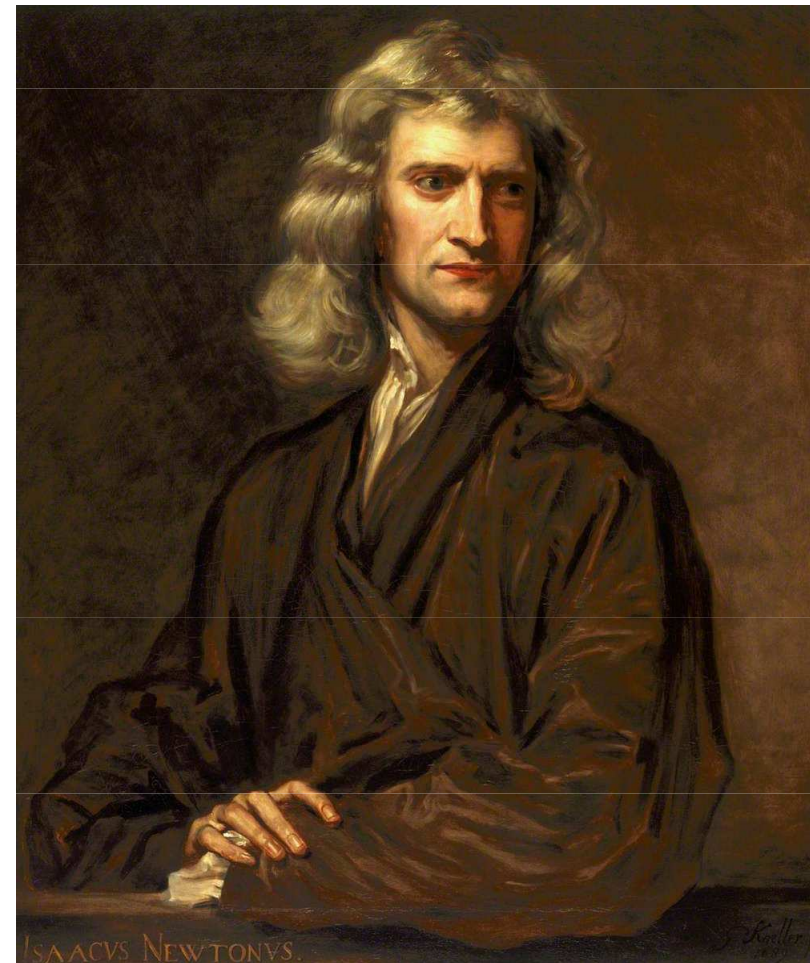


Molekulární dynamika

J. Fikar

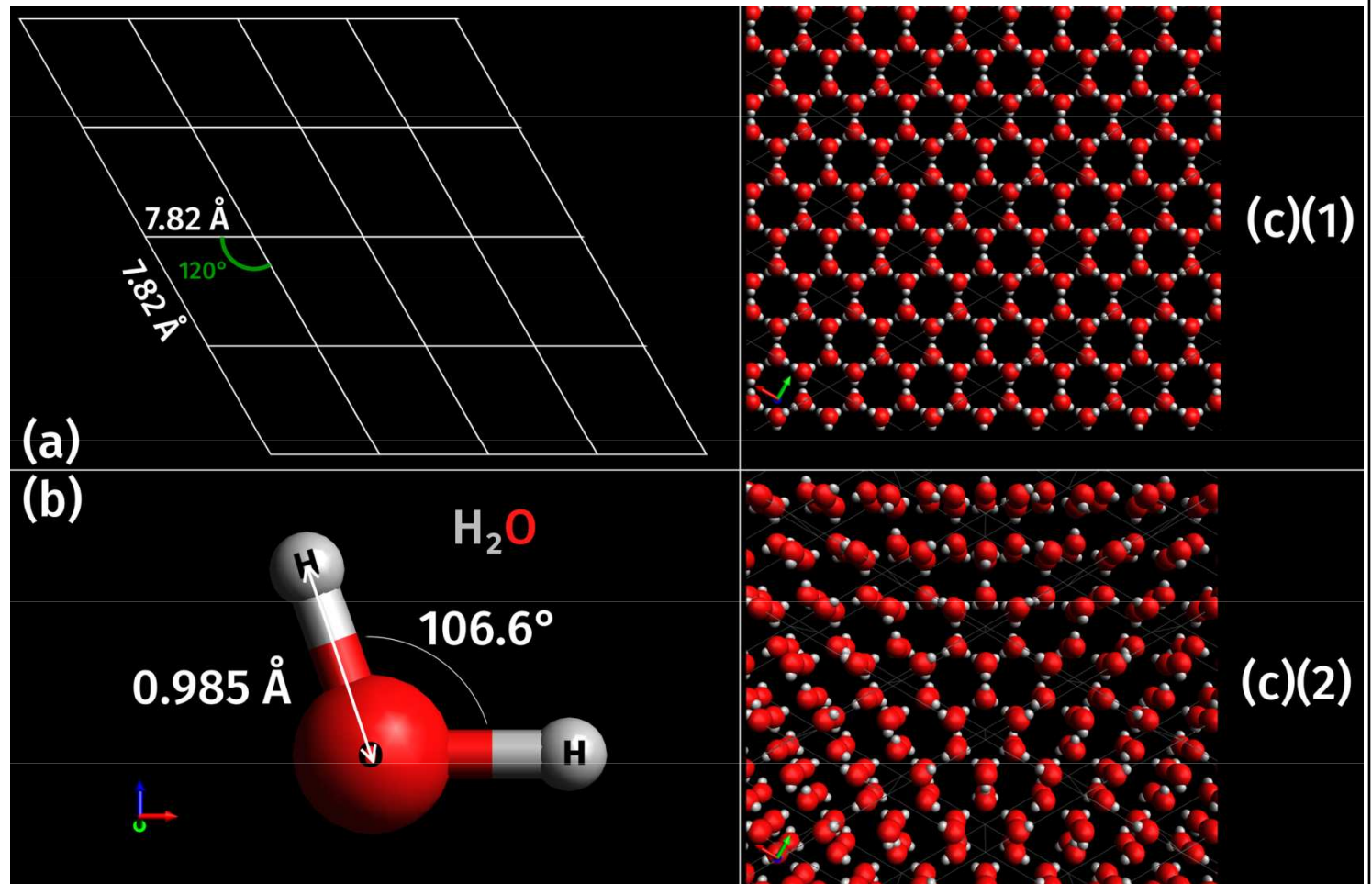


- 1) N-těles, x , x' , x''
- 2) Jaká tělesa?
- 3) Klasická mechanika
- 4) Empirické potenciály
- 5) Typy vazeb
- 6) Zákony zachování
- 7) Statistická termodynamika
- 8) Periodické okrajové podmínky



