Voids and 30000 atoms
~ Molecular dynamics (MD) simulations of ductile fracture ~

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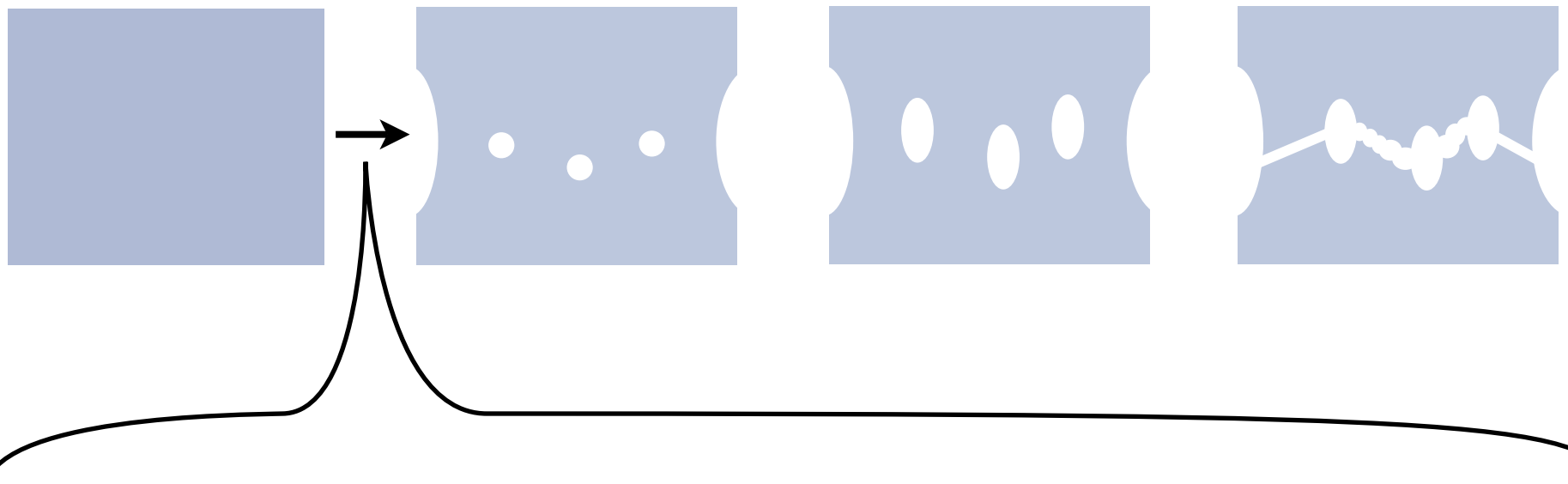
Outline

- Introduction
- Method of molecular-dynamics simulation
- Results & Discussion
  - Single crystal
  - Poly crystal
- Conclusions

Introduction

Ductile fracture

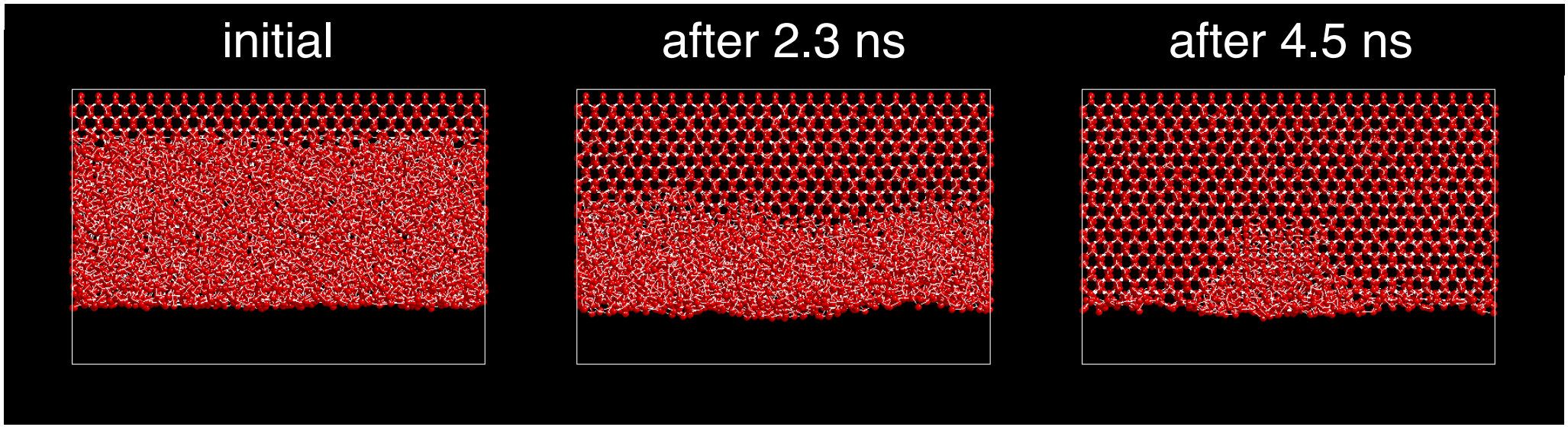


It is impossible to directly observe the process for the generation of voids in atomic scale.

