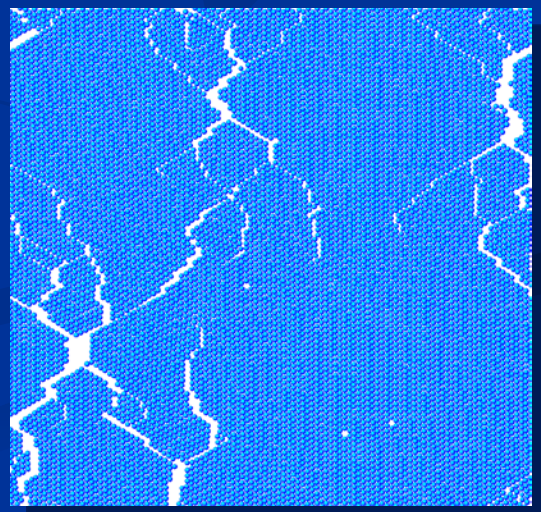
Russian Academy of Sciences
Institute for Problems in Mechanical Engineering
Laboratory Discrete Models in Mechanics
A. M. Krivtsov

Influence of defects type and chemical reaction on fracture initiation, molecular dynamics study



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V. A. Tsaplin

Introduction

- MEMS: require multiscale approach coupling continuum theories for creep and fatigue with discrete modeling based on atomic consideration and molecular dynamics simulation.
- Molecular dynamics simulation technique – important tool at nano- and microscale

Molecular dynamics equations of motion

$$m\ddot{\underline{r}}_k = \sum_{n=1}^{N} \frac{f(|\underline{r}_k - \underline{r}_n|)}{|\underline{r}_k - \underline{r}_n|} (\underline{r}_k - \underline{r}_n) - B\,\dot{\underline{r}}_k\,, \qquad k = 1, 2, ..., N\,;$$

where

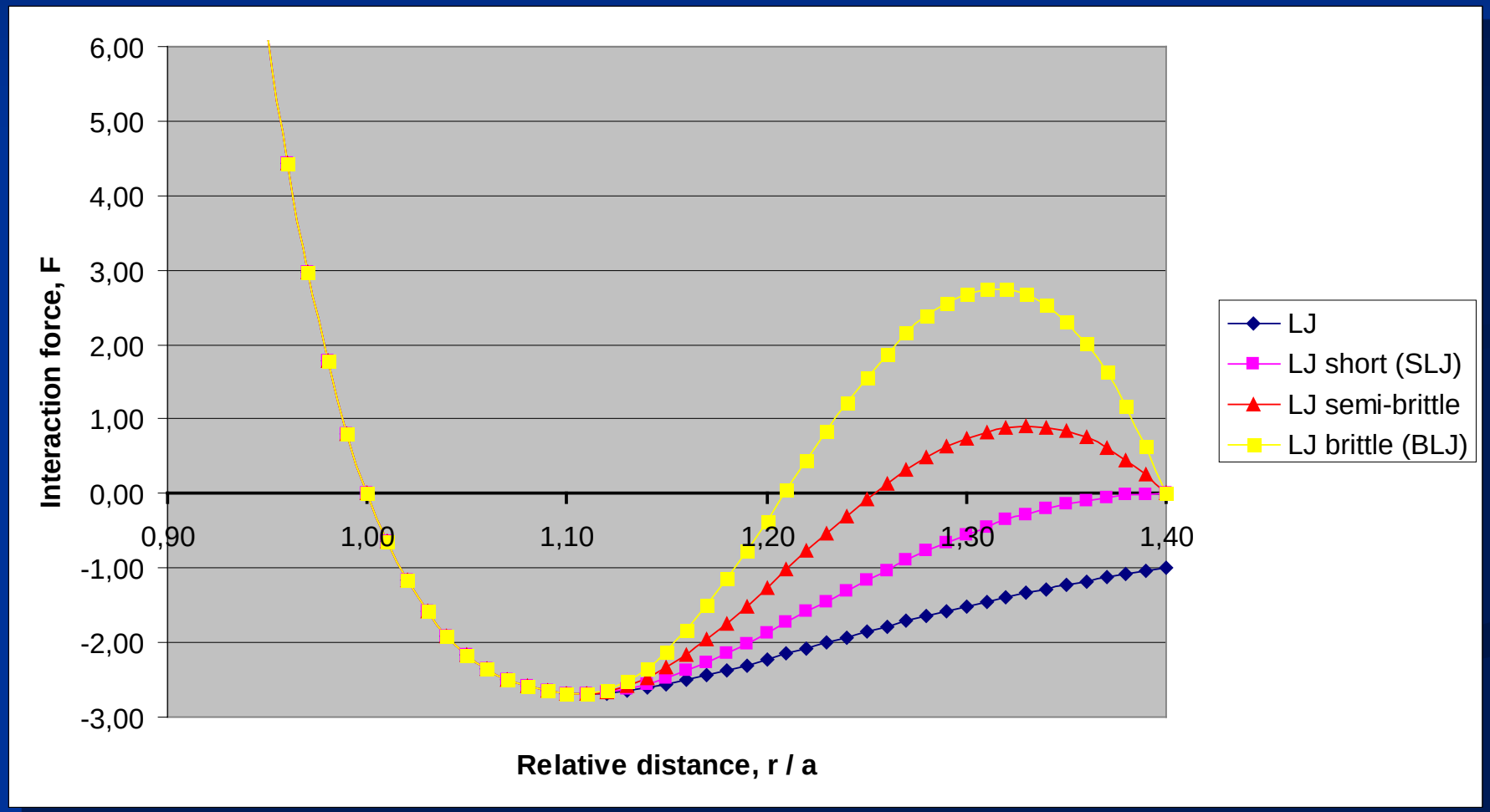
$\underline{r}_k$ — radius-vector of the particle number k,
m — mass of the particle,
N — total number of particles,
$f(r) = -\Pi'(r)$ — force of interaction,
B — cooling coefficient.

Lennard-Jones law of interaction

$$f(r) = -\Pi'(r), \qquad \Pi(r) = D\left[\left(\frac{a}{r}\right)^{12} - 2\left(\frac{a}{r}\right)^{6}\right].$$

where D — bond energy, a — bond length.

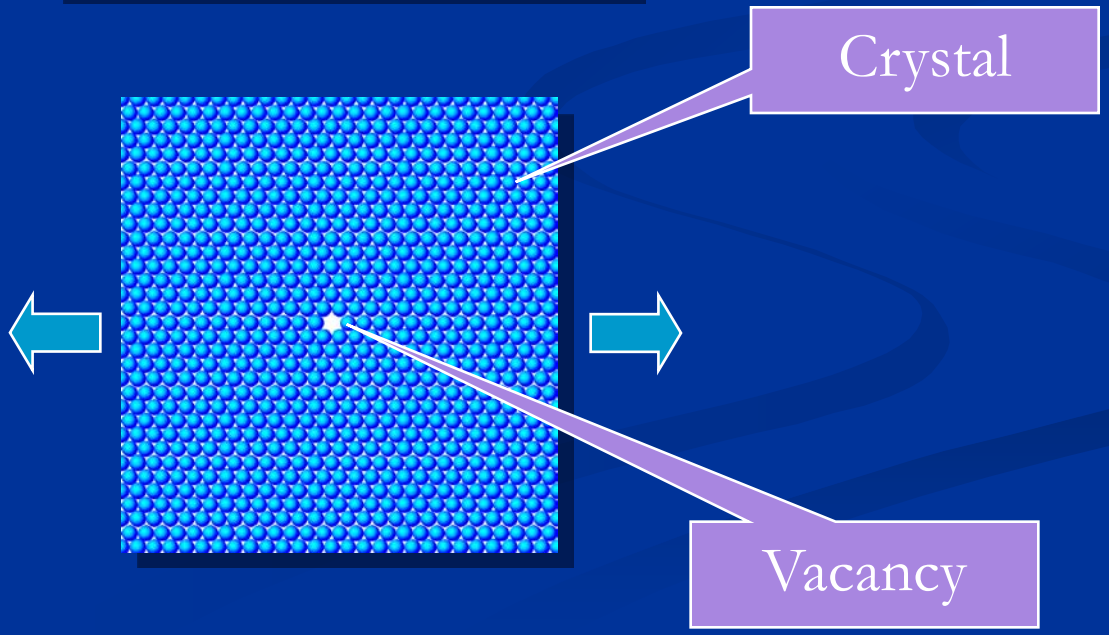
Modified LJ interactions



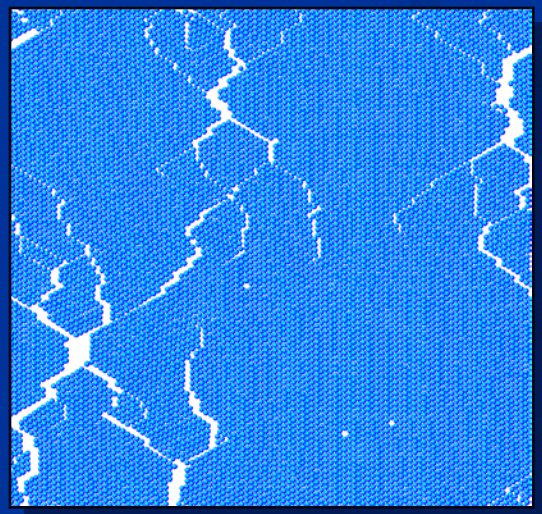
Periodical loading

$$\varepsilon_x = \frac{1}{4}\varepsilon_{\max}\left(3 - \cos\left(2\pi\frac{t}{T}\right)\right), \qquad \varepsilon_y = 0$$

$$\varepsilon_{\max}/2 \le \varepsilon_x \le \varepsilon_{\max}$$



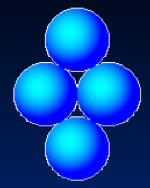
2D simulation



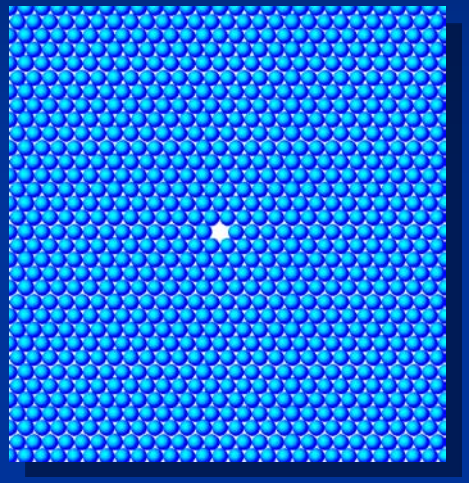
The model

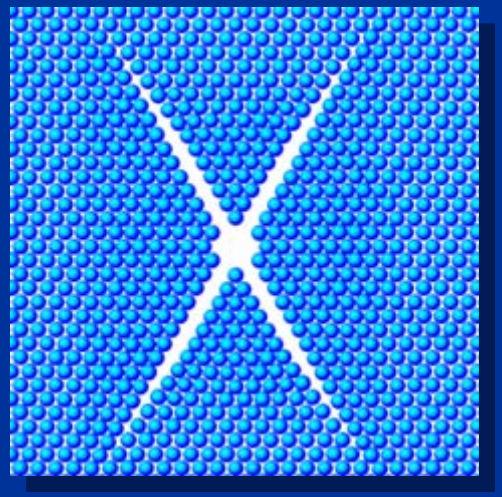
- Triangular crystal lattice
- SLJ (Shortened Lennard-Jones interaction) or BLJ (Brittle Lennard-Jones interaction)
- Predefined defects (vacancies)
- Periodic boundary conditions
- Cyclic uniaxial loading