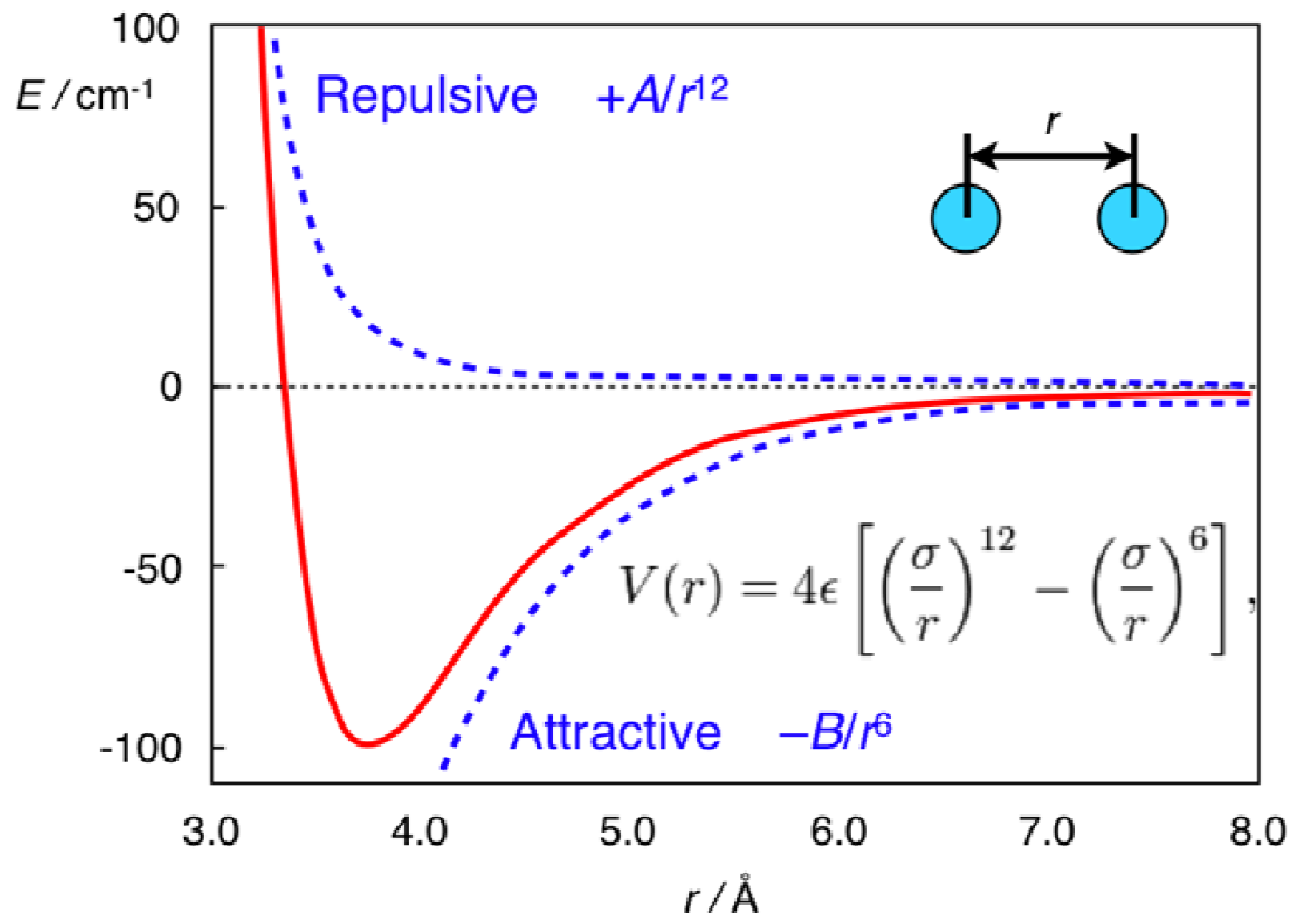
Typy vazeb

- 1) Iontová
- 2) Kovalentní
- 3) Kovová
- 4) Vodkový můstek
- 5) Van der Waals

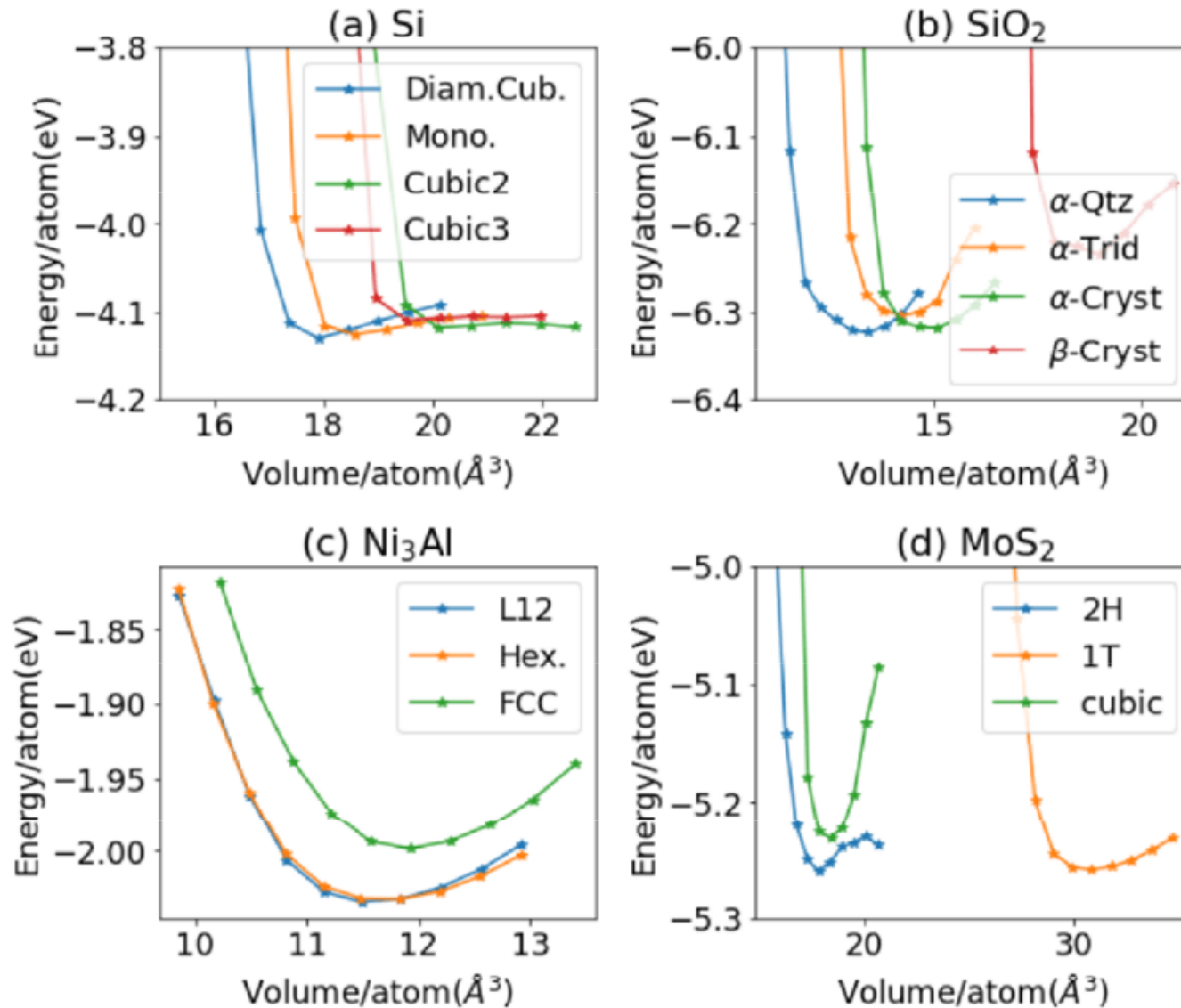


Empirické potenciály

- Lennard-Johnes

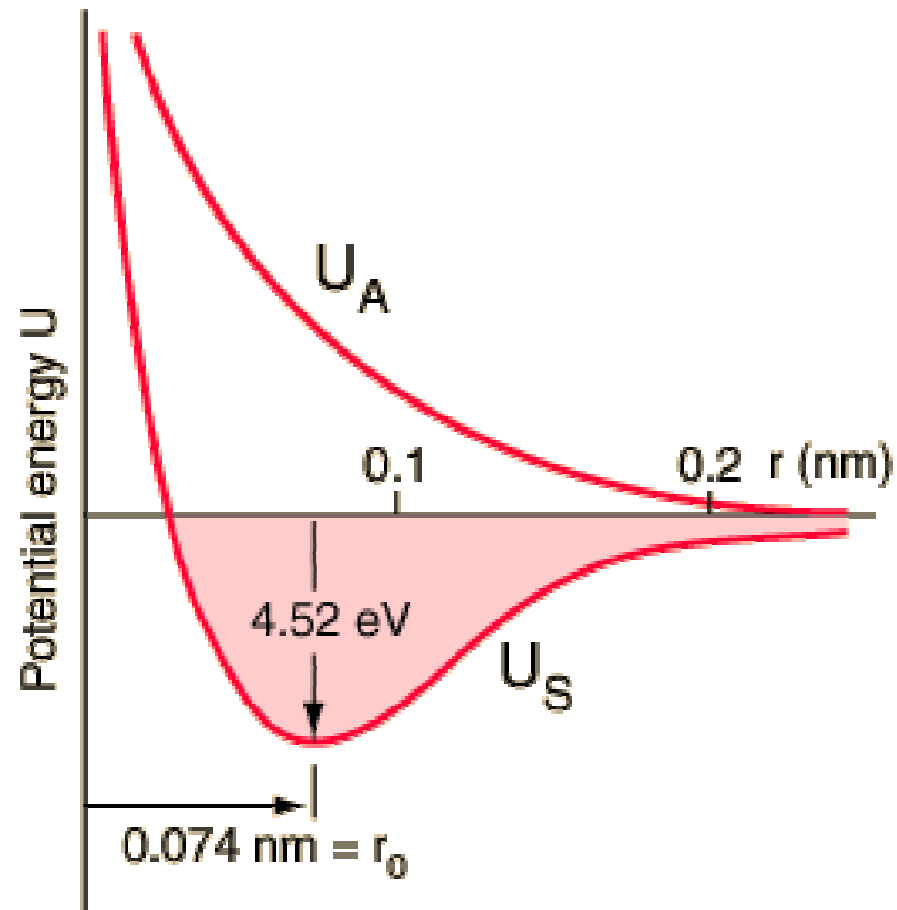


Křivka objem-energie



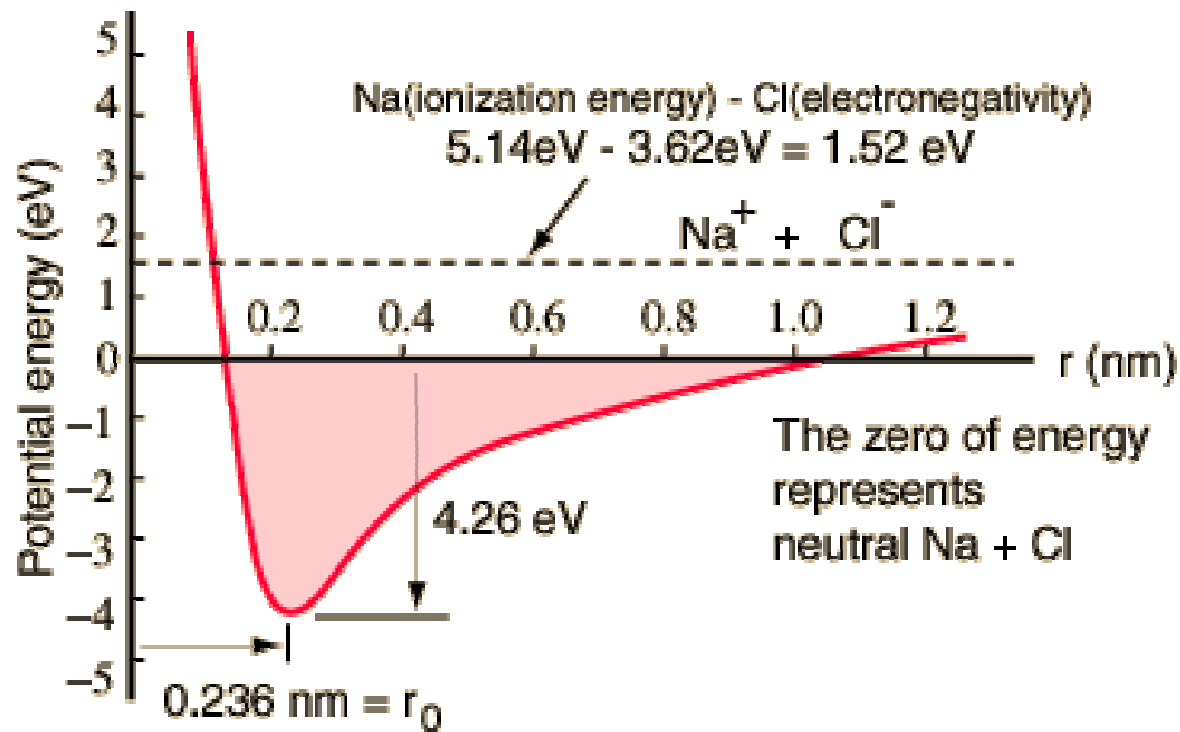
Empirické potenciály

◦ H₂



Empirické potenciály

- NaCl