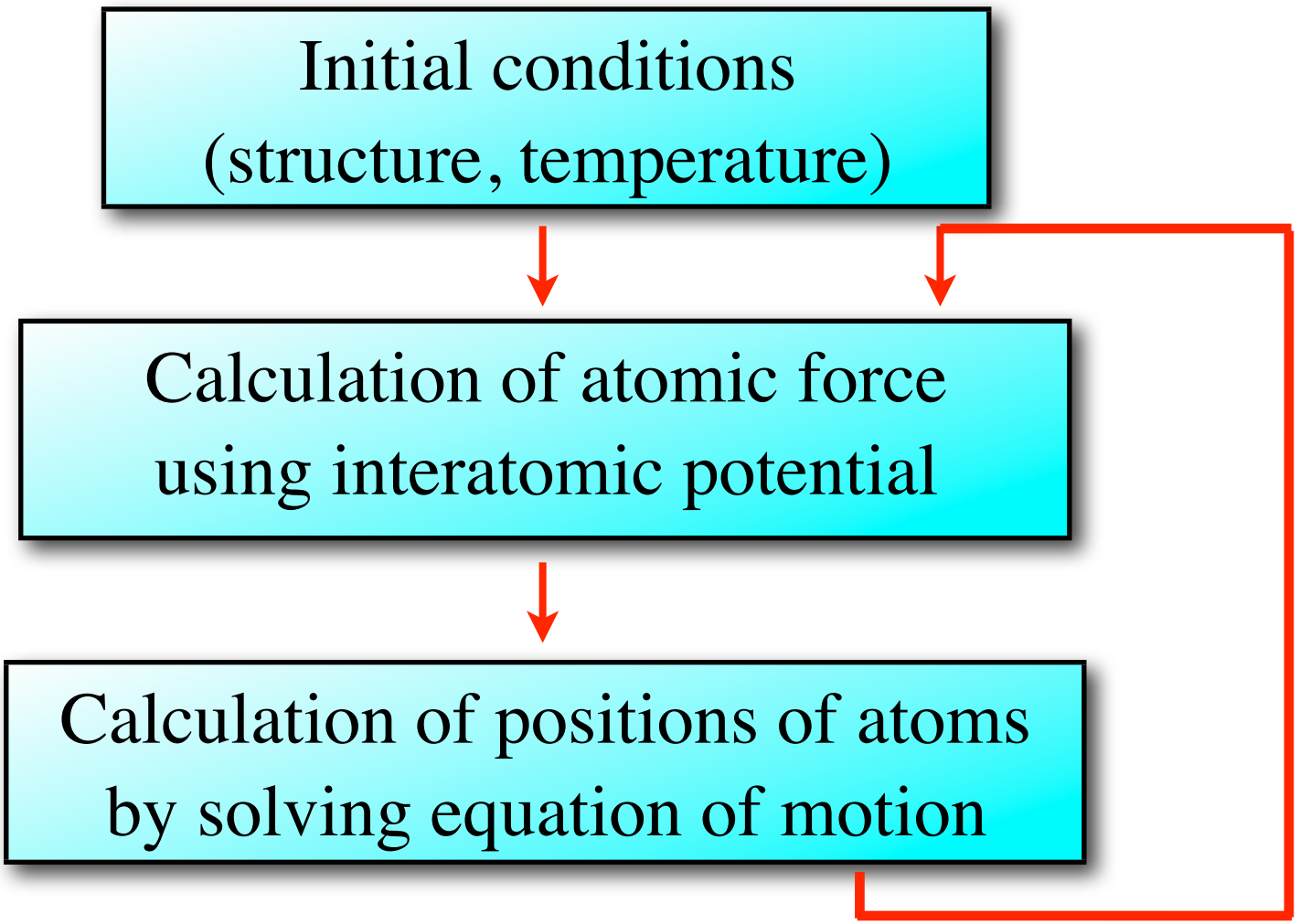
Molecular-dynamics simulation

- a powerful tool for analyzing the crystallization processes in atomic scale.

For example, Growth process of silicon....



