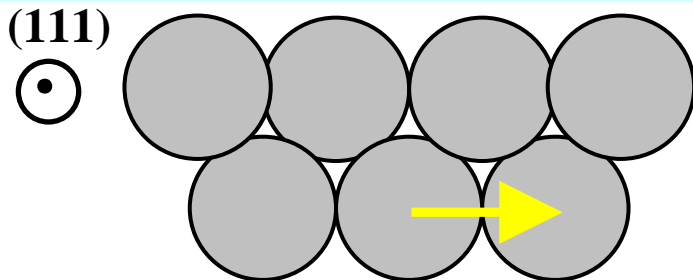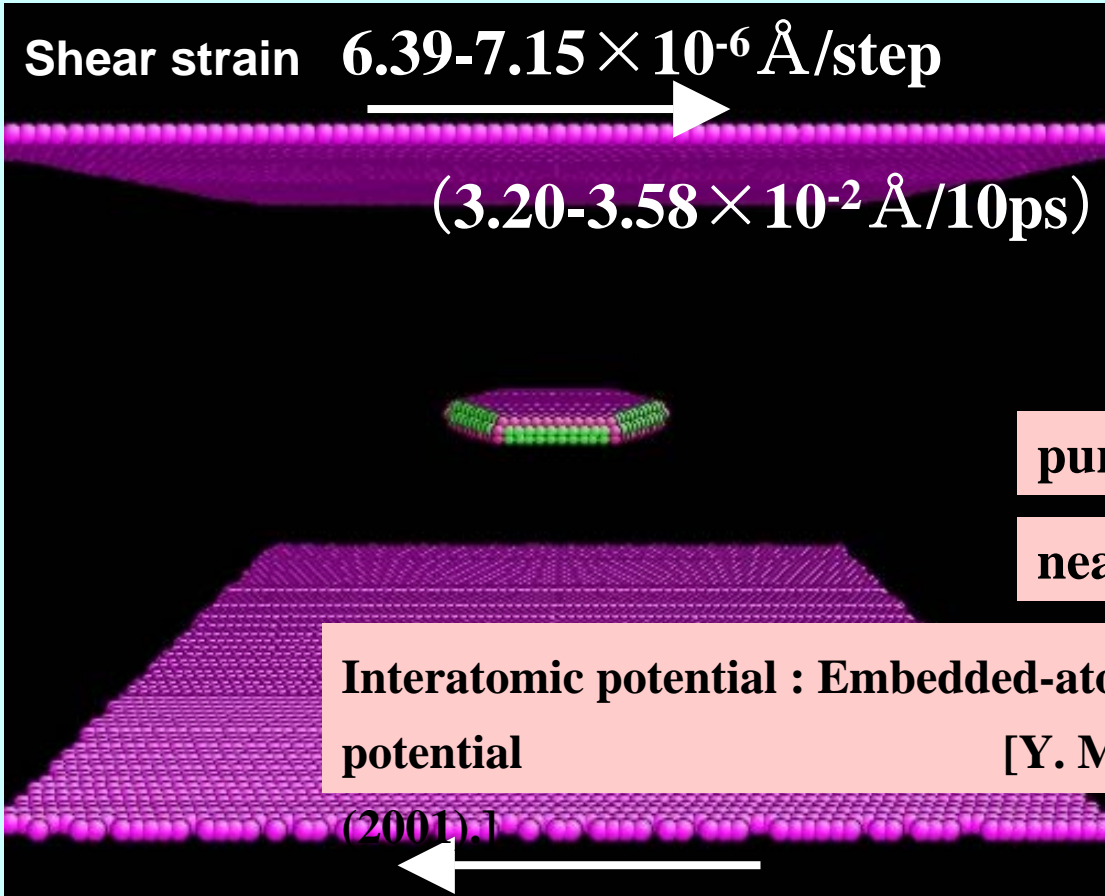# Molecular dynamics study on radiation hardening and fracture processes in FCC metals
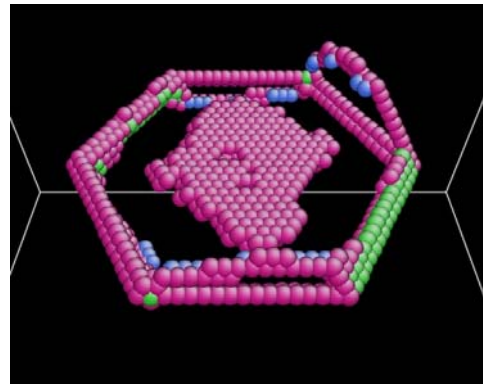
Hideo Kaburaki (JAERI)

Effect of external shear stress for unfaulting
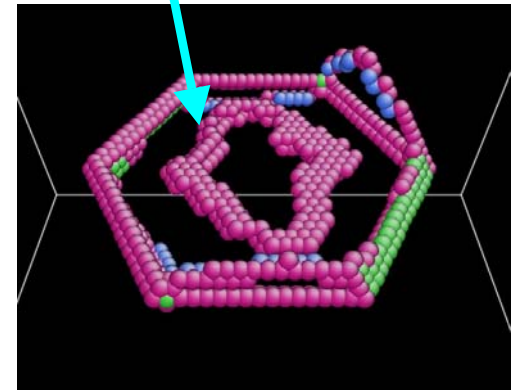
Shear strain $6.39\text{-}7.15 \times 10^{-6}$ Å/step

$(3.20\text{-}3.58 \times 10^{-2}$ Å/10ps$)$

$[1\underline{1}1]$ Z $[\underline{1}12]$ Y $[110]$ x

pure alminium

nearly 380,000 atoms

Interatomic potential : Embedded-atom method (EAM) potential   [Y. Mishin *et al.*, *PRB* (2001).]