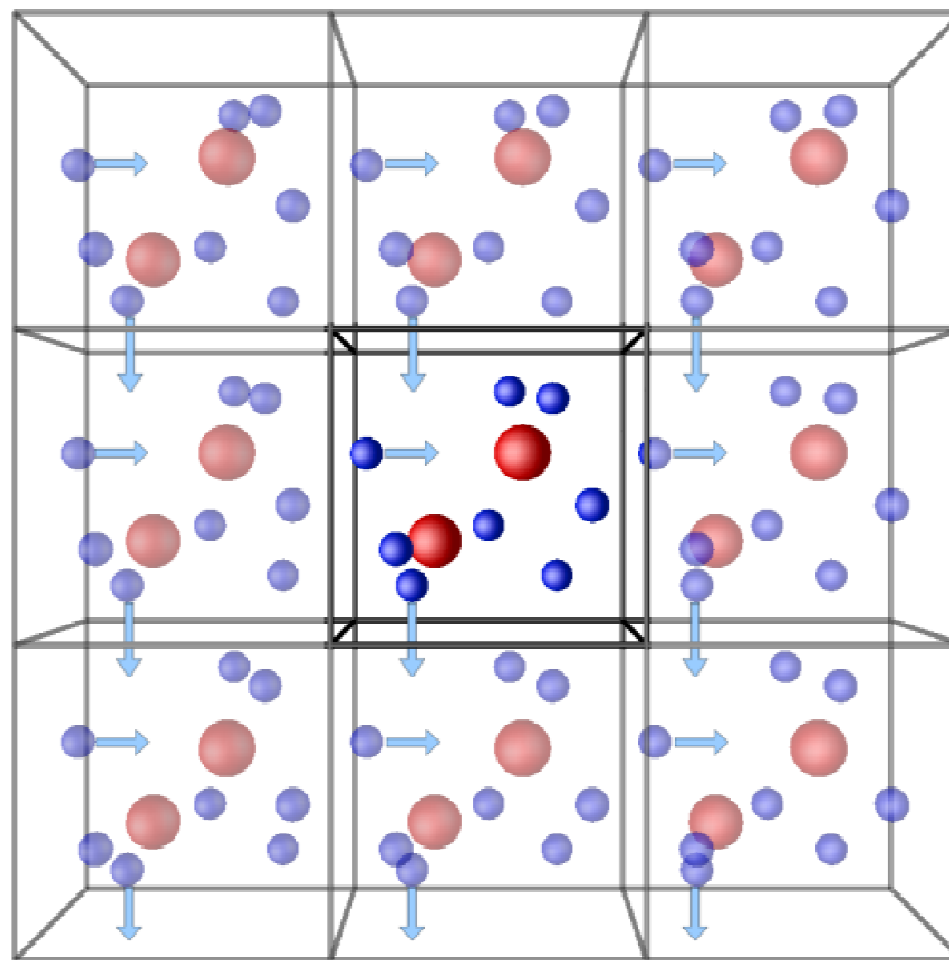


Embedded atom model

$$E_i = F_\alpha \left(\sum_{j \neq i} \rho_\beta(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij})$$

Property	Target value	Ackland <i>et al.</i> (1997) potential
a (Å), bcc at $T=0$ K	2.8553 ^a	2.8665
a (Å), bcc at $T=1820$ K	2.94	2.921
E_{coh} (eV atom ⁻¹), bcc	-4.316 ^a	-4.316
E_f^v (eV), bcc at $T=0$ K	1.84 ^a	1.89