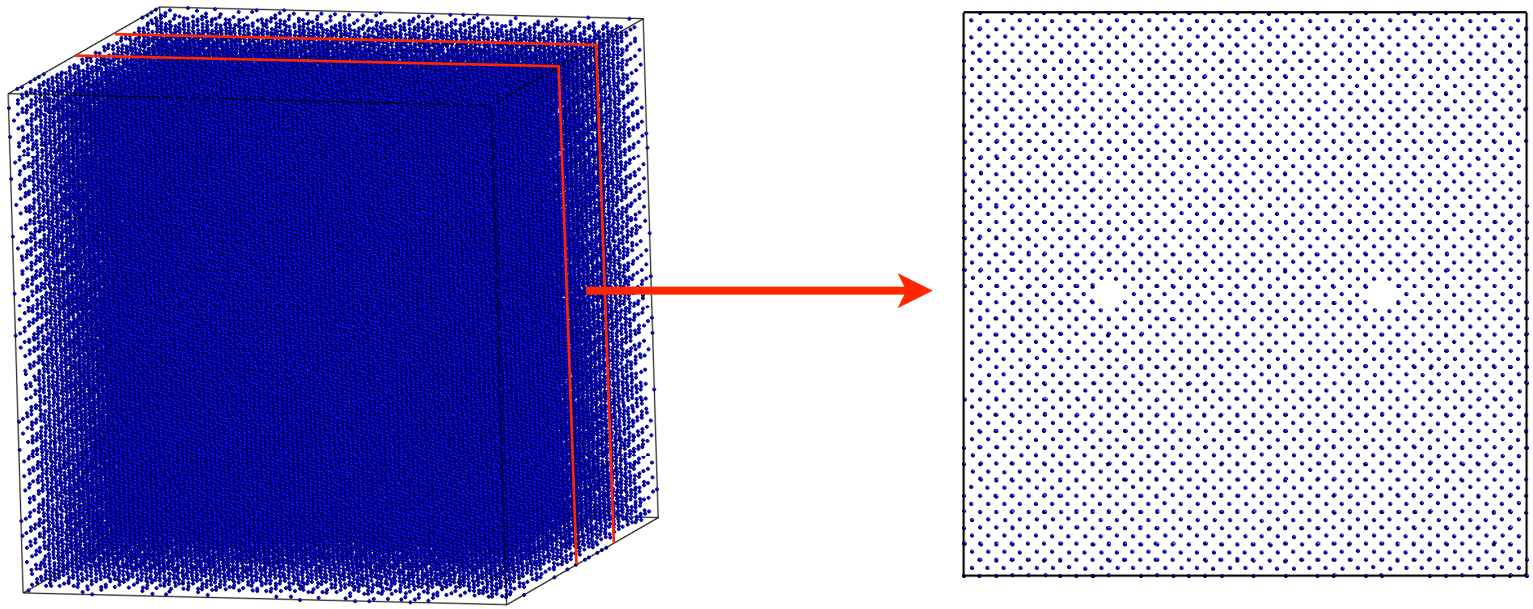
Method of molecular-dynamics simulation



Method of molecular-dynamics simulation

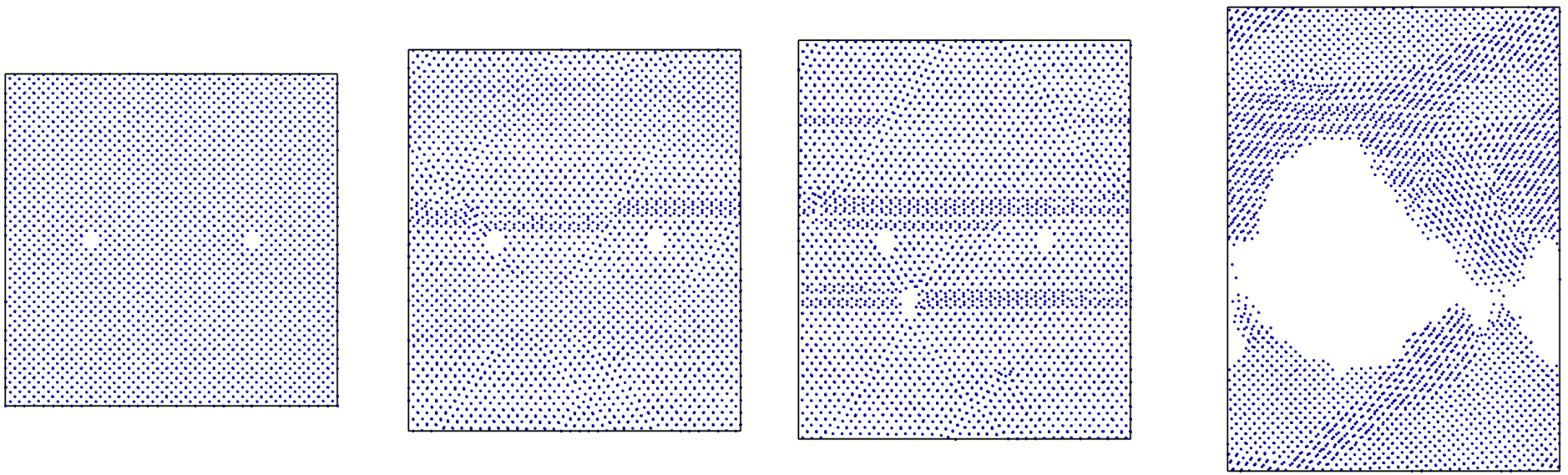
- Single crystal including vacancies
- Poly crystal (including grain boundary)