(111)
⊙

For 80ps (40,000steps)

Unfaulting process of H721 vacancy loop

Partial dislocation loop

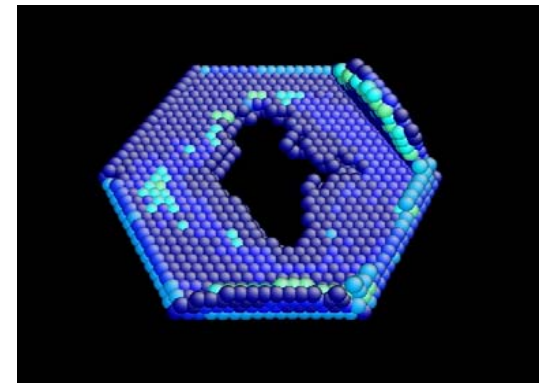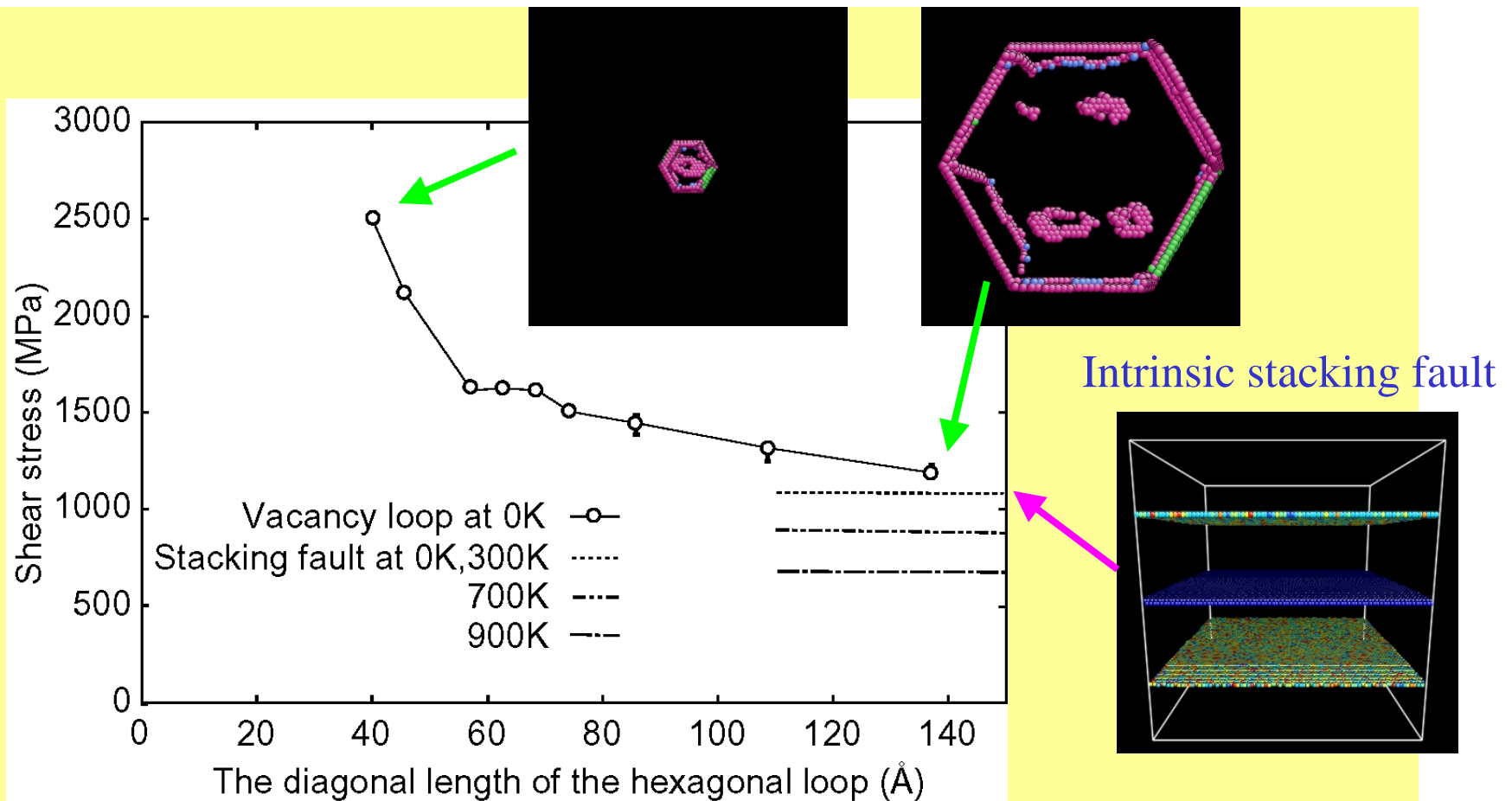**Coordination number representation**

Central symmetry parameter representation
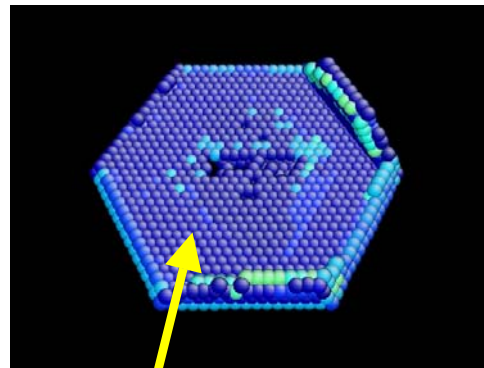
Stacking fault

Results of unfaulting critical shear stress for vacancy loops

Intrinsic stacking fault

Vacancy loop at 0K —○—
Stacking fault at 0K,300K ········
700K —·—
900K —··—

Shear stress (MPa)

The diagonal length of the hexagonal loop (Å)