E_D (eV atom ⁻¹), bcc at $T=0$ K	2.65 ^b	2.49
E_f^1 (eV), $\langle 100 \rangle$ bcc at $T=0$ K	4.37 ^d	6.12
E_f^1 (eV), $\langle 110 \rangle$ bcc at $T=0$ K	3.41 ^d	4.88
E_f^1 (eV), $\langle 111 \rangle$ bcc at $T=0$ K	4.11 ^d	5.02
C_{11} (GPa), bcc at $T=0$ K	243.4 ^a	243.4
C_{12} (GPa), bcc at $T=0$ K	145.0 ^a	145.0
C_{44} (GPa), bcc at $T=0$ K	116.0 ^a	116.0
γ_{100} (eV Å ⁻²), bcc at $T=0$ K	0.136 ^e	0.113
a (Å), fcc at $T=0$ K	3.6583 ^e	3.6800
$\Delta E_{\text{bcc} \rightarrow \text{fcc}}$ (eV atom ⁻¹)	0.122 ^e	0.054
ρ_{liquid} (GPa), $T=1820$ K	0.00 ^f	-0.460
PCF first peak position (Å), $T=1820$ K	2.49 ^g	2.53
PCF first peak height, $T=1820$ K	2.28 ^g	2.87
D_{liquid} (10 ⁻⁵ cm ² s ⁻¹), $T=1820$ K		1.19
ΔH_{melt} (eV atom ⁻¹), $T=1820$ K	0.143	0.188
R_{F1} (eV Å ⁻¹)	0.00	0.63
R_{F2} (eV Å ⁻¹)	0.00	0.66