Single crystal of BCC Fe including vacancies

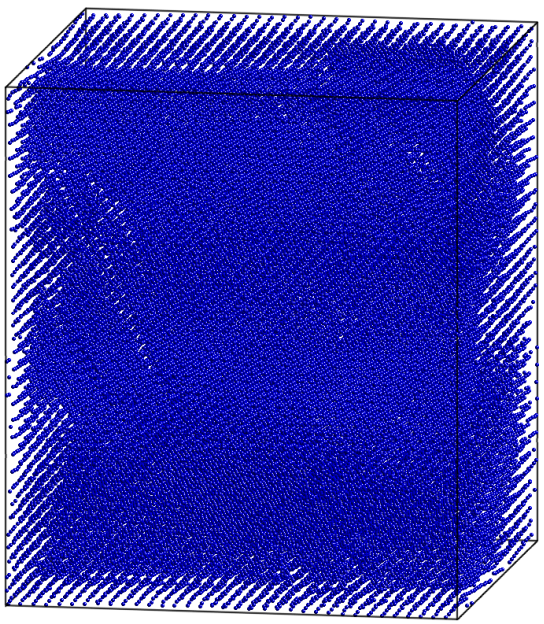


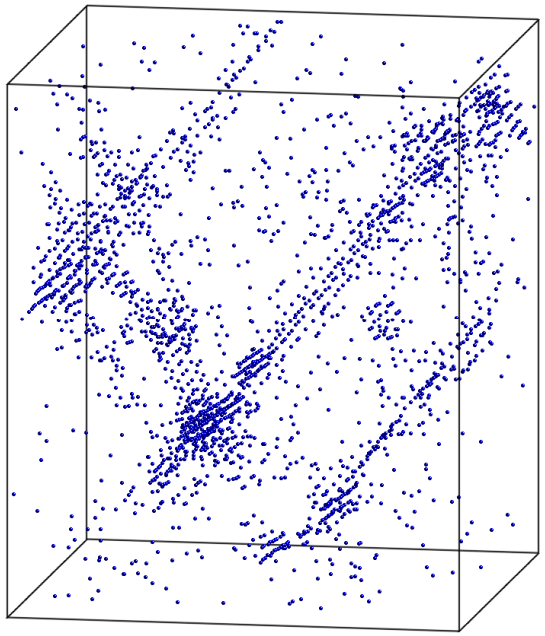
- MD cell : 100 x 100 x 100 $Å^3$
- 85,738 atoms
- Periodic boundary conditions for X,Y and Z direction
- Finnis-Sinclair potential