Hardening process --- the interaction of an edge dislocation with a hexagonal interstitial dislocation loop
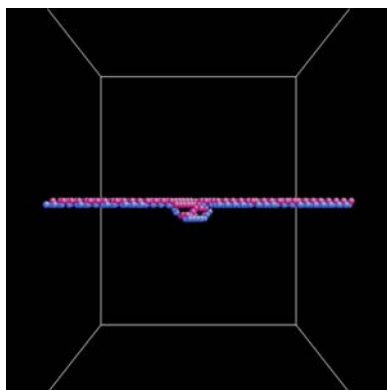
Simulation System

mixed free

$[1\underline{1}1]$ $[\underline{1}12]$

Z Y

$[110]$

x

$170\,\text{Å}$ $10\,\text{Å}$

$120\,\text{Å}$

periodic

$200\,\text{Å}$ **Number of atoms   3.8×10⁵**
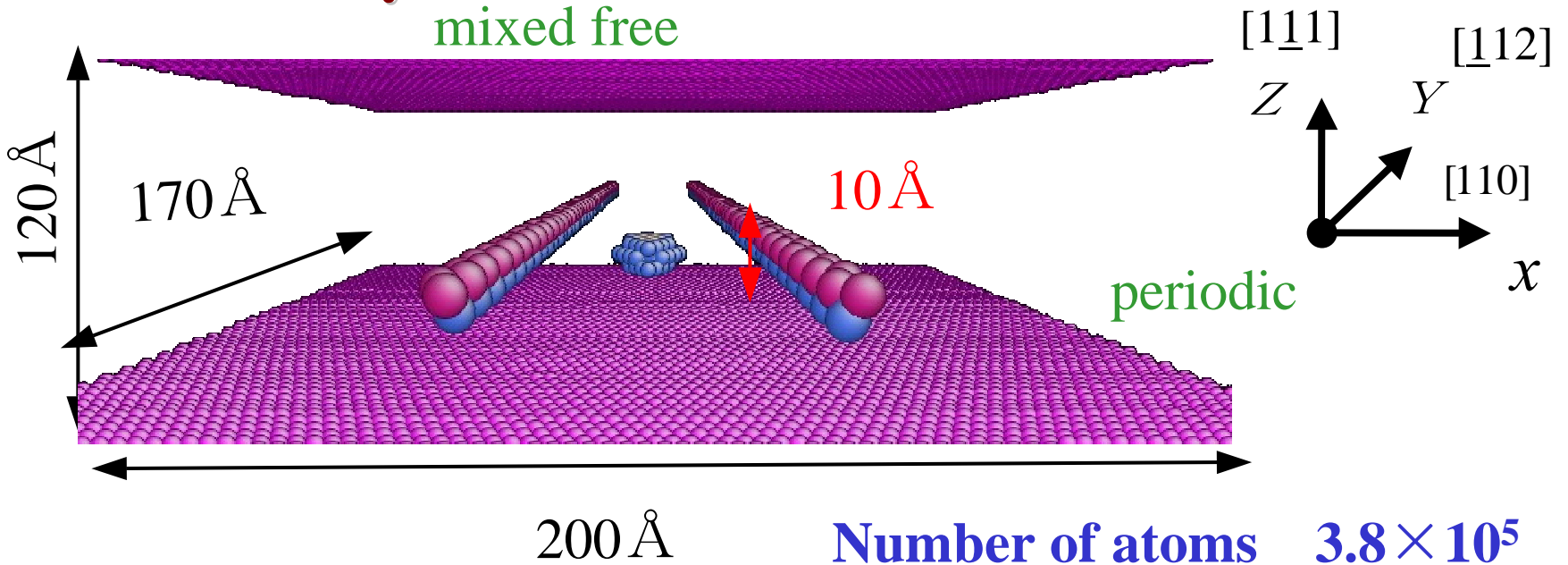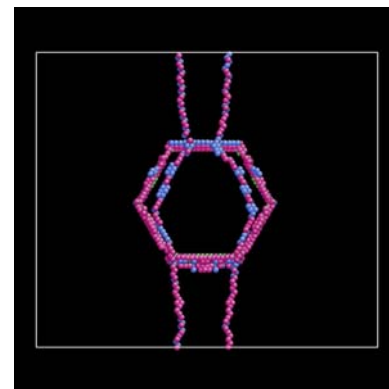
Interatomic potential : Embedded-atom method (EAM)
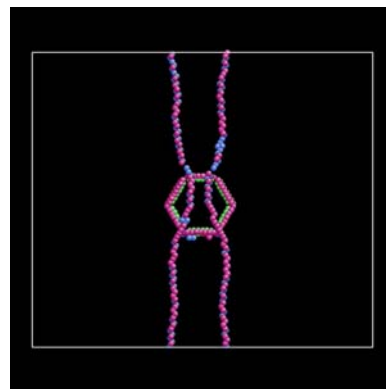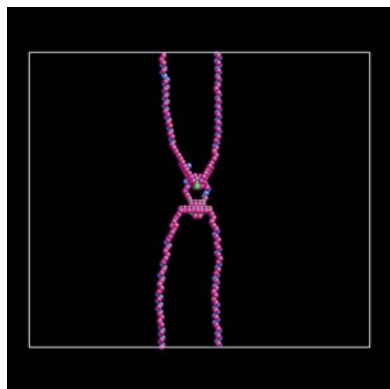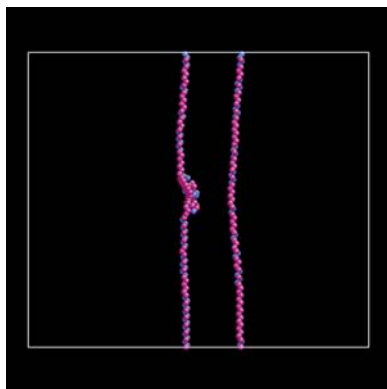
potential   **Cu, Al**   [Y. Mishin *et al., PRB* (2001).]

