - \frac{2^{3/2}(B_{T,2} - B_{T,3})}{<\vec{T}^{\vec{\nu}}_y>_{A_1}} d \right) \quad \Leftrightarrow$$

Criterion for growth

$$h < a(r - r_0)$$

Effect of heat treatment

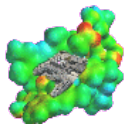


Effect of 815°C heat treatment on Cu.

DC Breakdown Conditioning and Breakdown Rate of Metals and Metallic Alloys under Ultrahigh Vacuum, Descouedres, Ramsvik, Calatroni, Taborelli, Wuensch, 2009

Voids would be annealed out in high temperatures...

Conclusions



Voids in copper

- Voids have been observed in the structures
- Kirkendall effect may create near-surface voids

Dislocation emission from voids is possible

- Forces used in simulation are huge
- Need to do further analysis

Criterion for growth

Growth will occur during timescale Δt if

$h < a(r - r_{\min})$

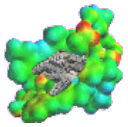
where

h is the depth of the void

r is the radius of the void

$r_{\min}$ is the minimum radius for the growth to occur

Discussion



• Dislocations are probably nucleated easier from a grain boundary void

• Dislocation emission from the void might initiate a growth on surface that would enhance the field

• Dislocation emission might lead to a detachment of a particle from the surface

-> Particle detachment from anode might create impact crater on cathode where the field would be enhanced