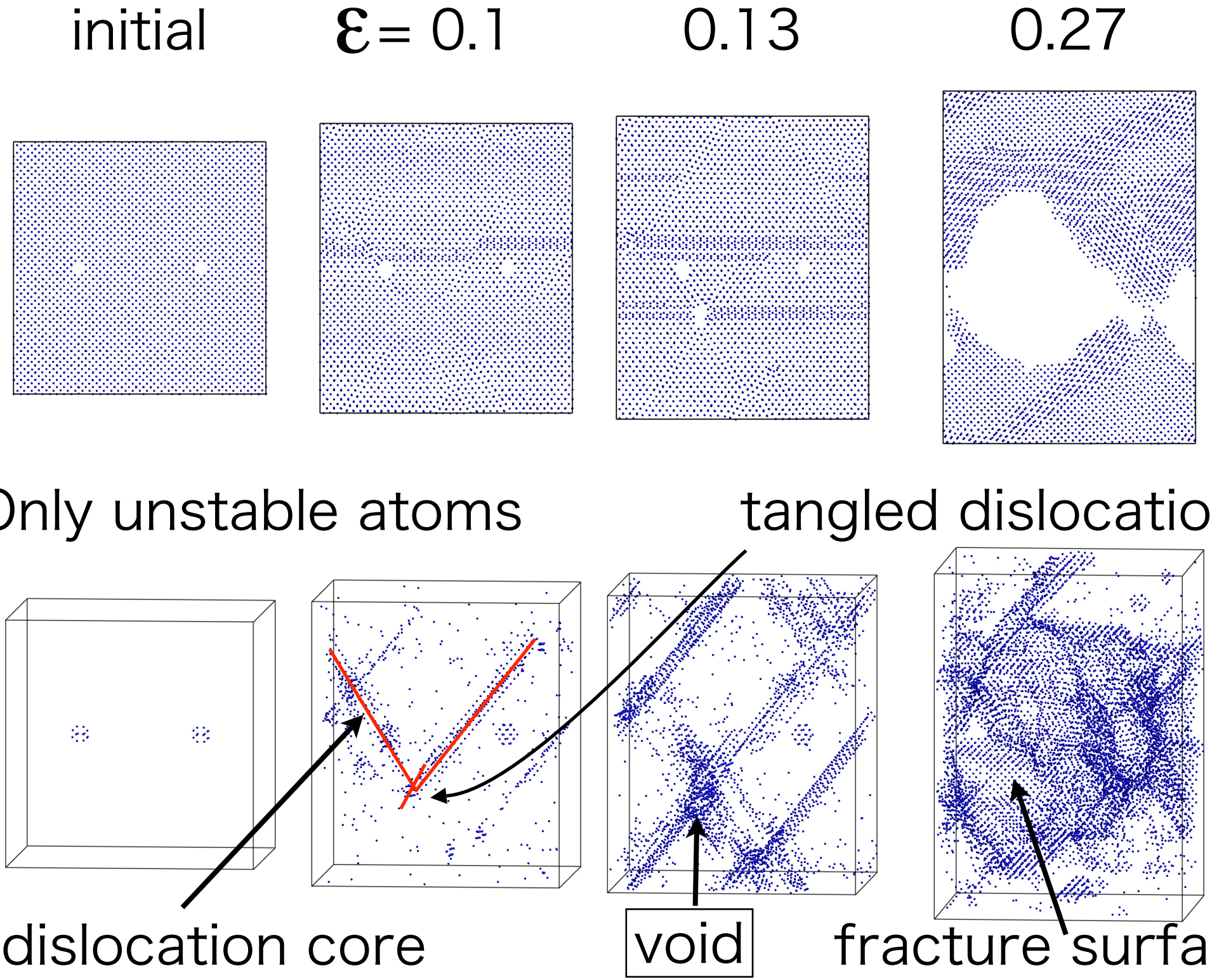
initial $\varepsilon = 0.1$ 0.13 0.27

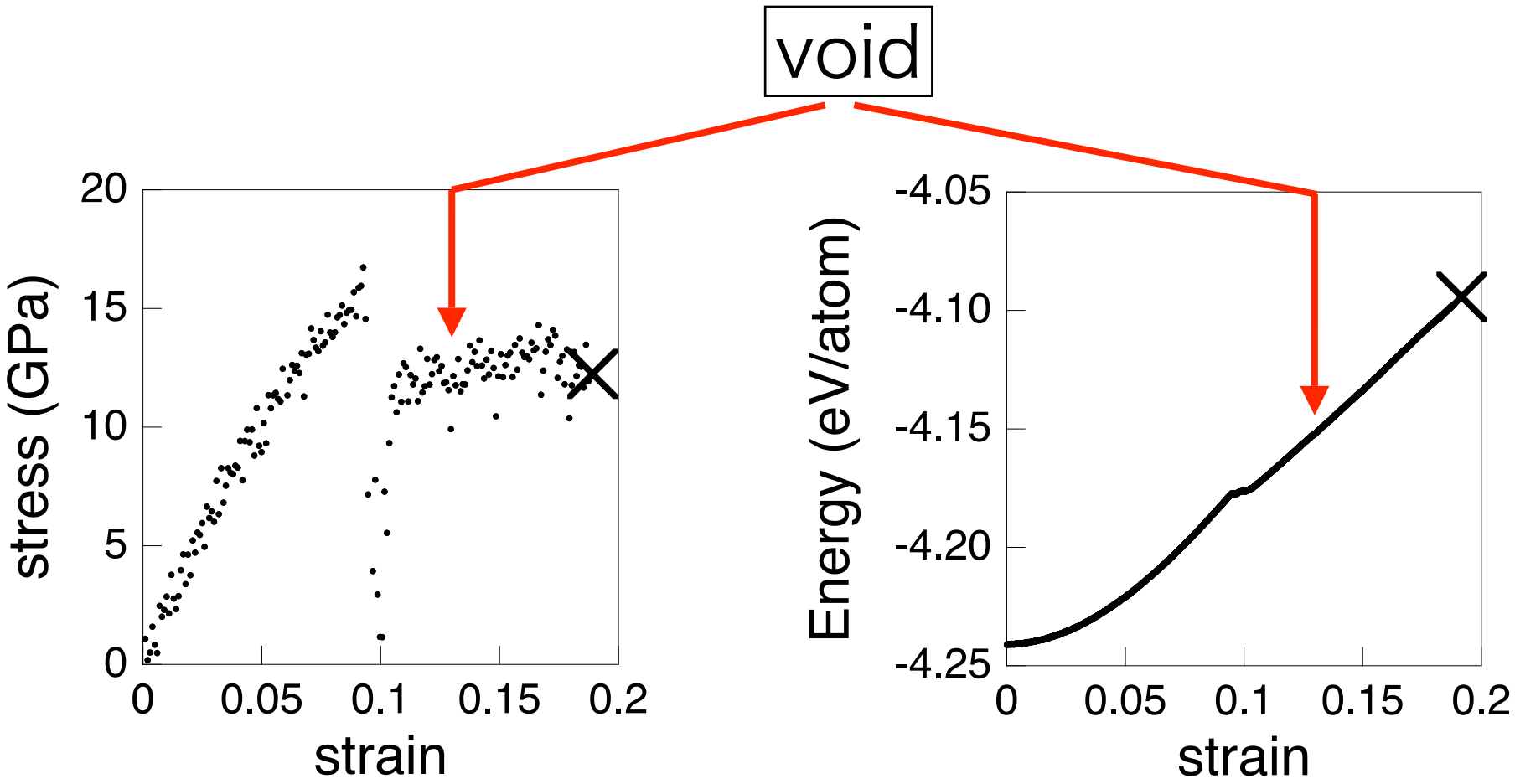


Only unstable atoms were monitored...