$$E_{tot} = \frac{1}{2}\sum_{ij} V(r_{ij}) + \sum_i F(\overline{\rho}_i)$$

V: Pair potential
F: Embedding energy

Pinning structure formed due to the interaction of an edge dislocation and an interstitial cluster in Cu
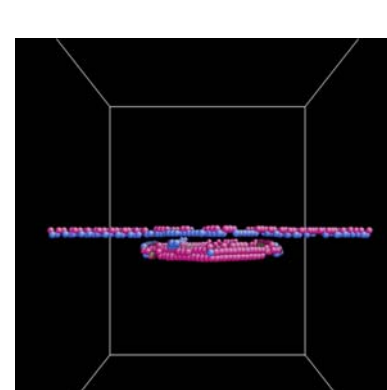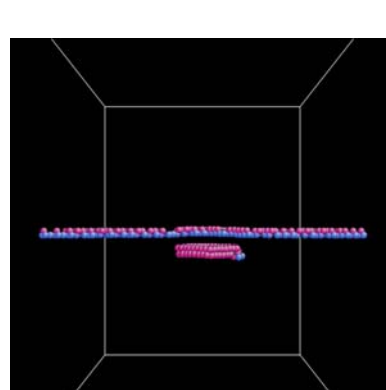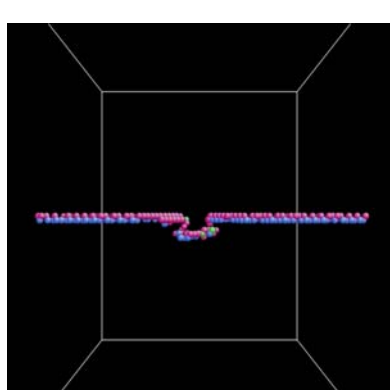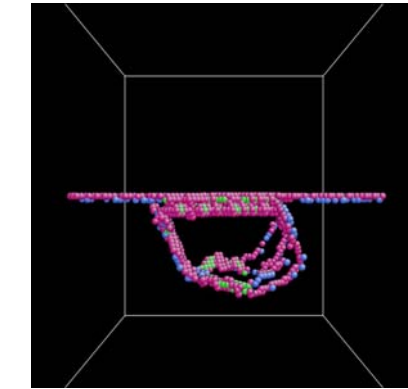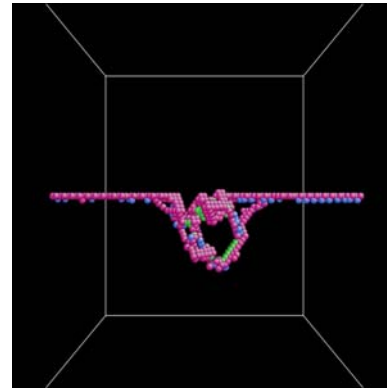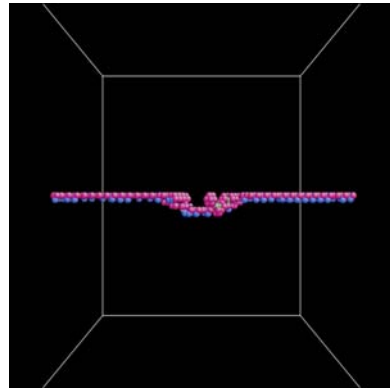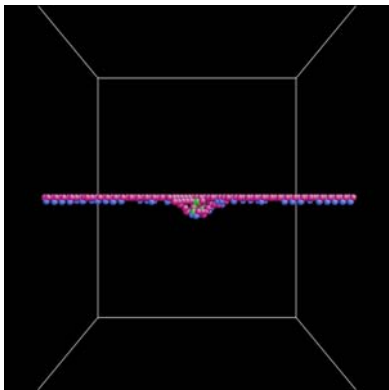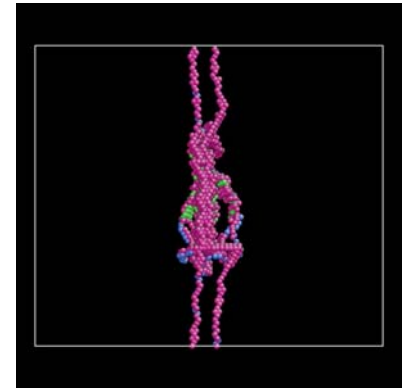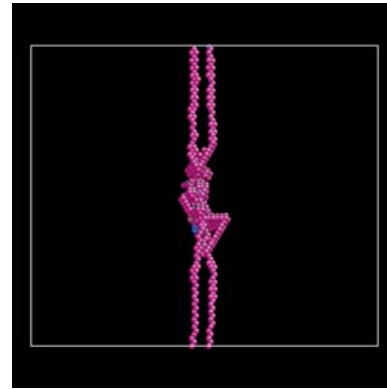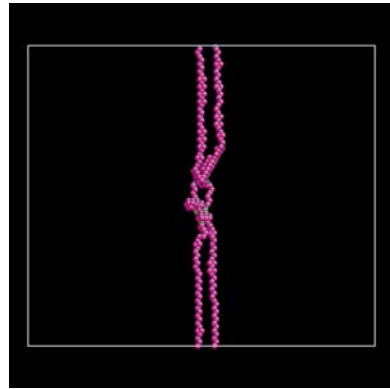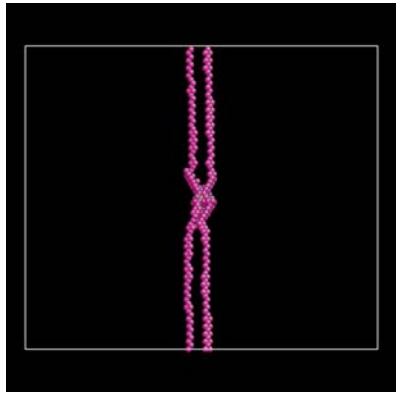