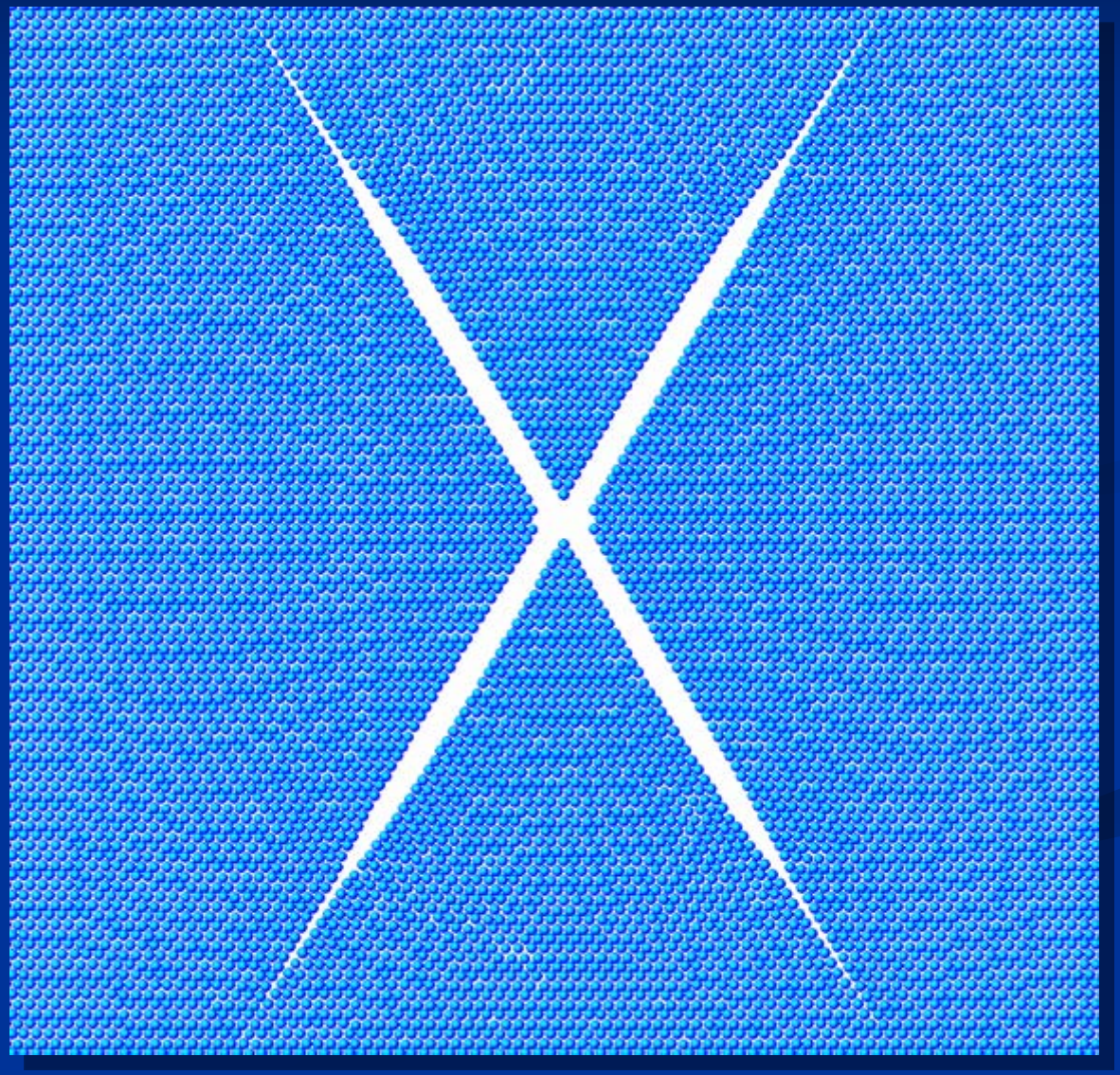
Crack initiation from a point defect



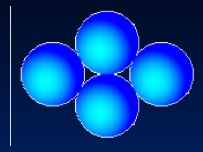
Vertical lattice



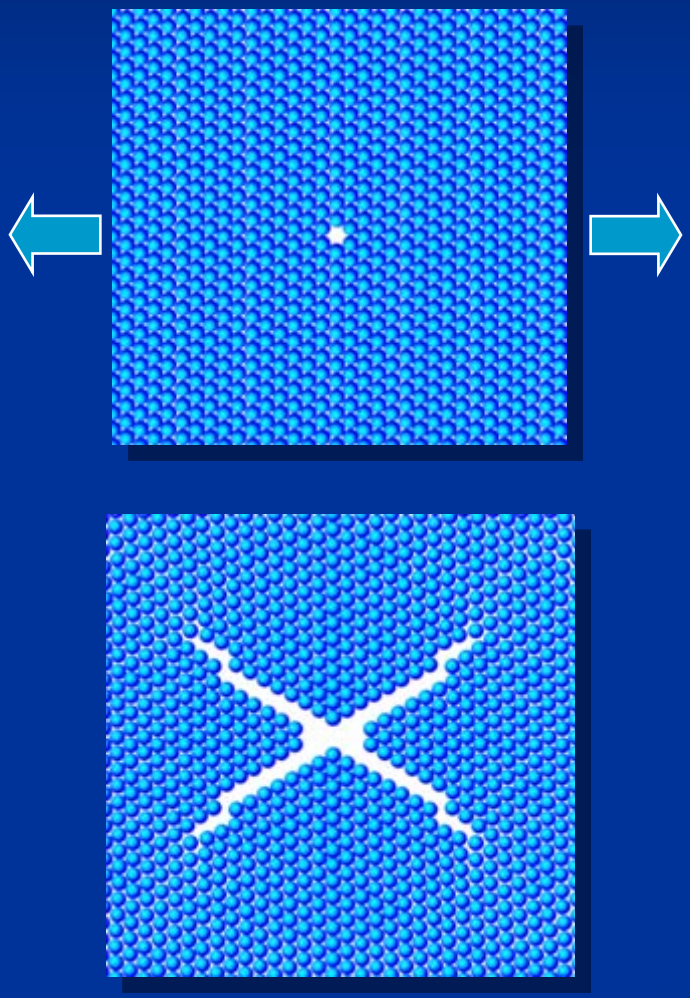


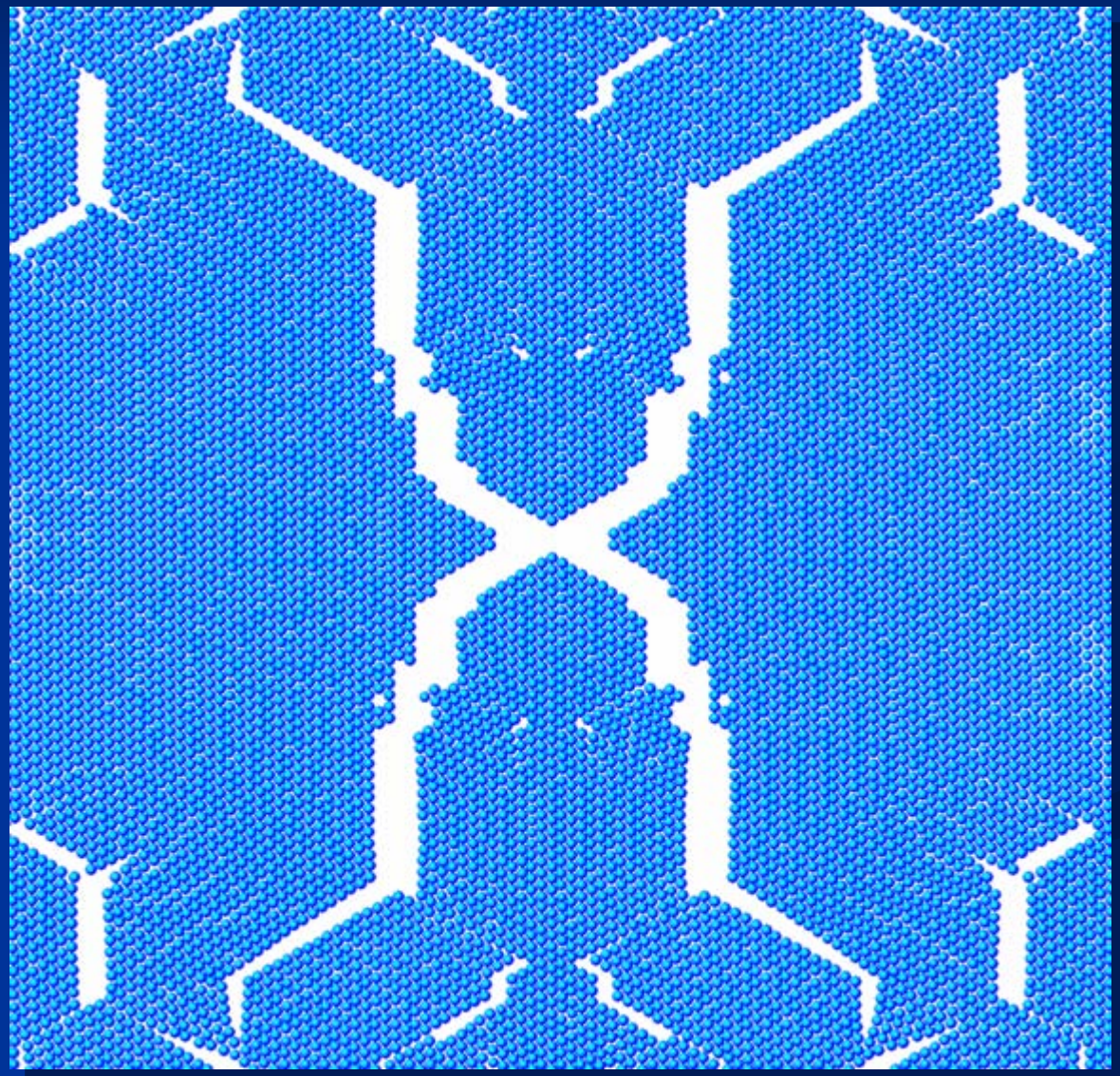


Crack initiation from a point defect

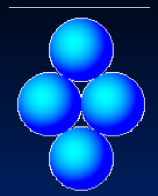


Horizontal lattice



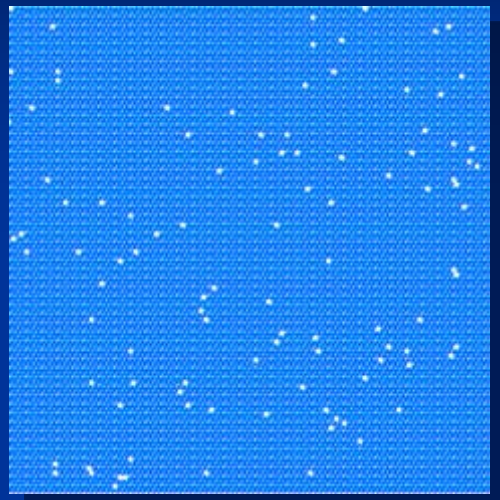


Influence of defect rate

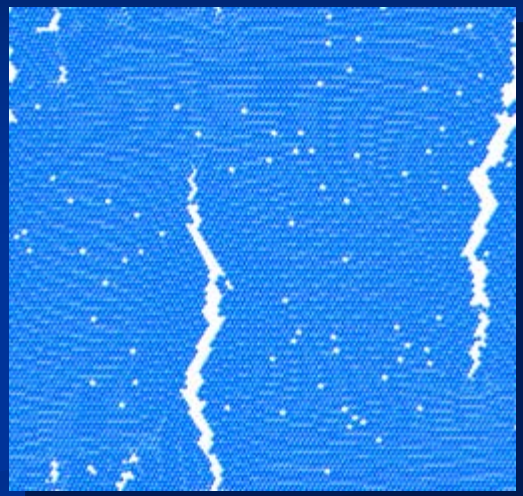


Vertical lattice

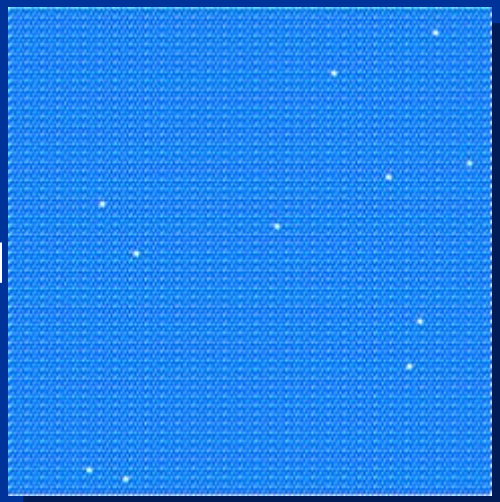
Initial configuration: 1.0% defects



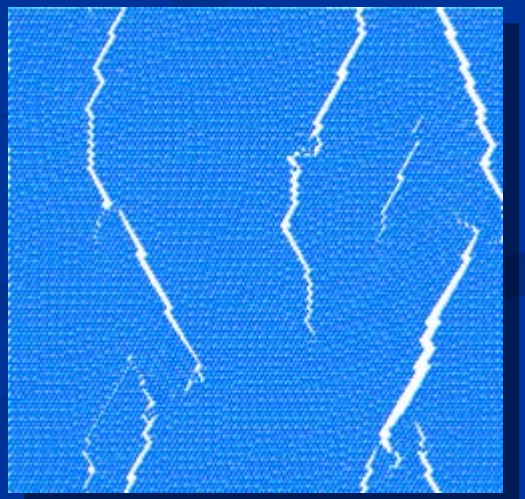
Crack development: 1.0% defects