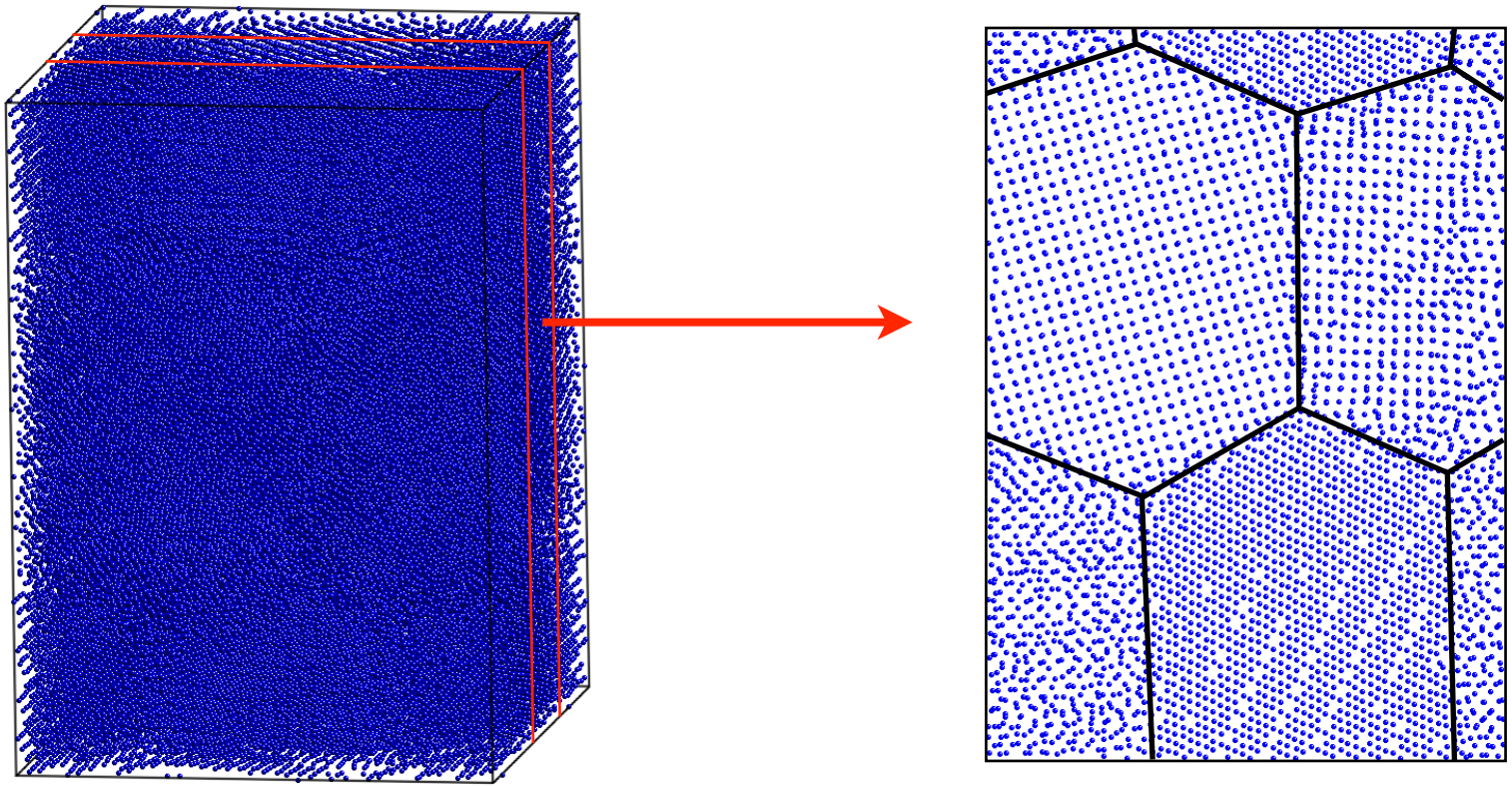




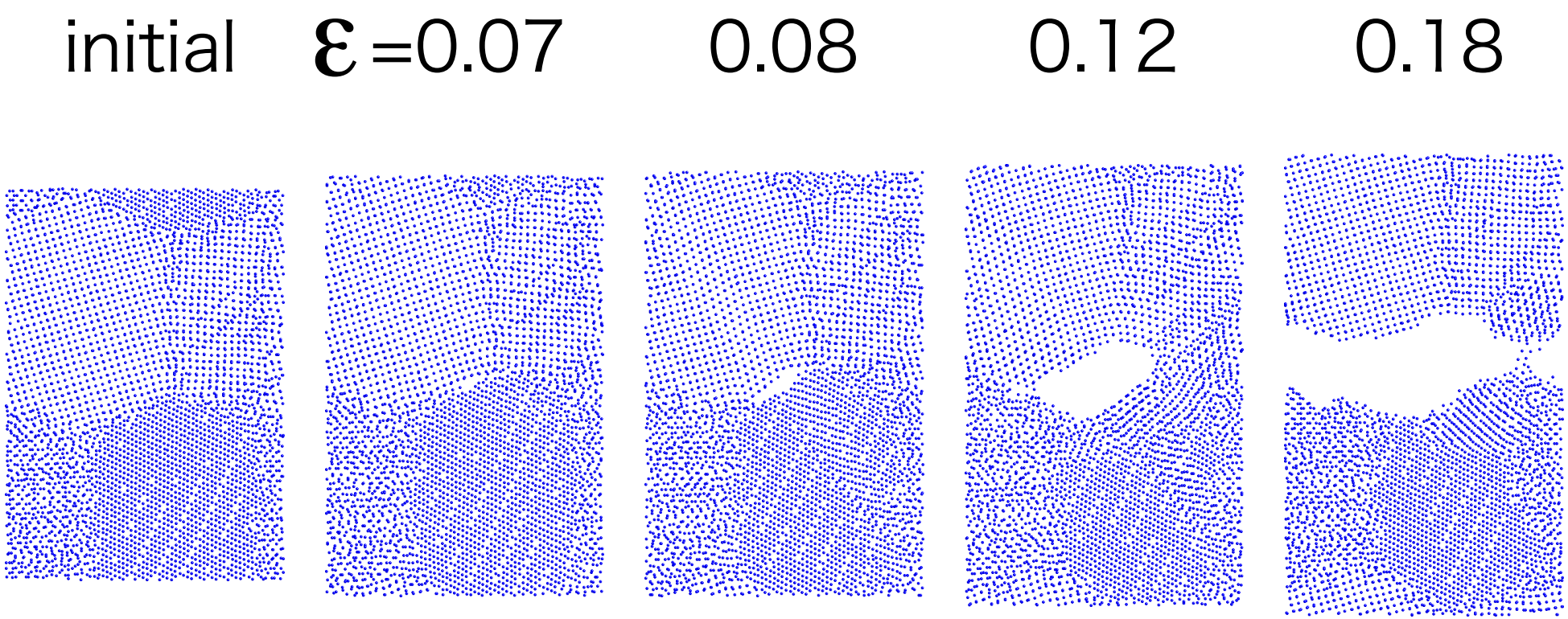

initial
ε= 0.1
0.13
0.27
Only unstable atoms
tangled dislocation
dislocation core
void
fracture surface


void
stress (GPa)
20
15
10
5
0
0
0.05
0.1
0.15
0.2
strain
Energy (eV/atom)
-4.05
-4.10
-4.15
-4.20
-4.25
0
0.05
0.1
0.15
0.2
strain