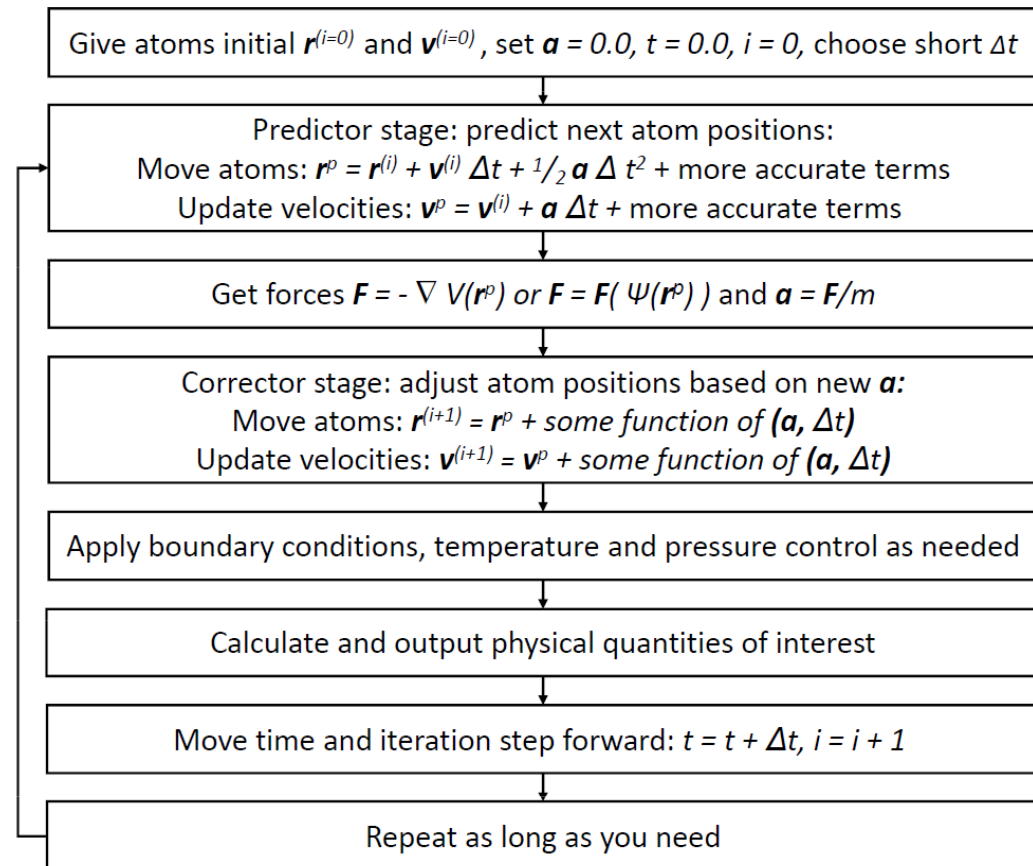
Periodické okrajové podmínky



Integrace - dynamika

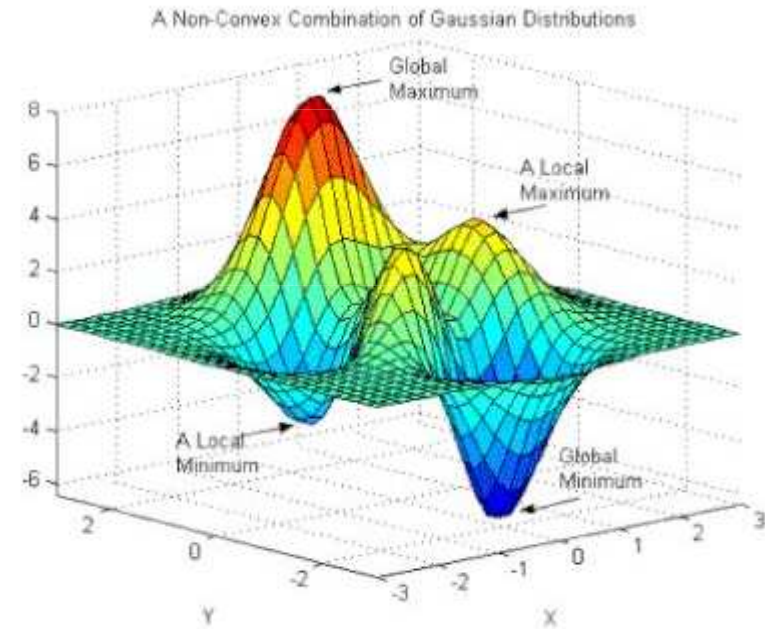
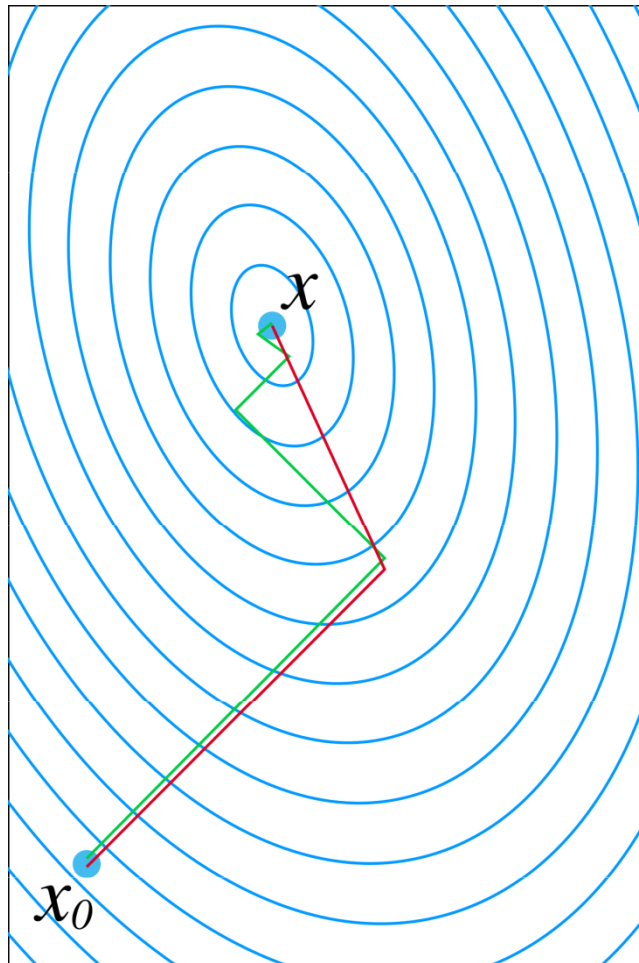
1. **Newtonovy rovnice**
2. **Predictor-corrector**
3. **Time-step 10^{-15} s**
4. **Debyeova frekvence**
5. **Teplota $E_k = 3/2 kT$**
6. **Maxwell-Boltzmannovo rozdělení**
7. **Termostat – škálování rychlostí**