Initial configuration: 0.1% defects

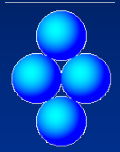


Crack development: 0.1% defects

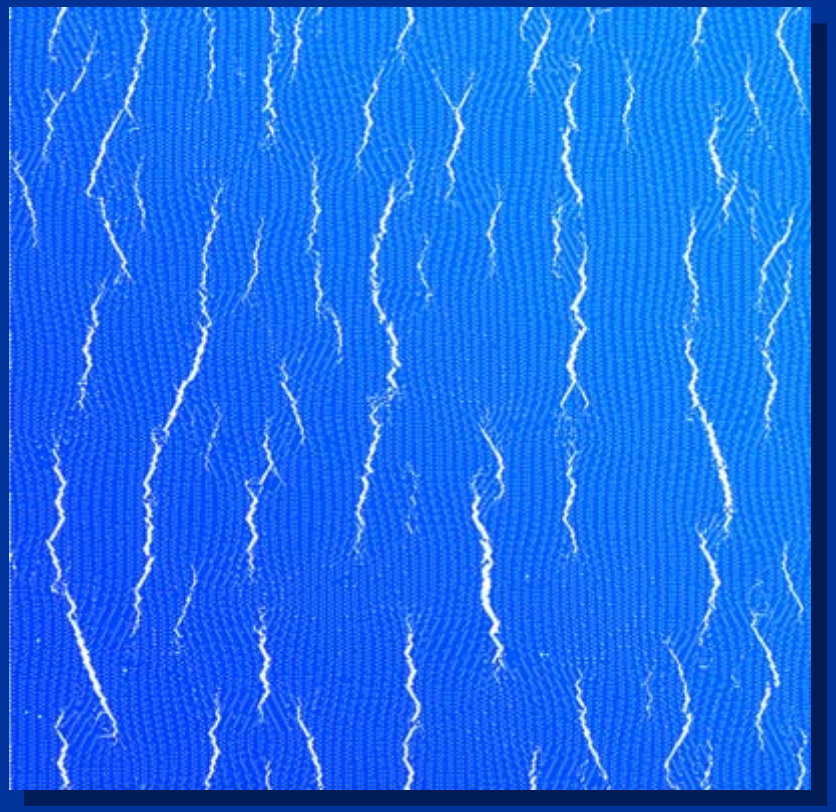


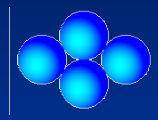
Influence of lattice orientation

(10^5 particles, 0.1% defects)

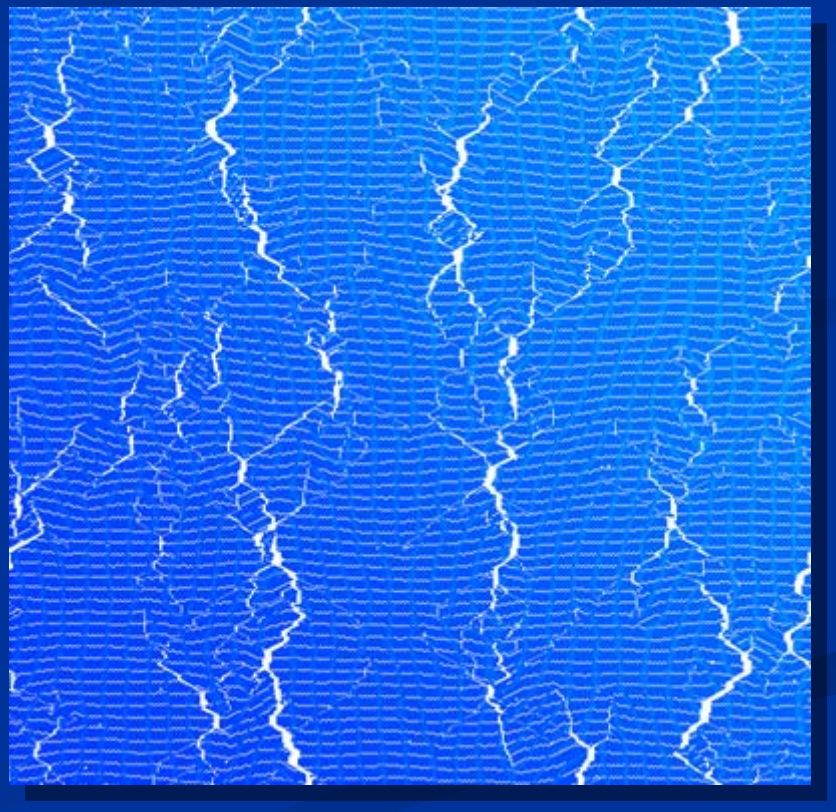


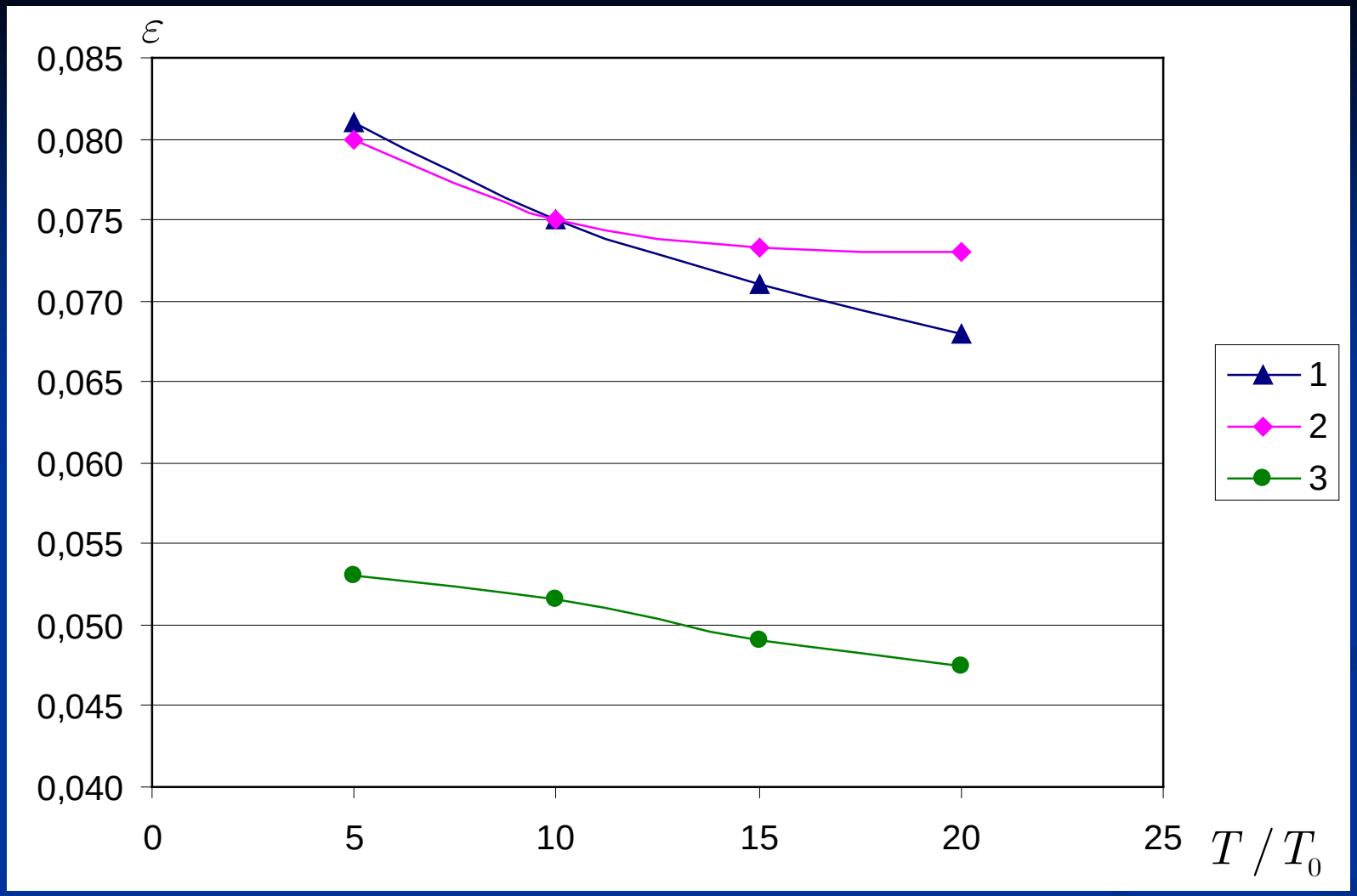
Vertical lattice





Horizontal lattice

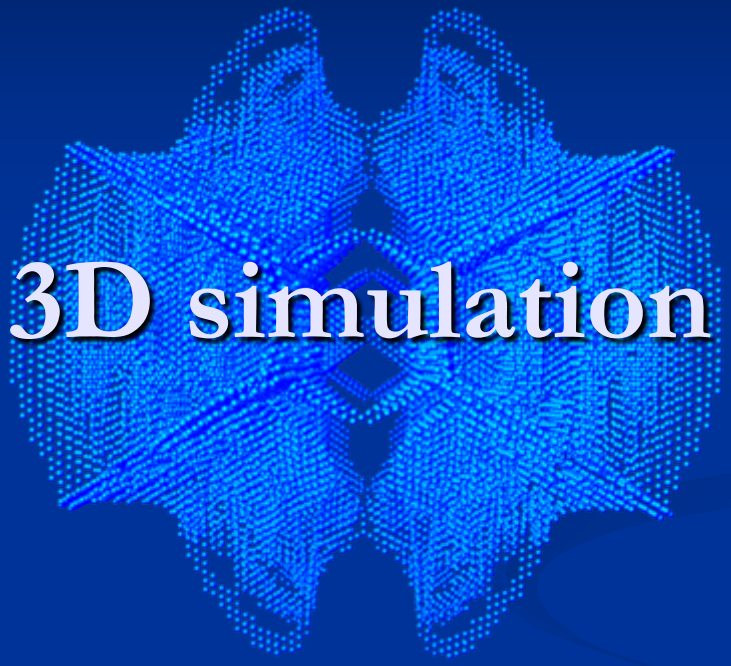




Dependence of the critical deformation on the period of loading:

1) single vacancy, vertical lattice;
2) single vacancy, horizontal lattice;
3) 1% vacancies, vertical lattice.