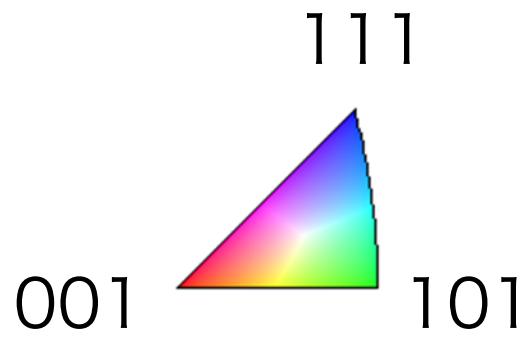
Single crystal of BCC Fe

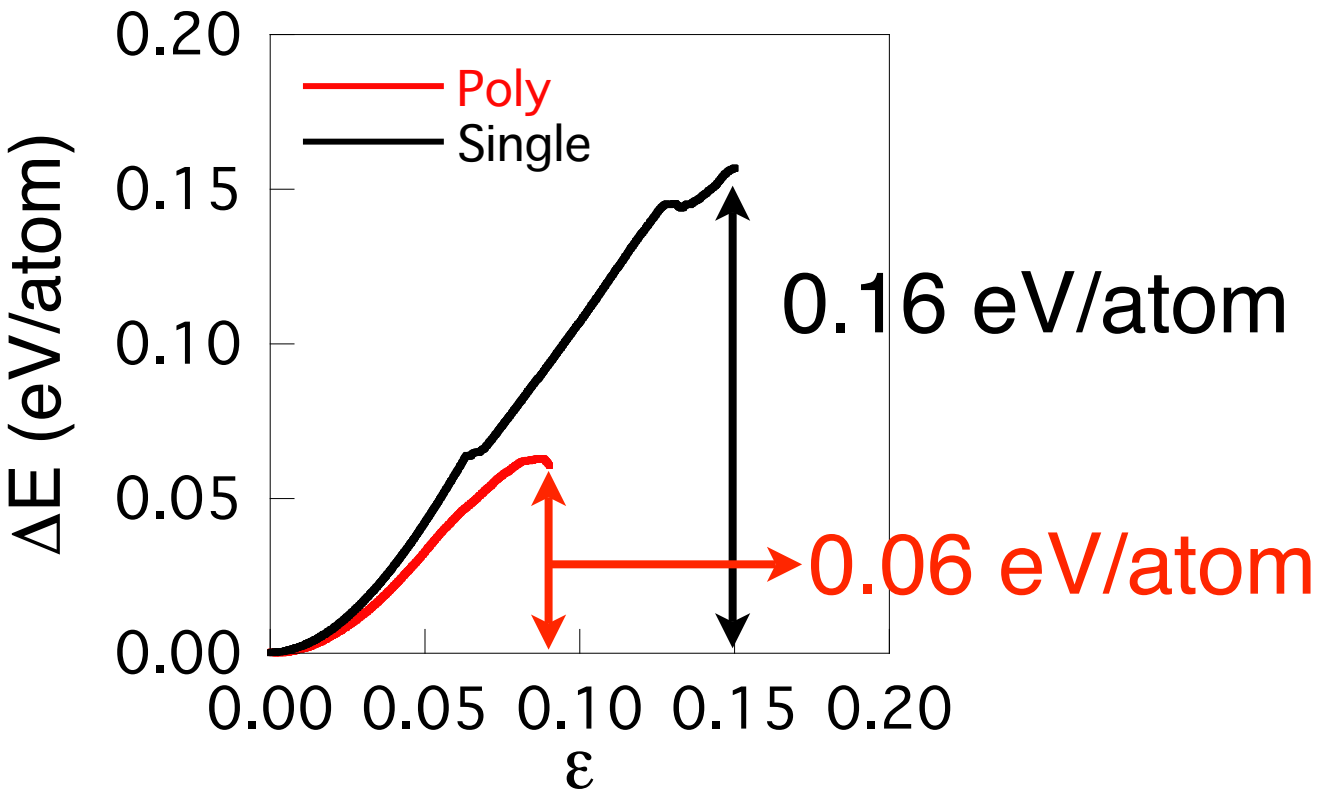


- MD cell : 81 x 94 x 115 $Å^3$
- 73,058 atoms
- Periodic boundary conditions for X,Y and Z direction
- Finnis-Sinclair potential


initial
ε=0.07
0.08
0.12
0.18

In the experiment...




0.20
0.15
0.10
0.05
0.00
ΔE (eV/atom)
Poly
Single
0.16 eV/atom
0.06 eV/atom