H007   H037   H169   H721

Pinning structure formed due to the interaction of an edge dislocation and an interstitial cluster in Al
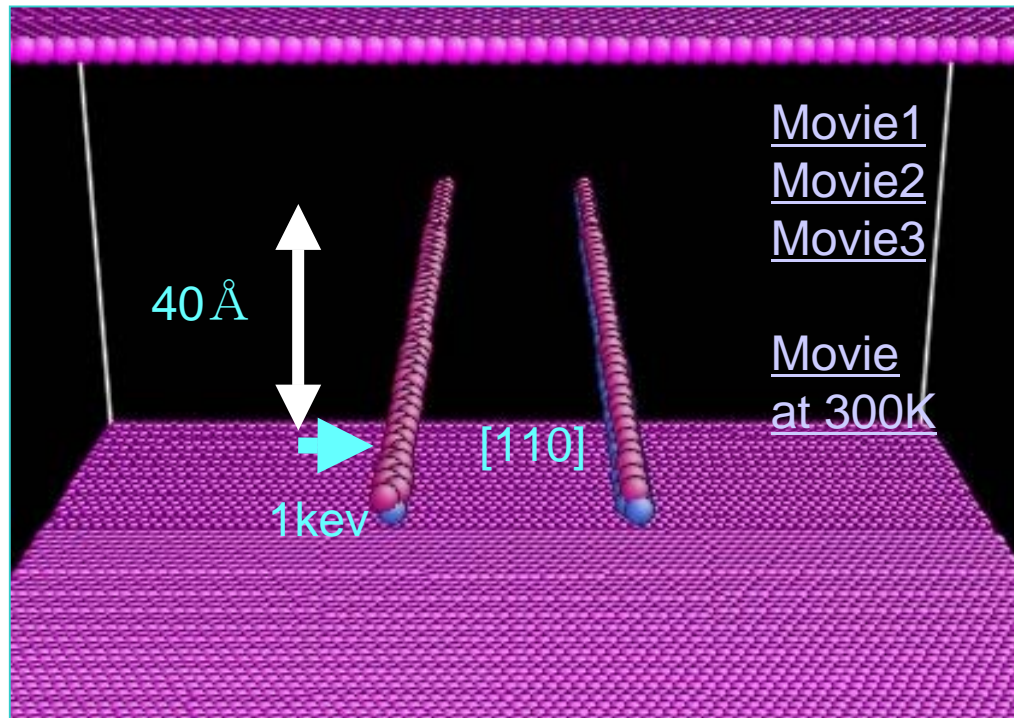

H007 **H037** **H169** **H721**

A molecular dynamics study on displacement cascades in the strain field of an edge dislocation in Cu
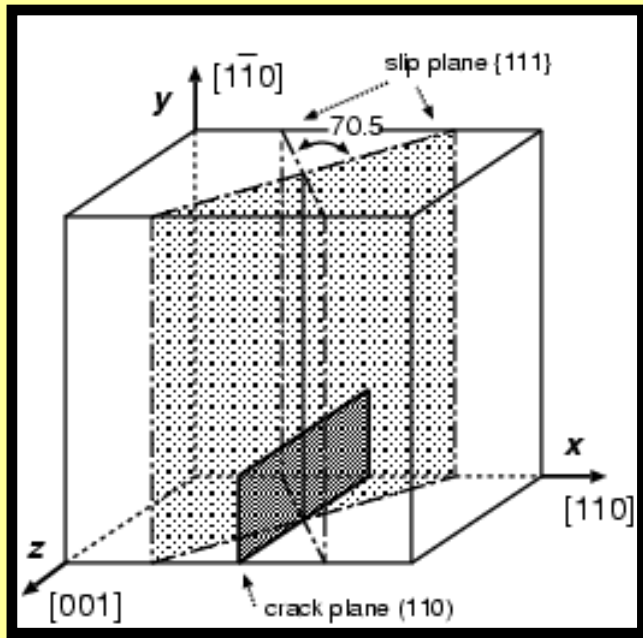

$205 \times 177 \times 125 \text{Å}$

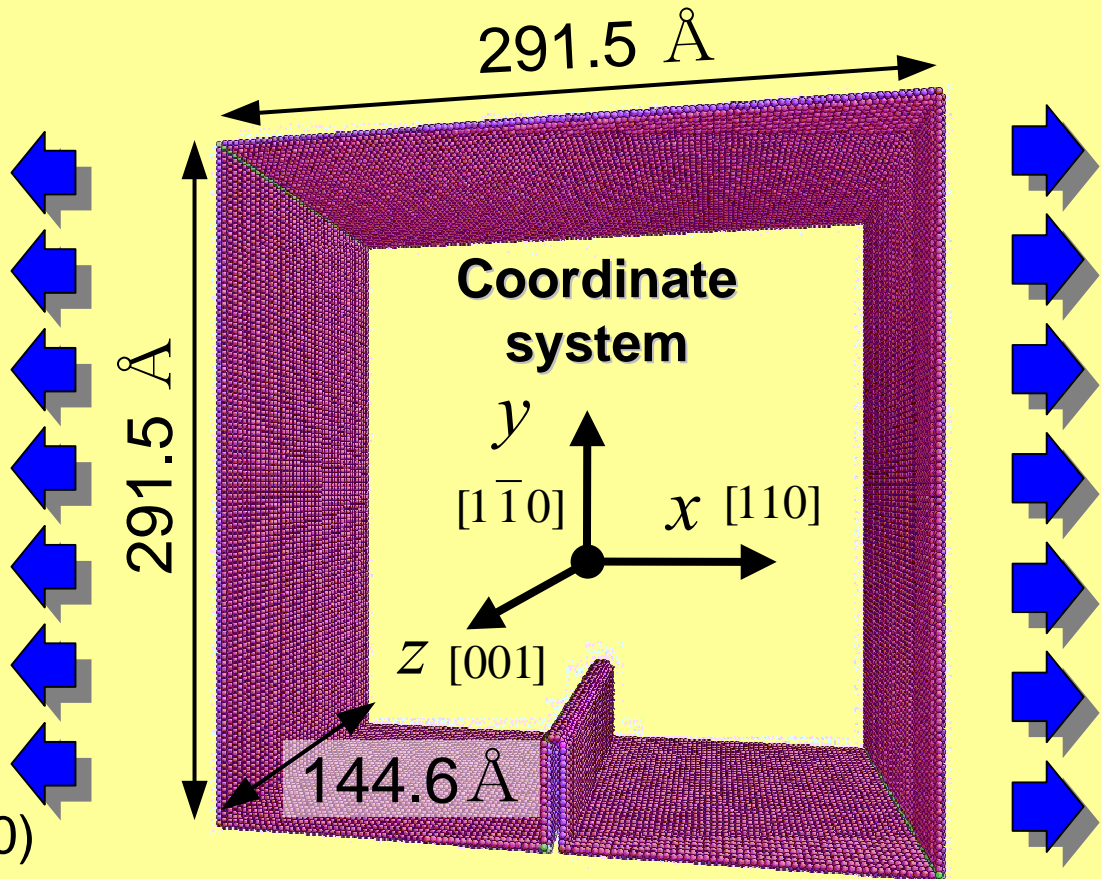# Fracture process --- development of crack-tip microstructures