3D simulation



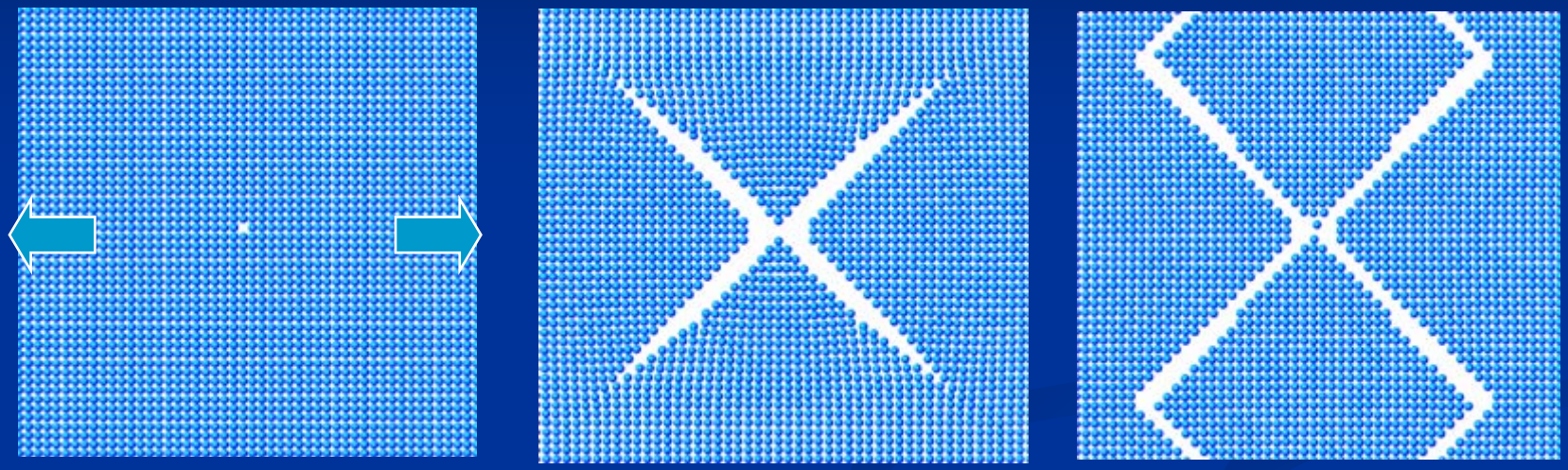
The model

- FCC (Face Centered Cubic lattice)
- SLJ (Shortened Lennard-Jones interaction) or BLJ (Brittle Lennard-Jones interaction)
- Predefined defects (vacancies)
- Periodic boundary conditions
- Cyclic uniaxial loading

Crack initiation from vacancy (SLJ)

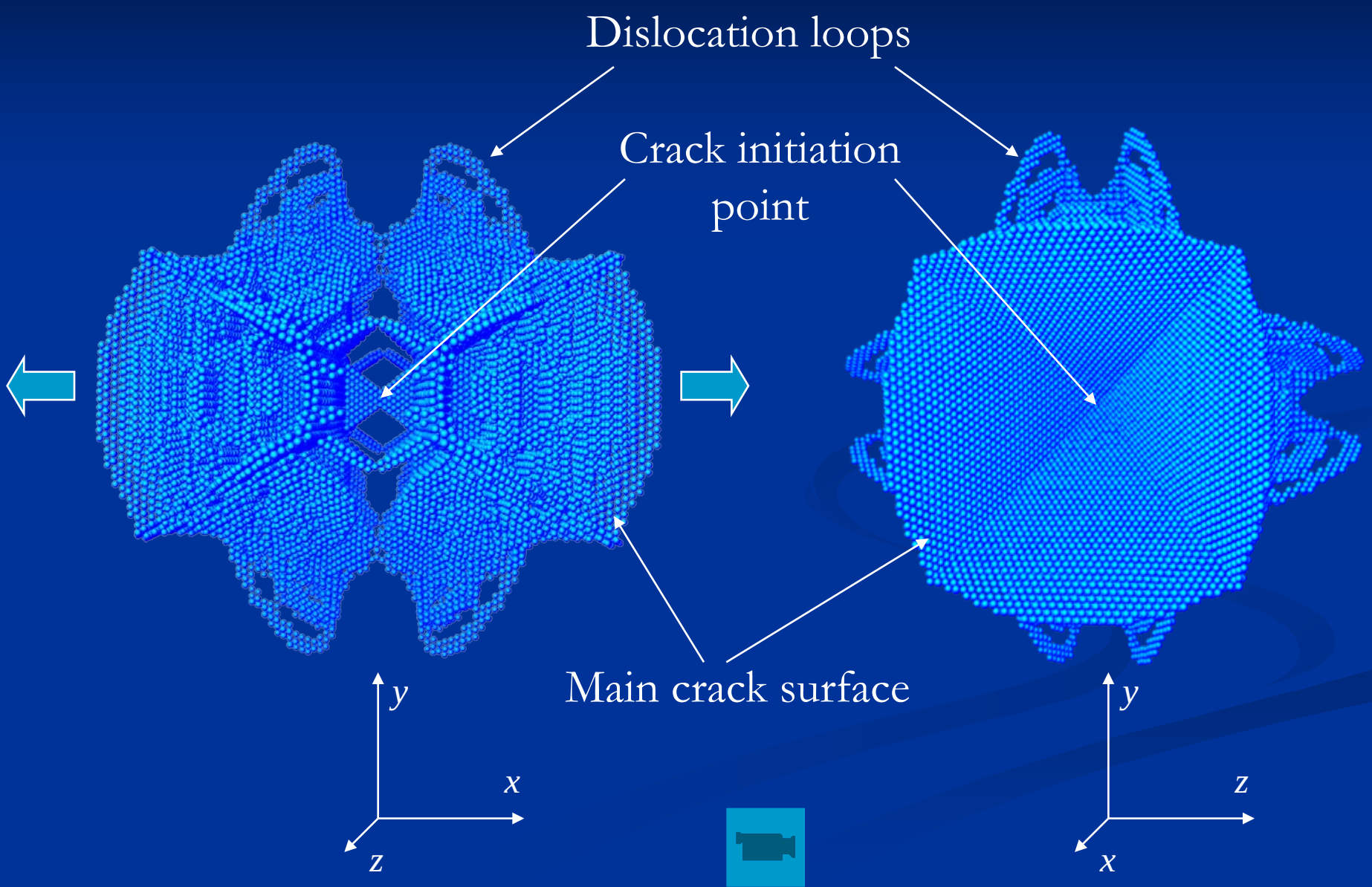
Initial vacancy | Crack propagation | Developed crack

Cross-sections of the crystal



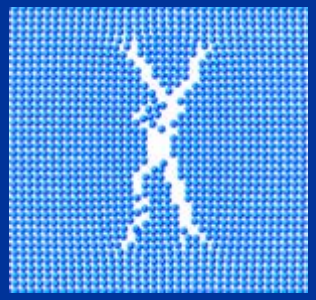
Crack surfaces

Crack initiation from vacancy (SLJ)

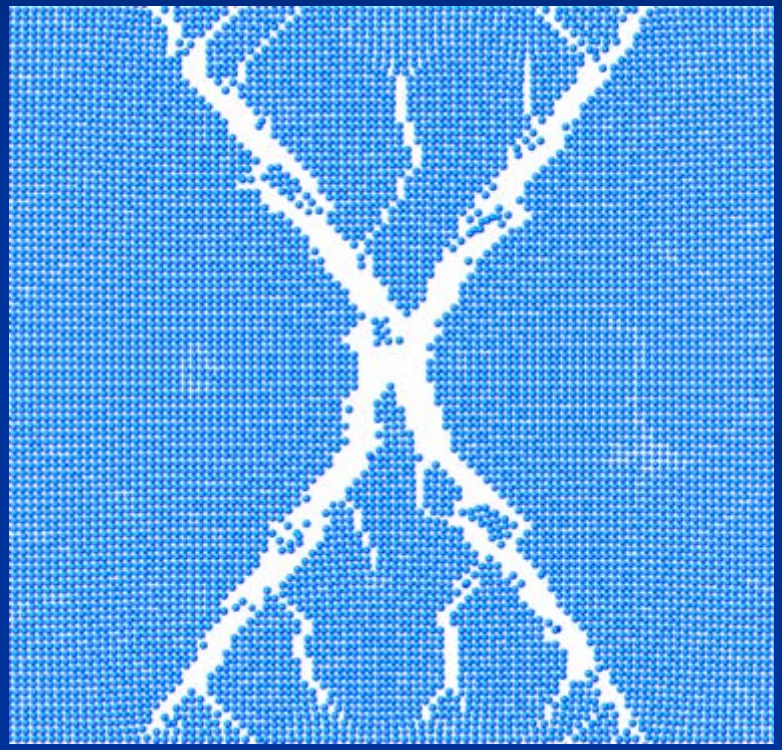


Crack branching

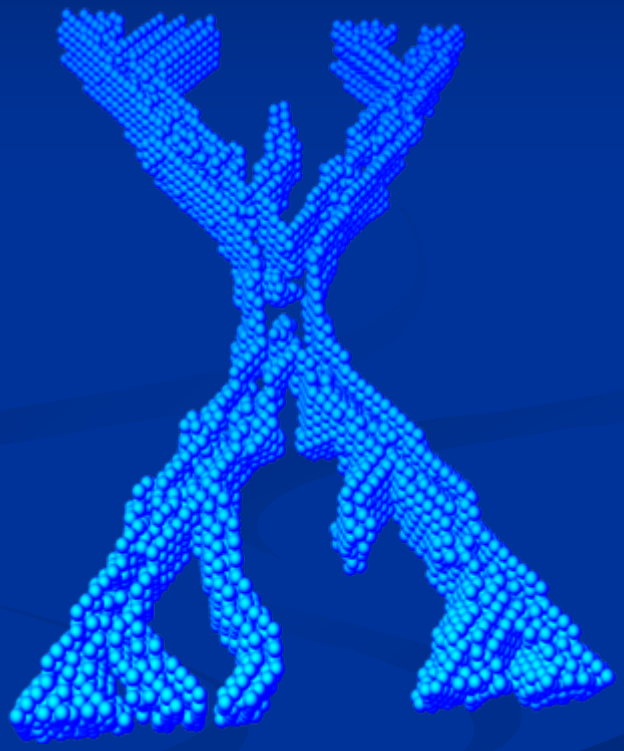
(BLJ + thermal motion)