Simplified schematic of the molecular dynamics algorithm



Minimalizace - statika

Conjugate-gradient



Termodynamické soubory

<u>École Polytechnique</u>	<u>Glasgow school</u>	<u>Berlin school</u>	<u>Edinburgh school</u>
			
<u>Sadi Carnot</u> (1796-1832)	<u>William Thomson</u> (1824-1907)	<u>Rudolf Clausius</u> (1822-1888)	<u>James Maxwell</u> (1831-1879)
<u>Vienna school</u>	<u>Gibbsian school</u>	<u>Dresden school</u>	<u>Dutch school</u>
			
<u>Ludwig Boltzmann</u> (1844-1906)	<u>Willard Gibbs</u> (1839-1903)	<u>Gustav Zeuner</u> (1828-1907)	<u>Johannes van der Waals</u> (1837-1923)

Termodynamické soubory

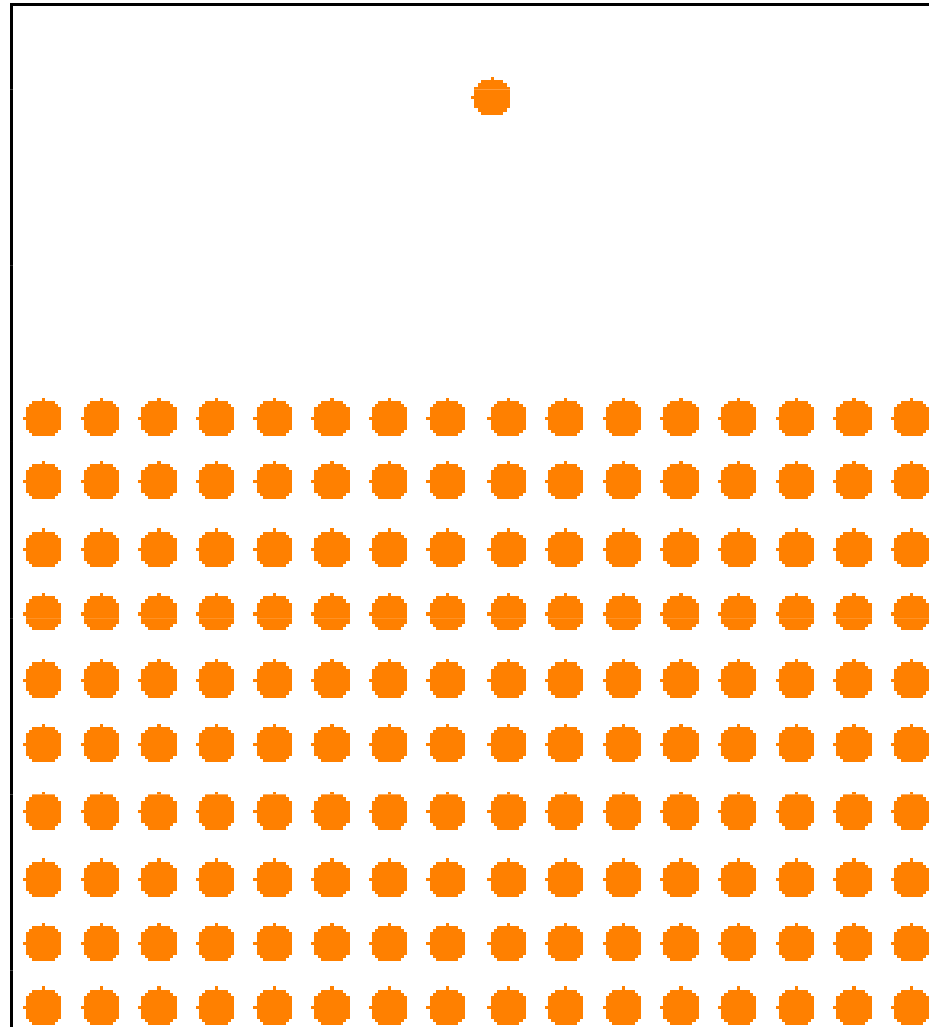
1. Mikrokanonický soubor (NVE soubor)
2. Kanonický soubor (NVT soubor, někdy též **Gibbsův kanonický soubor**) - termostat
3. Izotermicko-izobarický soubor (NpT soubor) – termostat a barostat