## Mode I crack in a single fcc crystal

Simulation Cell

slip plane {111}
70.5
[1$\bar{1}$0]
y
x
[110]
[001]
crack plane (110)
z

Slip plane = {111}

The slip planes and the (110) crack plane intersect obliquely at 70.5° x ½

291.5 Å

291.5 Å

Coordinate system

y
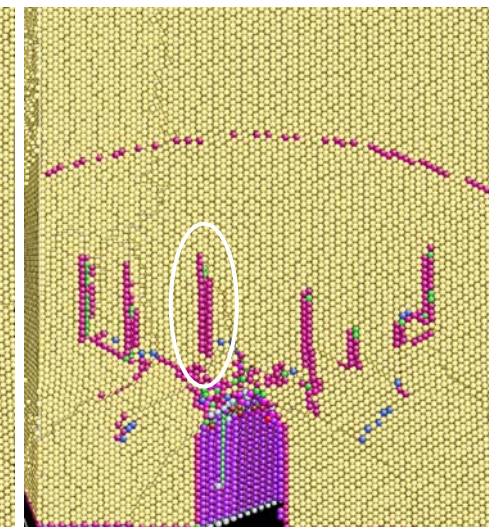$[1\bar{1}0]$ x [110]

z [001]

144.6 Å

# of atoms : 1,036,960

Temperature dependence on the crack-tip dislocation nanostructures (Cu)