Crack embryo

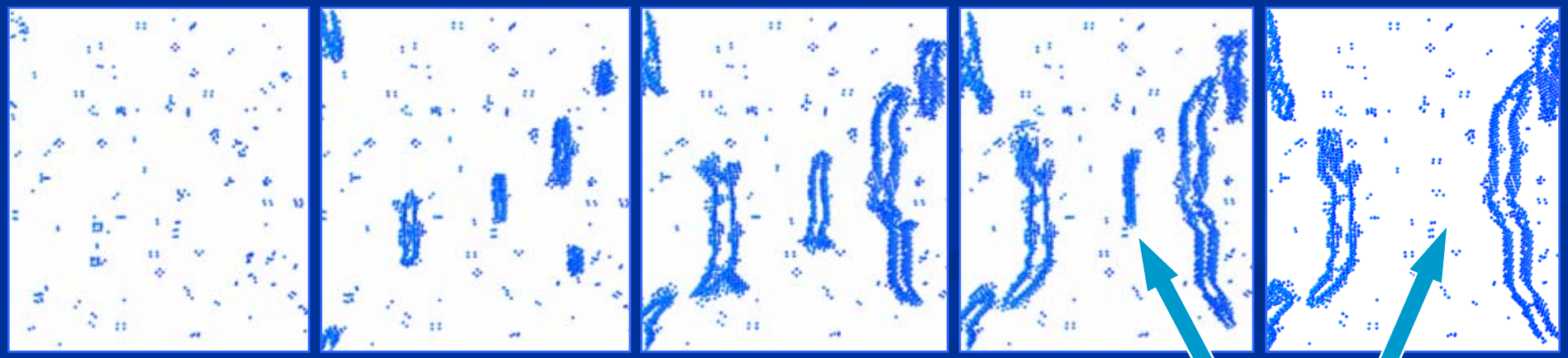


Developed crack



3D view of surface particles

Crack development in crystal with defects (cross-section)



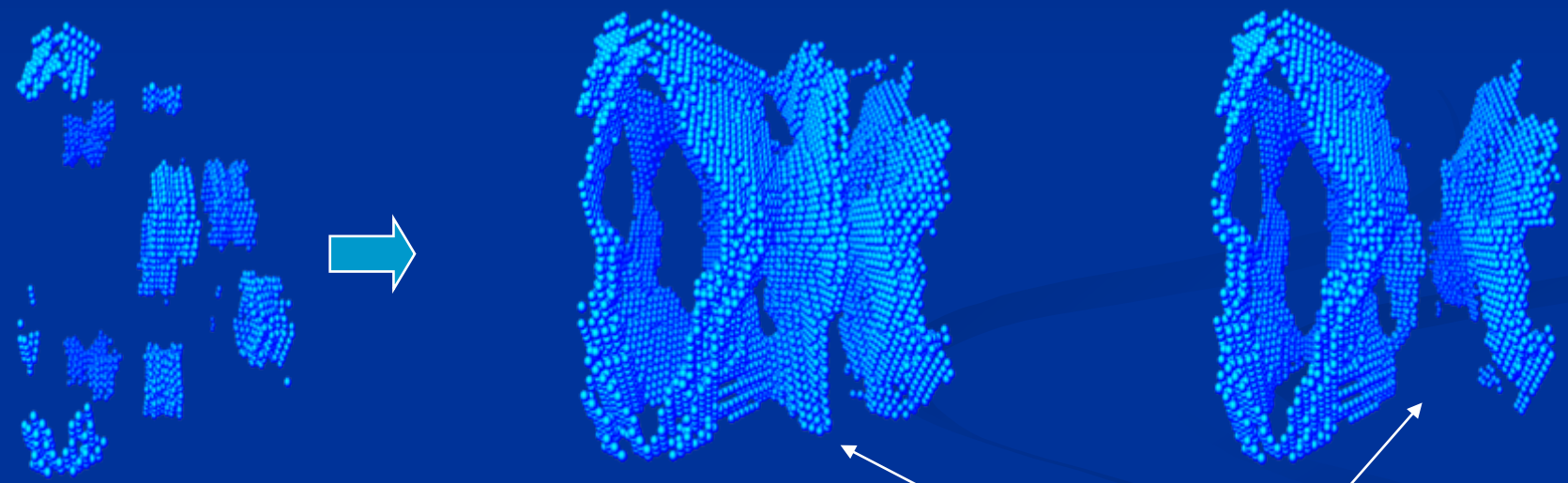
Initial defects

Crack initiation

Developed cracks

Disappearance of the crack

Crack development in crystal with defects (crack surfaces)

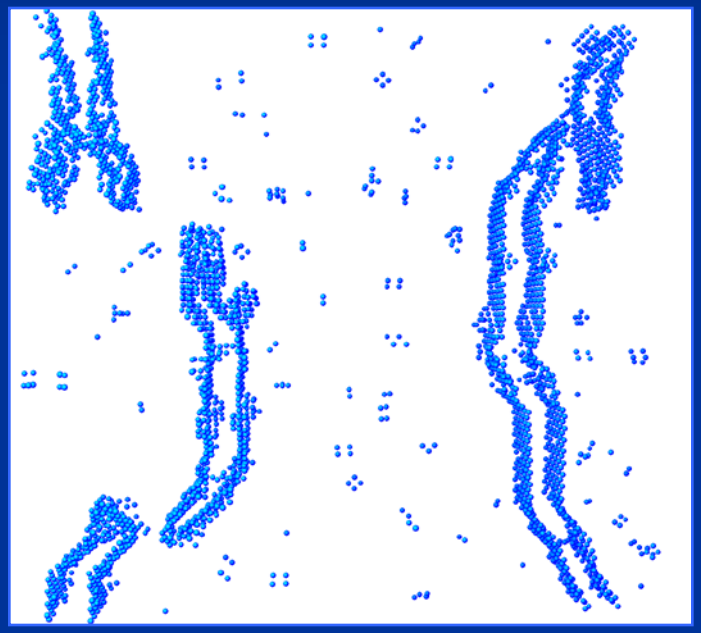


Crack initiation

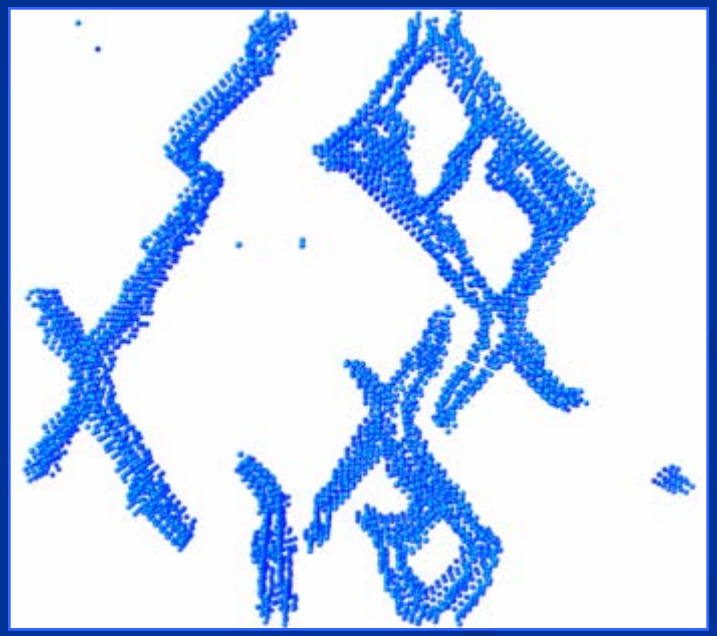
Developed cracks

Disappearance of the crack

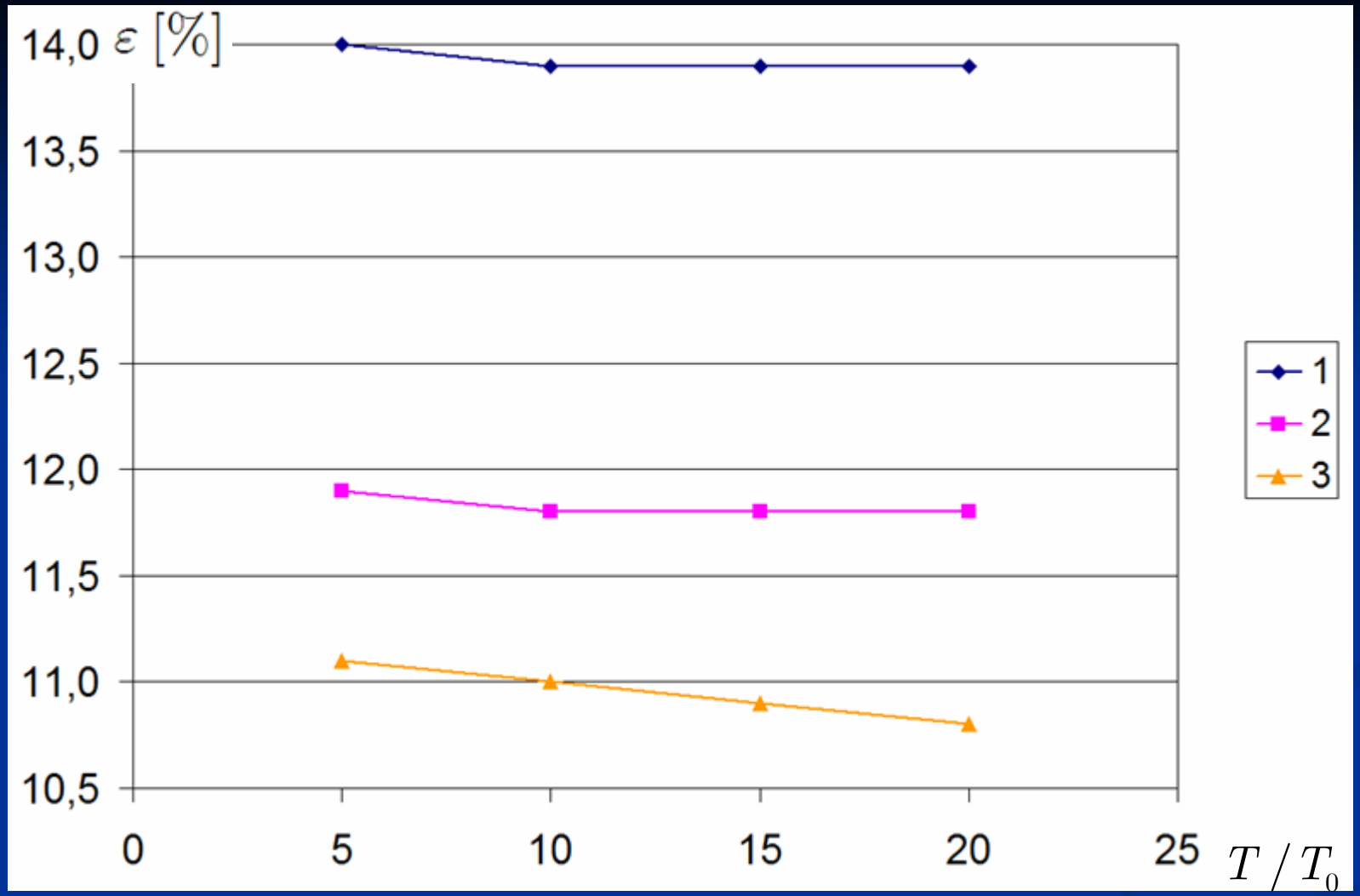
Crack development in different crystals



Shortened Lennard-Jones (SLJ)