0.00 0.05 0.10 0.15 0.20
ε

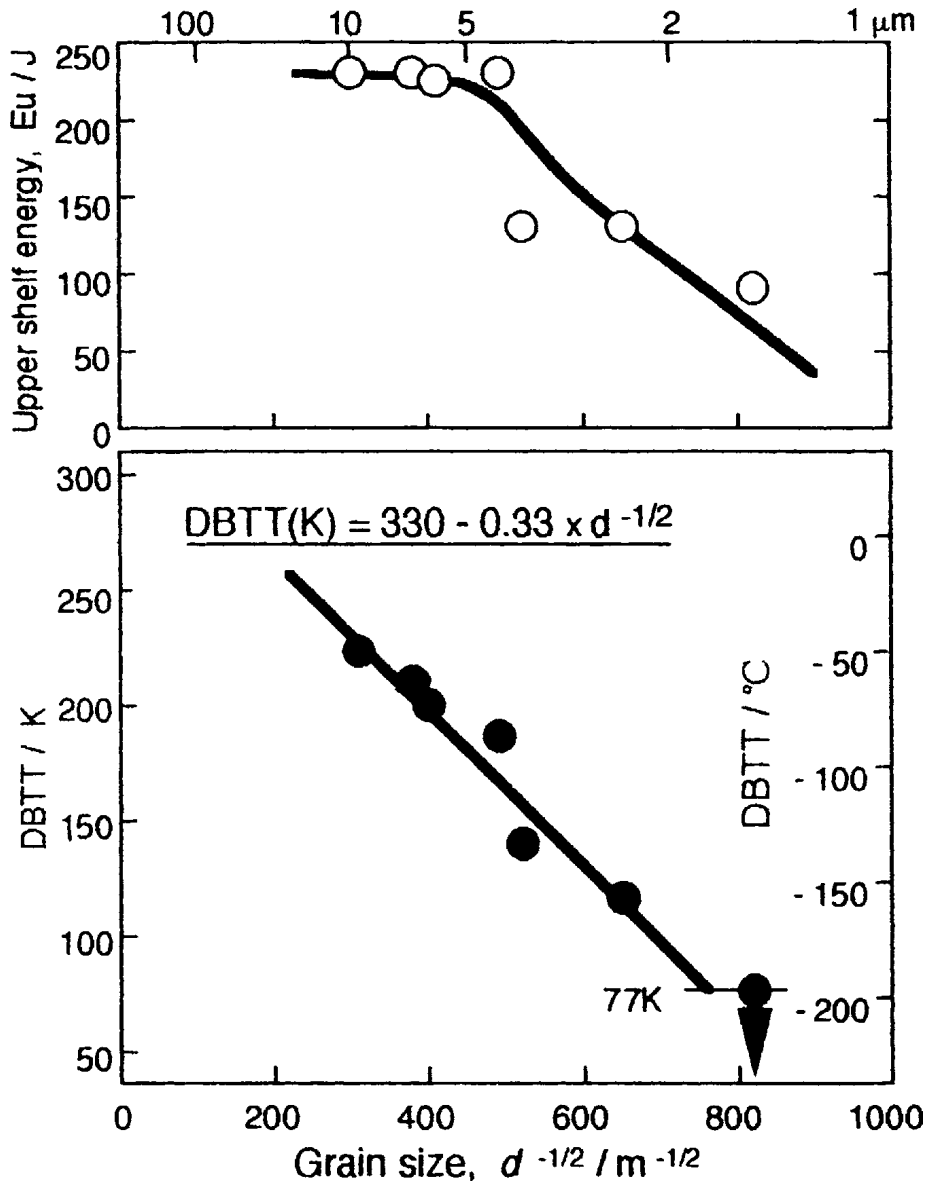


Fig. 9. Changes in upper shelf energy and DBTT as a function of grainsize.

Conclusions

We have performed MD simulation of ductile fracture...

- In the case of single crystal, a void was generated from a position tangled with dislocations.
- In the case of poly crystal, a void was generated from grain boundary.