16 ps

24 ps

Initial crack length

0 K   50 K   150 K   300 K
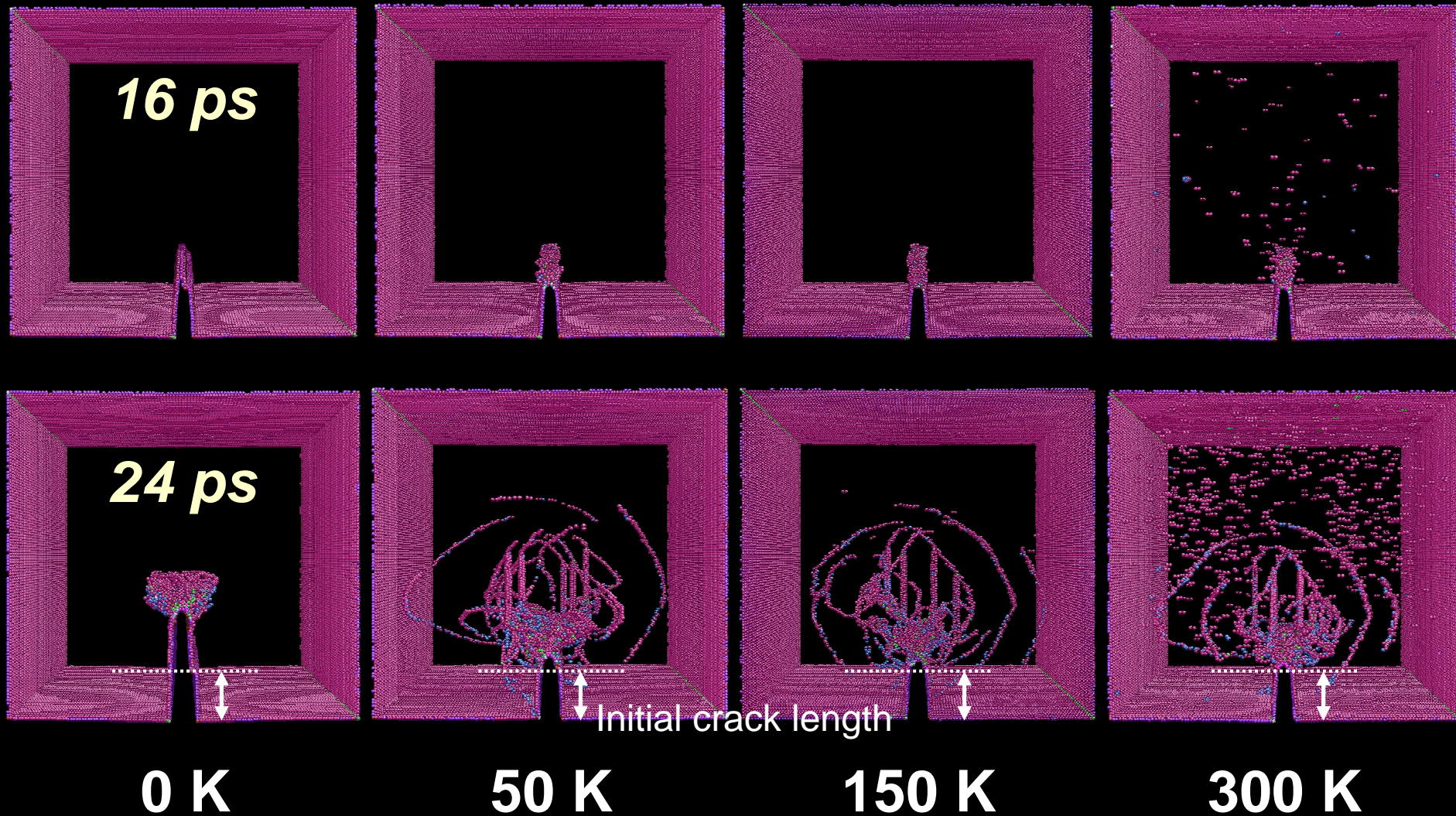
Disl. motion on the slip plane (Cu, 50K)

$[1\bar{1}0]$

$[1\bar{2}\bar{1}]$

$[2\bar{1}1]$

16 ps   **18 ps**   **20 ps**   **22 ps**
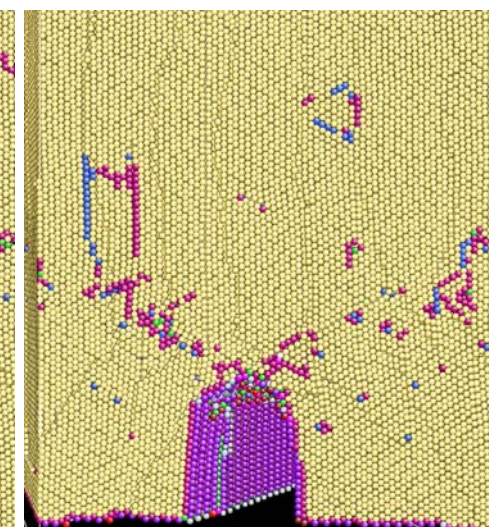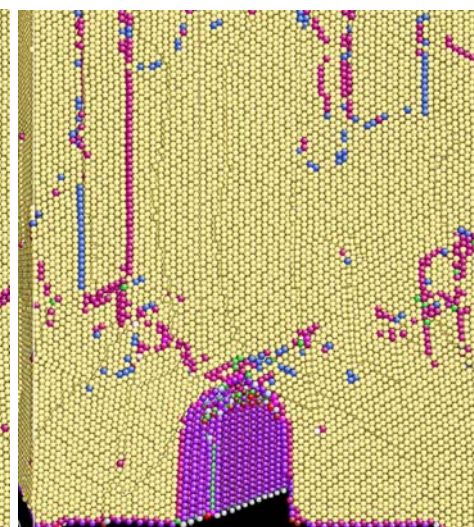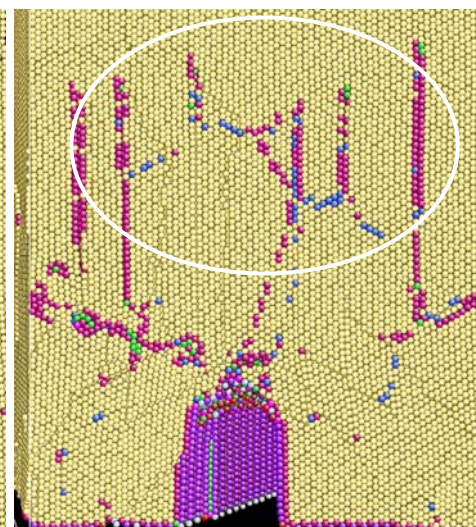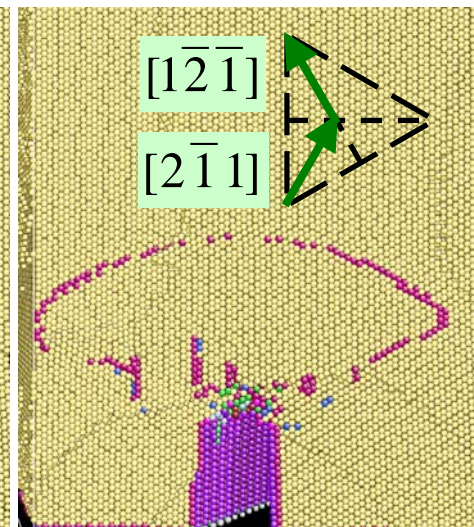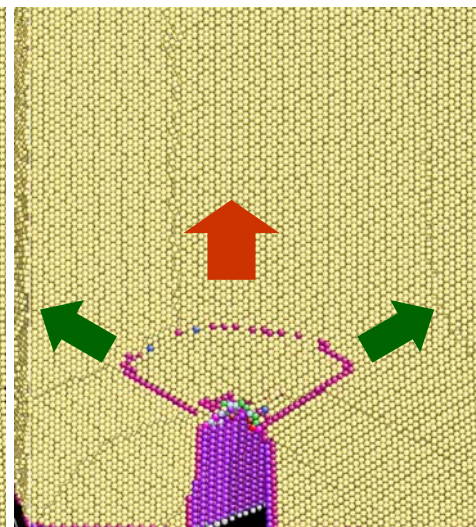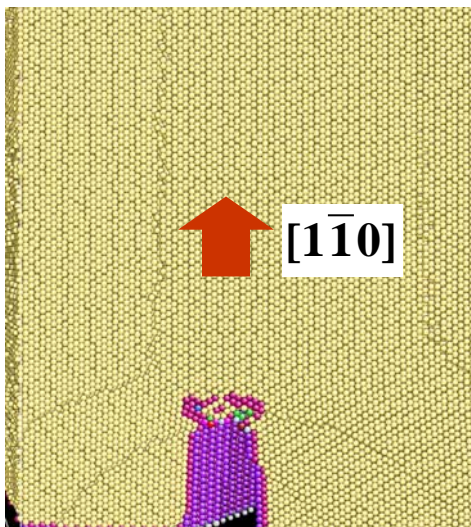
24 ps   **26 ps**   **28 ps**   **30 ps**