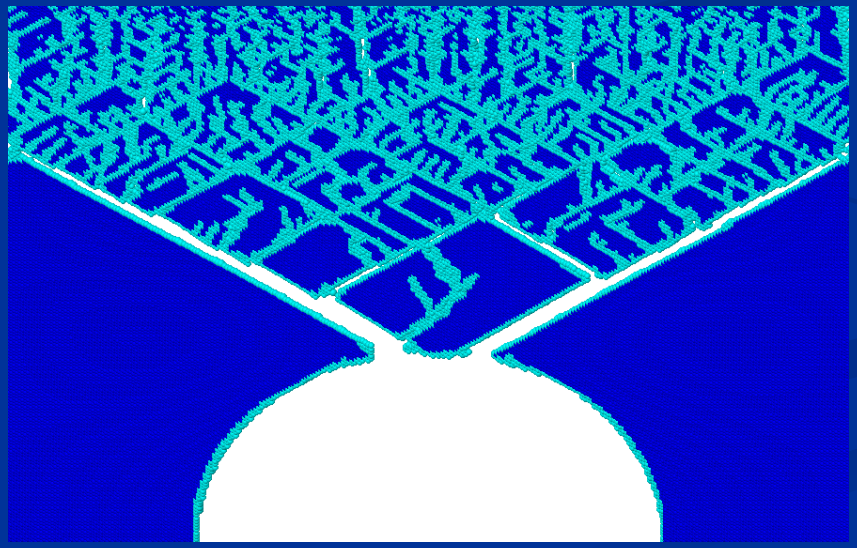
Brittle Lennard-Jones (BLJ)



Dependence of the critical deformation on the period of loading:

1) single vacancy;
2) pare of vacancies;
3) 0.3% vacancies.

Chemical reaction



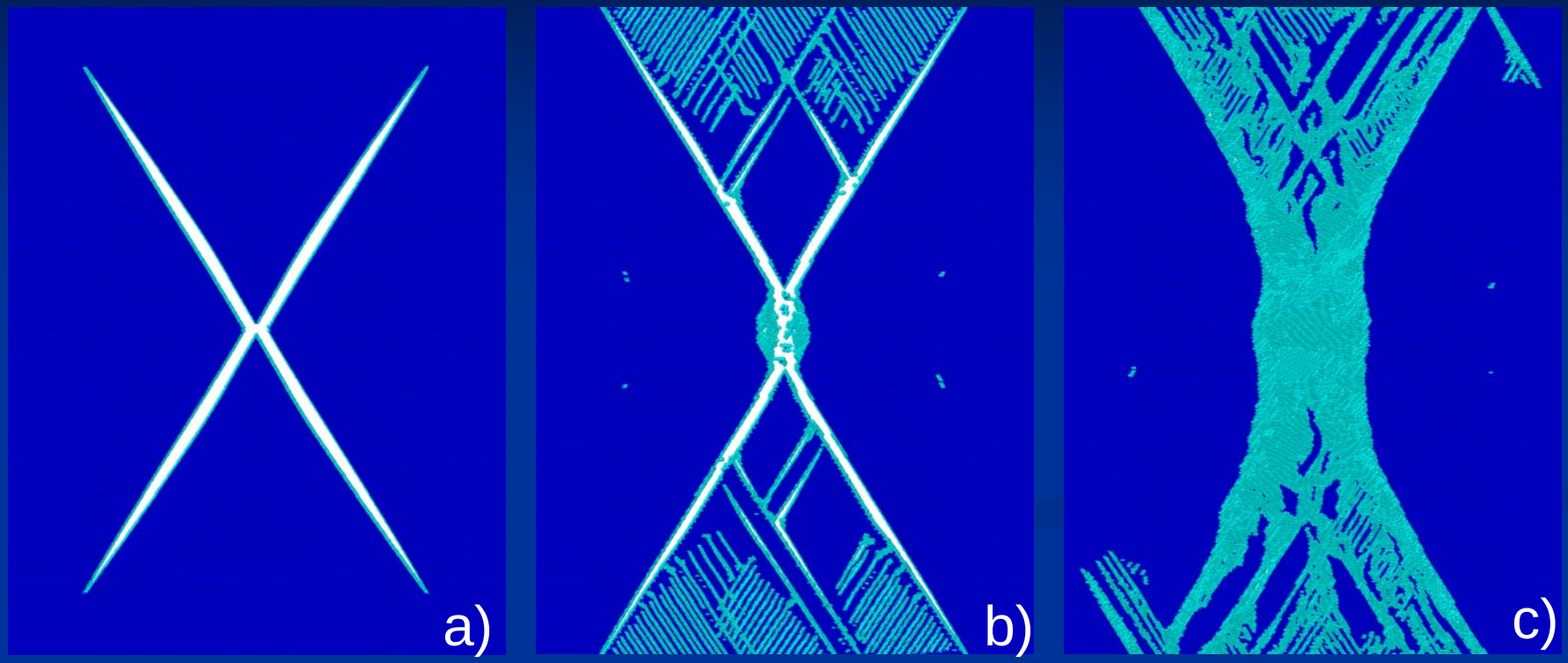
The model

- Triangular crystal lattice
- Shortened Lennard-Jones interaction
- Predefined defects (vacancies)
- Periodic boundary conditions
- Uniaxial loading
- Immediate oxidation of the boundary particles
- Size and strength change for the oxidized particles

Parameters of simulation

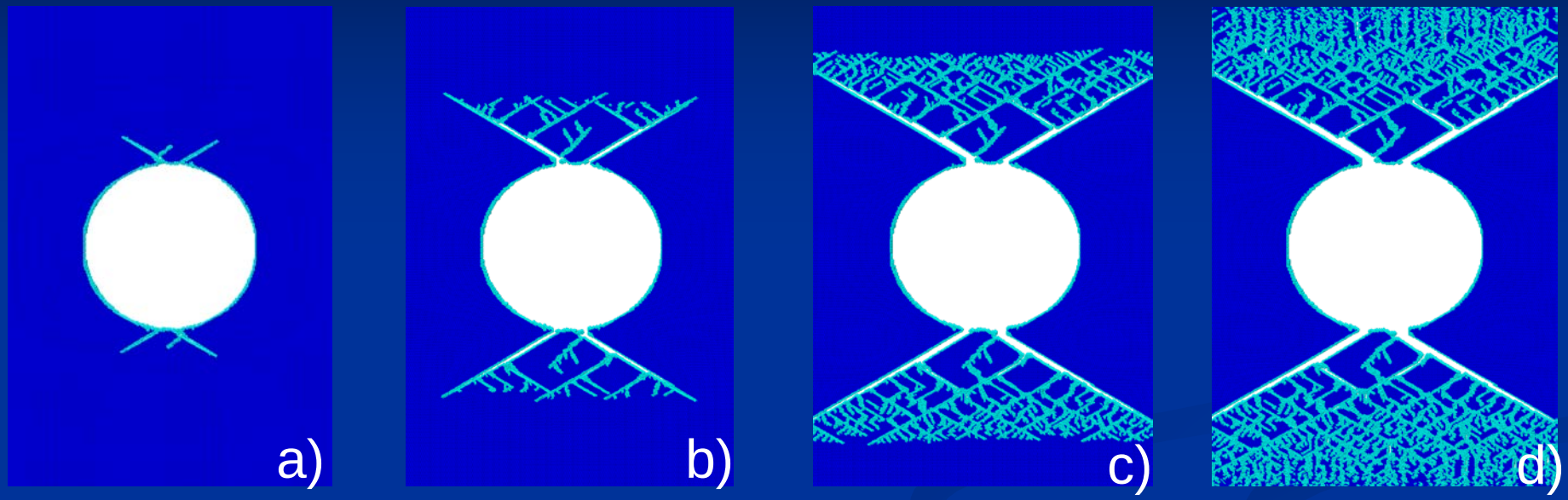
Parameter	Symbol	Value
Number of particles	N	10^5
Cut-off radius	a_{cut}	$1.4a$
Initial velocity deviation	Δv	$0.005v_d$
Integration step	Δt	$0.02T_0$
Maximum strain	ε_{max}	0.15
Strain rate	$\varepsilon_{max}/t_{max}$	$0.002T_0^{-1}$
Oxidation distance		1.2a
Chemical inflation	a_2 / a_1	1.10
Chemical strengthening	Q_2 / Q_1	1/3

Crack initiation from a single vacancy



Comparison of the computational results for different rate of chemical inflation:
a) no chemical reaction, b) 10% chemical inflation, c) 15% chemical inflation

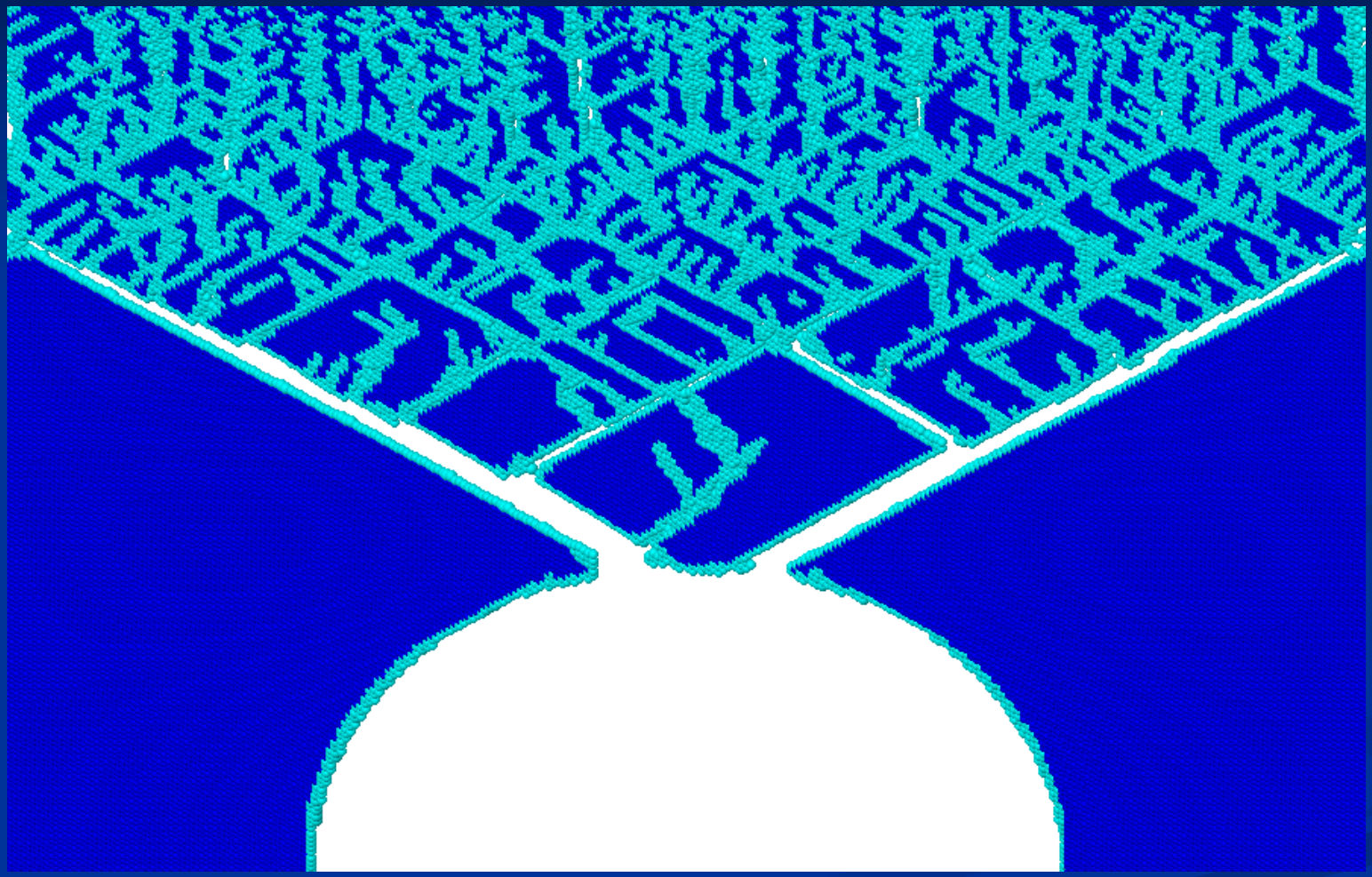
Crack initiation from a circular hole



Sequential stages of extension for the specimen with circular hole:

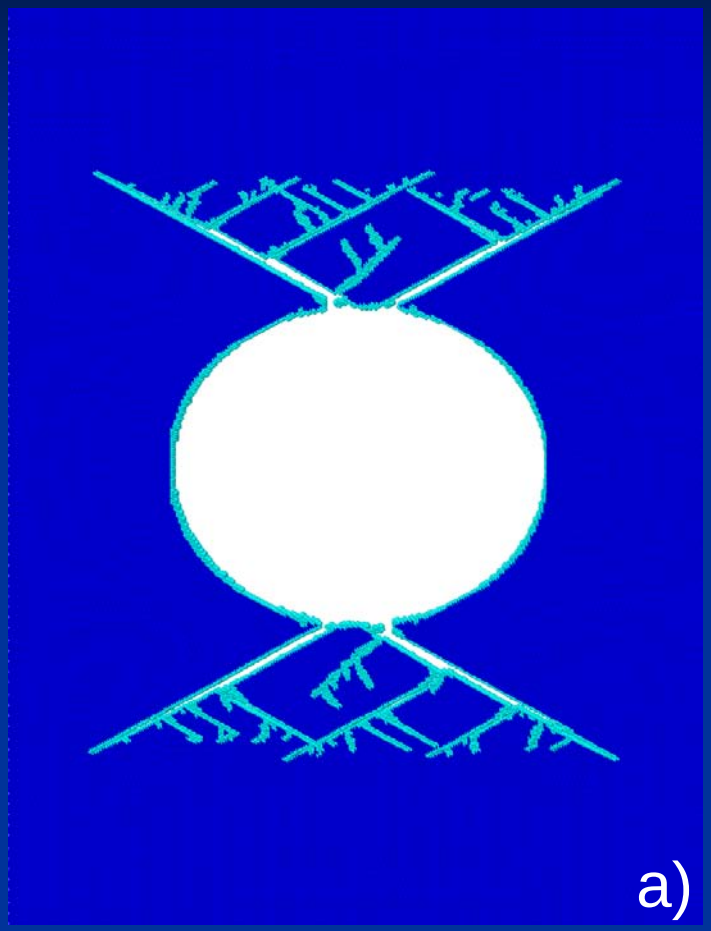
a) $\varepsilon = 7\%$, b) $\varepsilon = 10\%$, c) $\varepsilon = 13\%$, d) $\varepsilon = 15\%$.

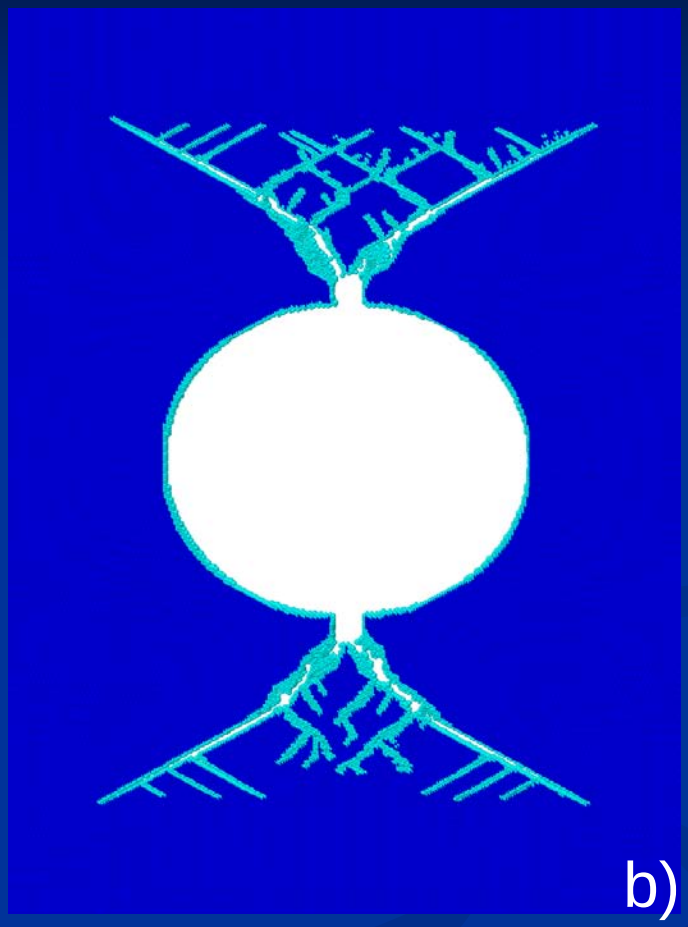
Crack initiation from a circular hole



Zoom-up of the specimen with the developed crack

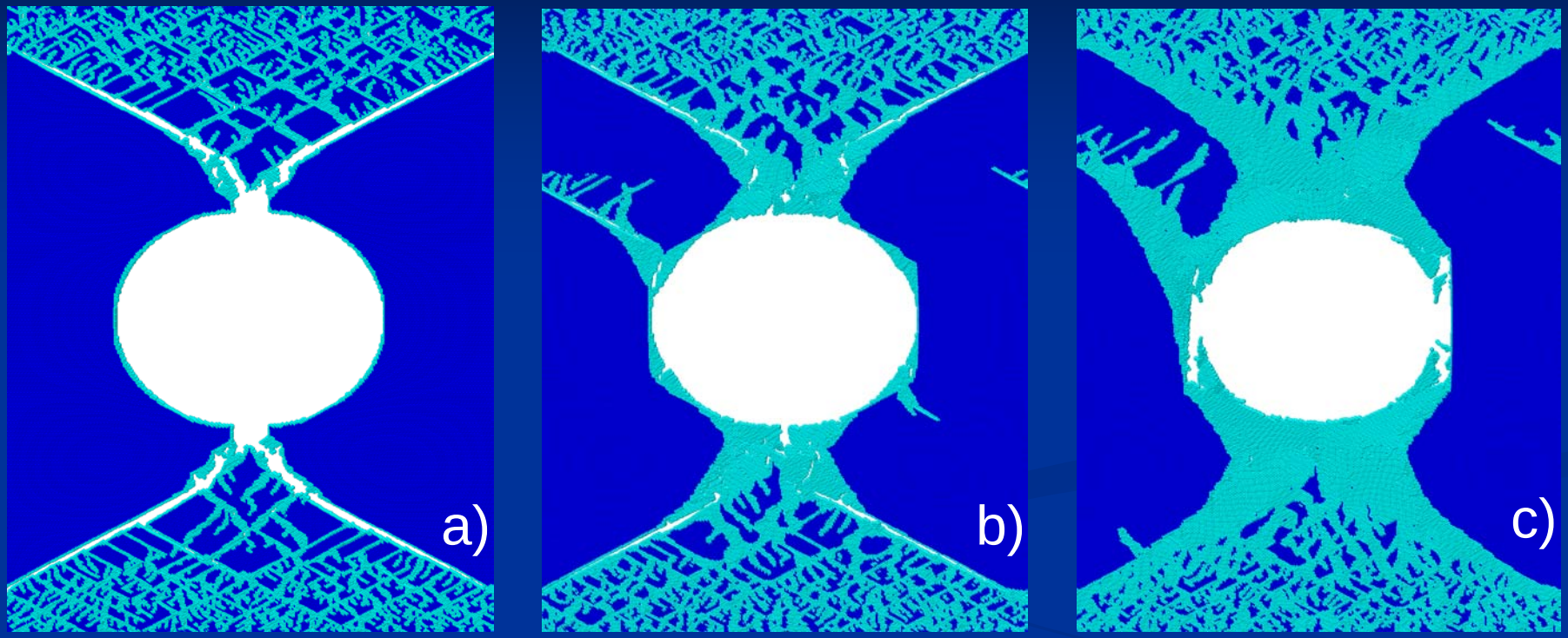
Crack initiation from a circular hole





Comparison of 10% extension for the specimen:
a) without predefined crack, b) with predefined crack.

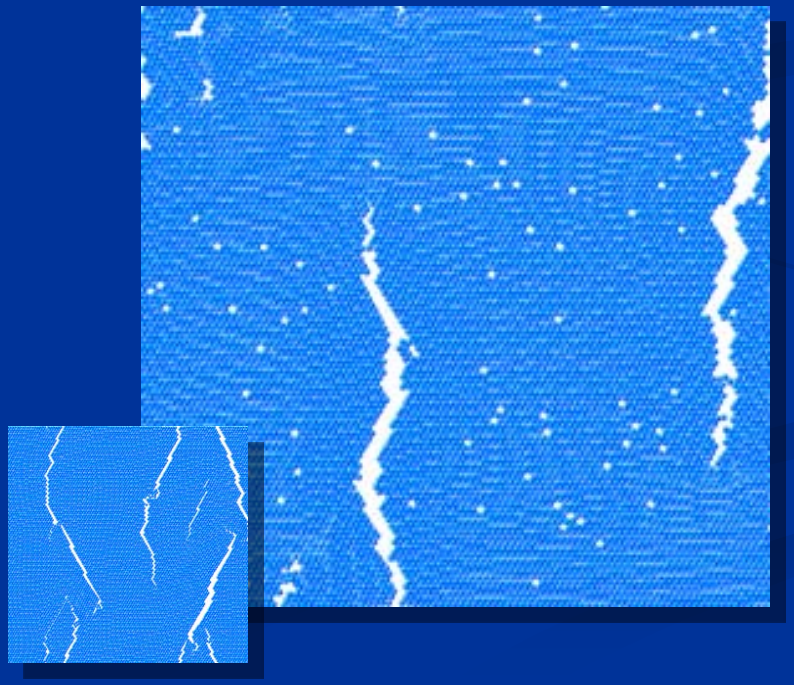
Crack initiation from a circular hole



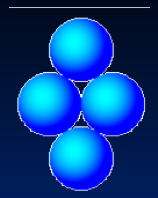
Comparison of results for different chemical inflation:

a) 10%, b) 12%, c) 15%.