Expansion and emission process of stacking-fault loops

Cu

Al

fcc

fcc

hcp

Shockley partial

$\frac{1}{6}\langle 112 \rangle$

hcp

fcc
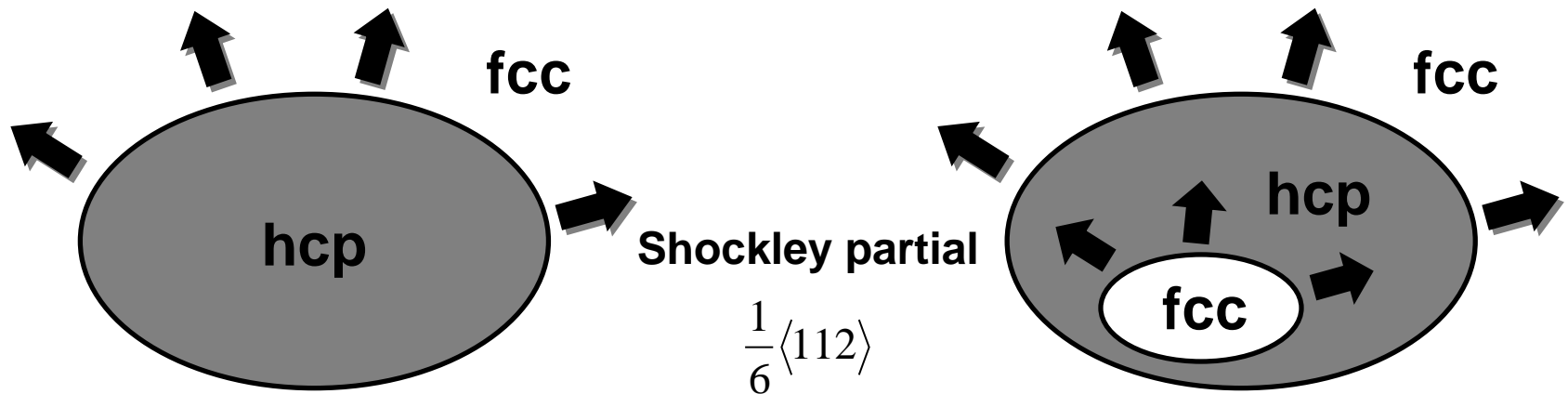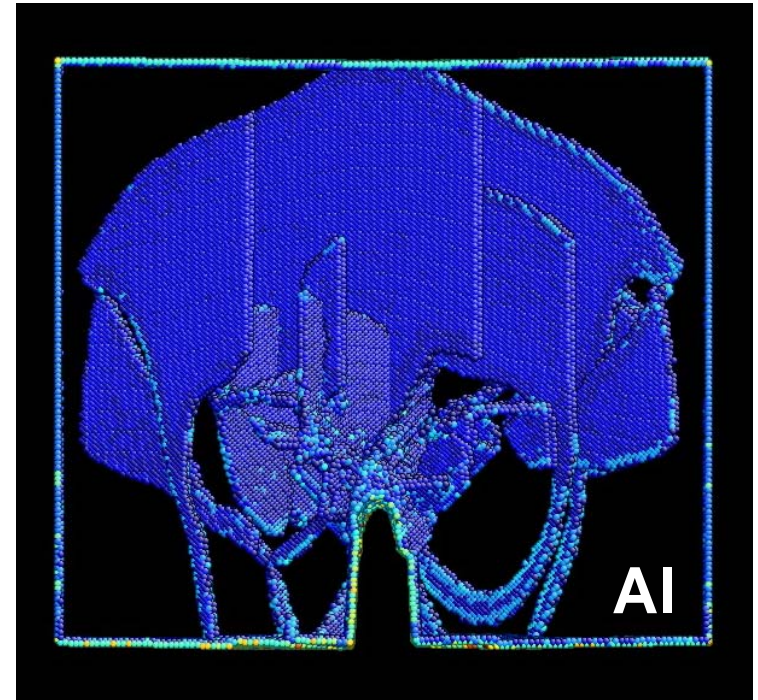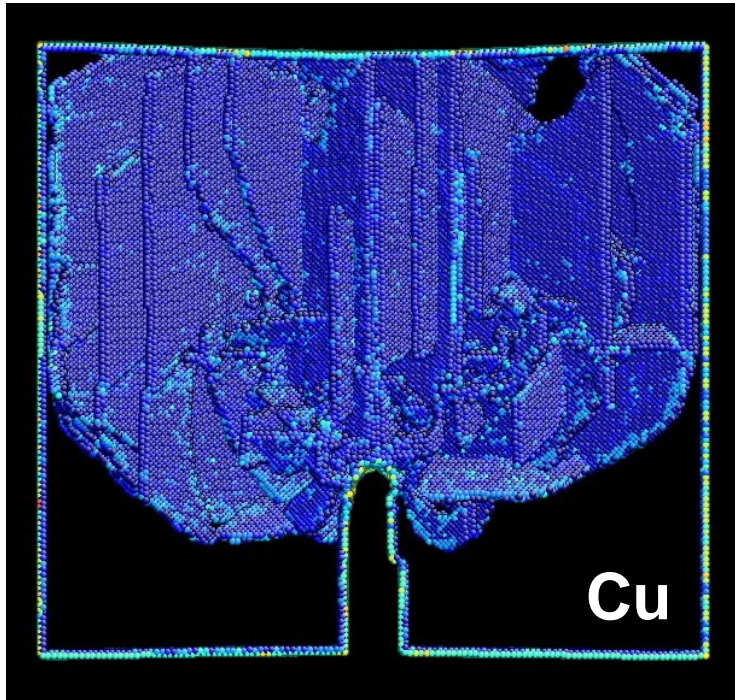
C.N. = 10 : Green
11 : Red
12 : omitted (f.c.c.)
13 : Blue

10.0 ps

18.4 ps

21.6 ps