Scale dependence of fracture

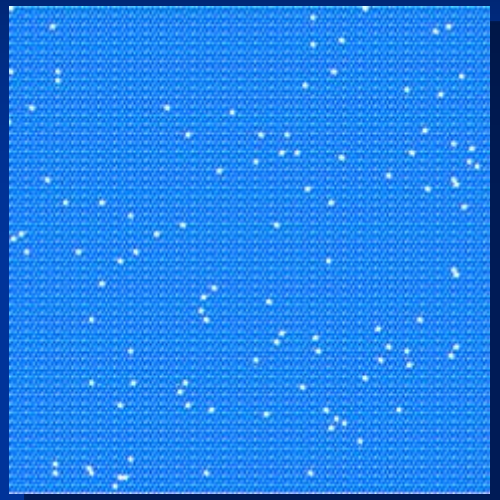


Influence of the defect rate on fracture

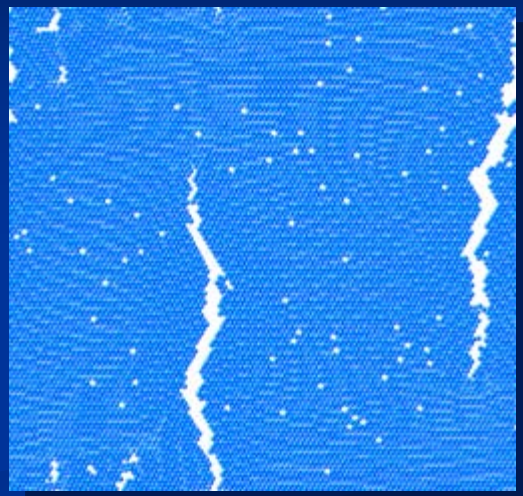


Vertical lattice

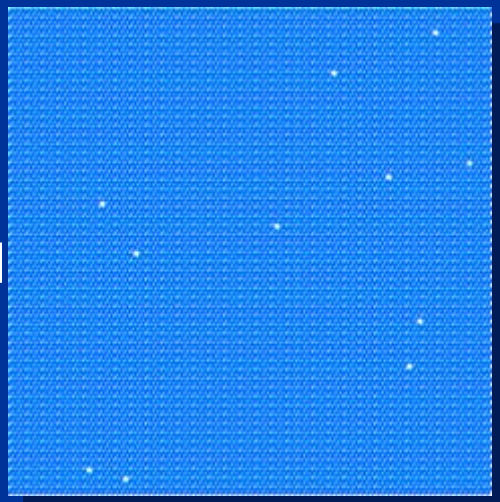
Initial configuration: 1.0% defects



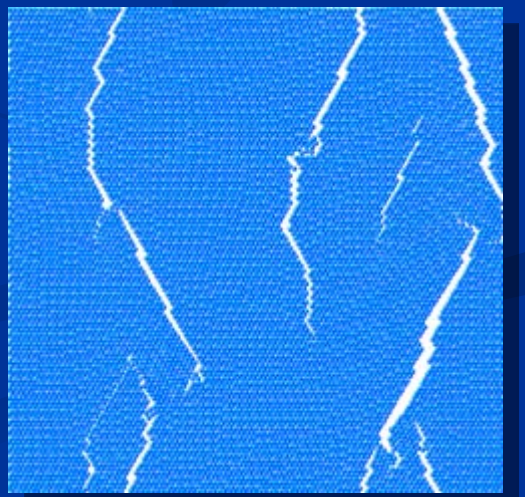
Crack development: 1.0% defects



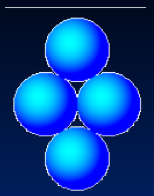
Initial configuration: 0.1% defects



Crack development: 0.1% defects

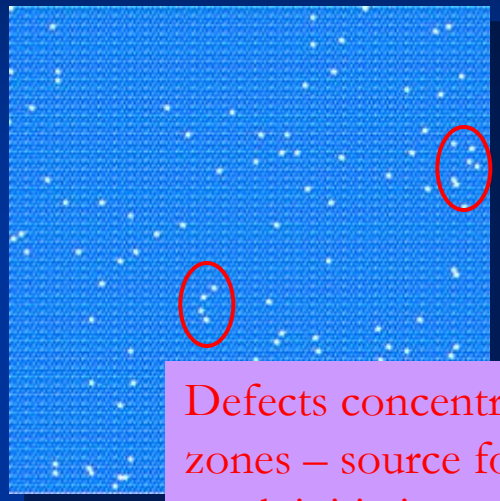


Influence of the defect rate on fracture



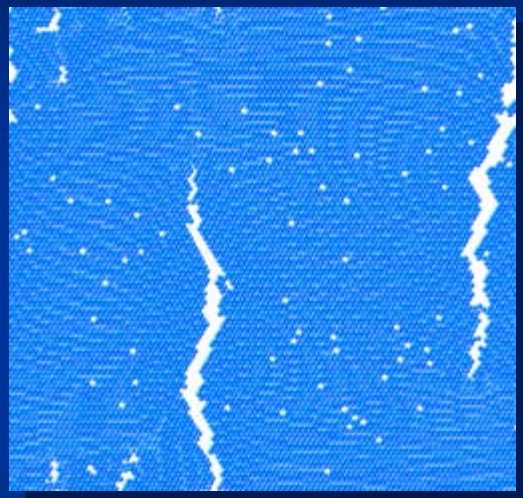
Vertical lattice

Initial configuration: 1.0% defects

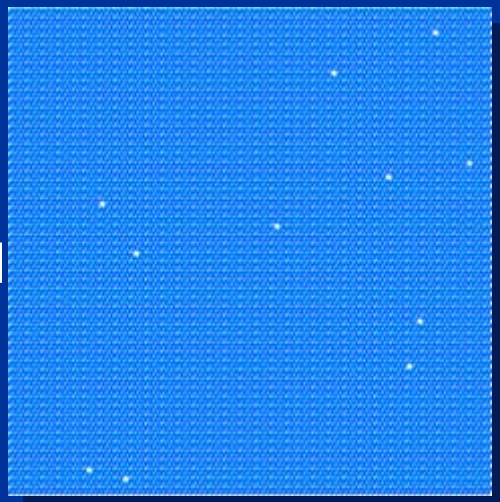


Defects concentration zones – source for the crack initiation

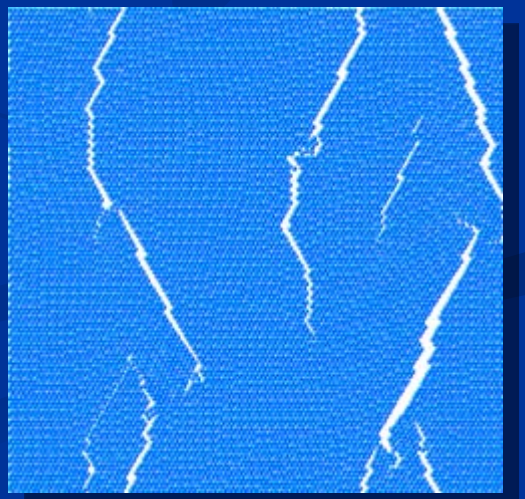
Crack development: 1.0% defects



Initial configuration: 0.1% defects



Crack development: 0.1% defects



Scale dependence of the fracture

Probability determination of the critical deformation

$$\varepsilon(p,N) = \varepsilon_1 + (\varepsilon_2 - \varepsilon_1)\xi(p,N), \qquad \xi(p,N) = 1 - e^{-\frac{1}{2}MNp^2}, \qquad p \ll \frac{1}{M}$$

Critical deformation

for single vacancy

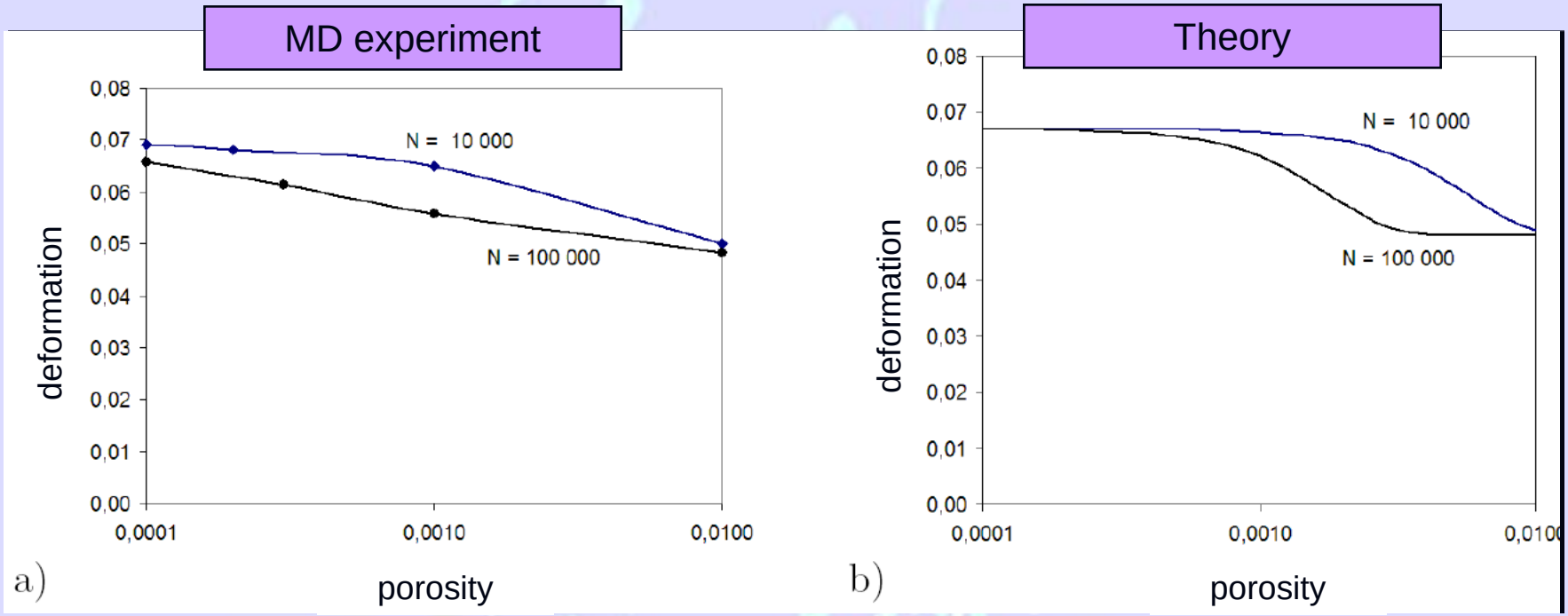
for double vacancy

Probability for the double vacancy

co-ordination number

number of particles

porosity



Concluding remarks

1. Influence of density of vacancies, lattice orientation, loading amplitude, loading period, and interaction characteristics on the fracture process were analyzed.
2. The computations showed that the lattice orientation and type of interaction have great influence on the shape and topology of cracks.
3. The critical deformation is decreasing with the period increase, which is in good correspondence with the numeric and experimental results of material strength dependence on the speed of deformation.
4. The critical deformation for the single crystal material with 1% of vacancies is approximately 70-80% of the critical deformation of a single vacancy.
5. Crack topology in 3D is much more complicated, however in many cases cross-sections of 3D specimens are in good agreement with results of 2D simulation.

Concluding remarks

6. Oxidation substantially stimulates the fracture.
7. The cracks are producing fractal-like branches.
8. If the rate of the chemical inflation is over the break extension then a self-generating process is realized, where the chemical reaction and fracture stimulate each other.
9. For the greater values of the chemical inflation this process can take place without external loading at all, resulting in a very fast oxidation of the whole specimen.
10. Generally there is no similarity in fracture for the specimens of the different size and scale, and therefore a representative volume for the material strength properties does not exist.

Thank you!