<u>École Polytechnique</u>	<u>Glasgow school</u>	<u>Berlin school</u>	<u>Edinburgh school</u>
			
<u>Sadi Carnot</u> (1796-1832)	<u>William Thomson</u> (1824-1907)	<u>Rudolf Clausius</u> (1822-1888)	<u>James Maxwell</u> (1831-1879)
<u>Vienna school</u>	<u>Gibbsian school</u>	<u>Dresden school</u>	<u>Dutch school</u>
			
<u>Ludwig Boltzmann</u> (1844-1906)	<u>Willard Gibbs</u> (1839-1903)	<u>Gustav Zeuner</u> (1828-1907)	<u>Johannes van der Waals</u> (1837-1923)

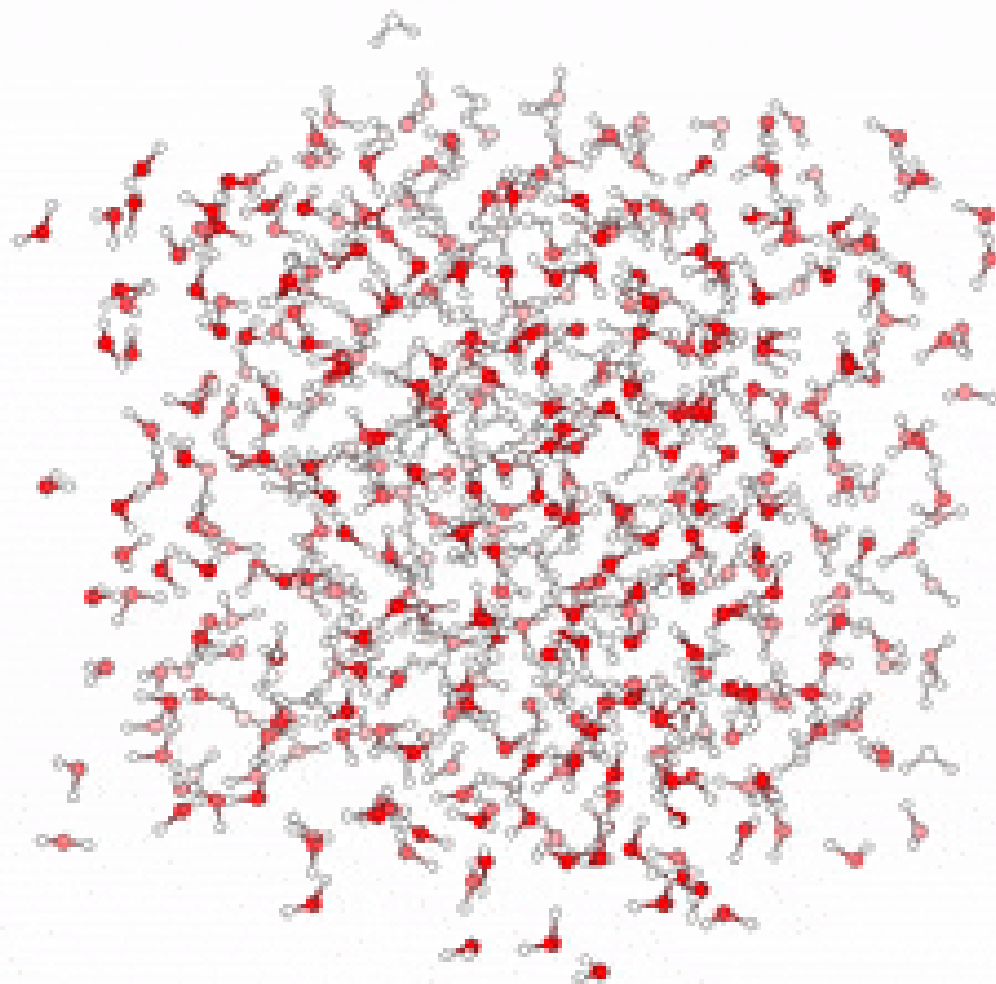
MD

time 0.0041 ps

Cu <100> depozice

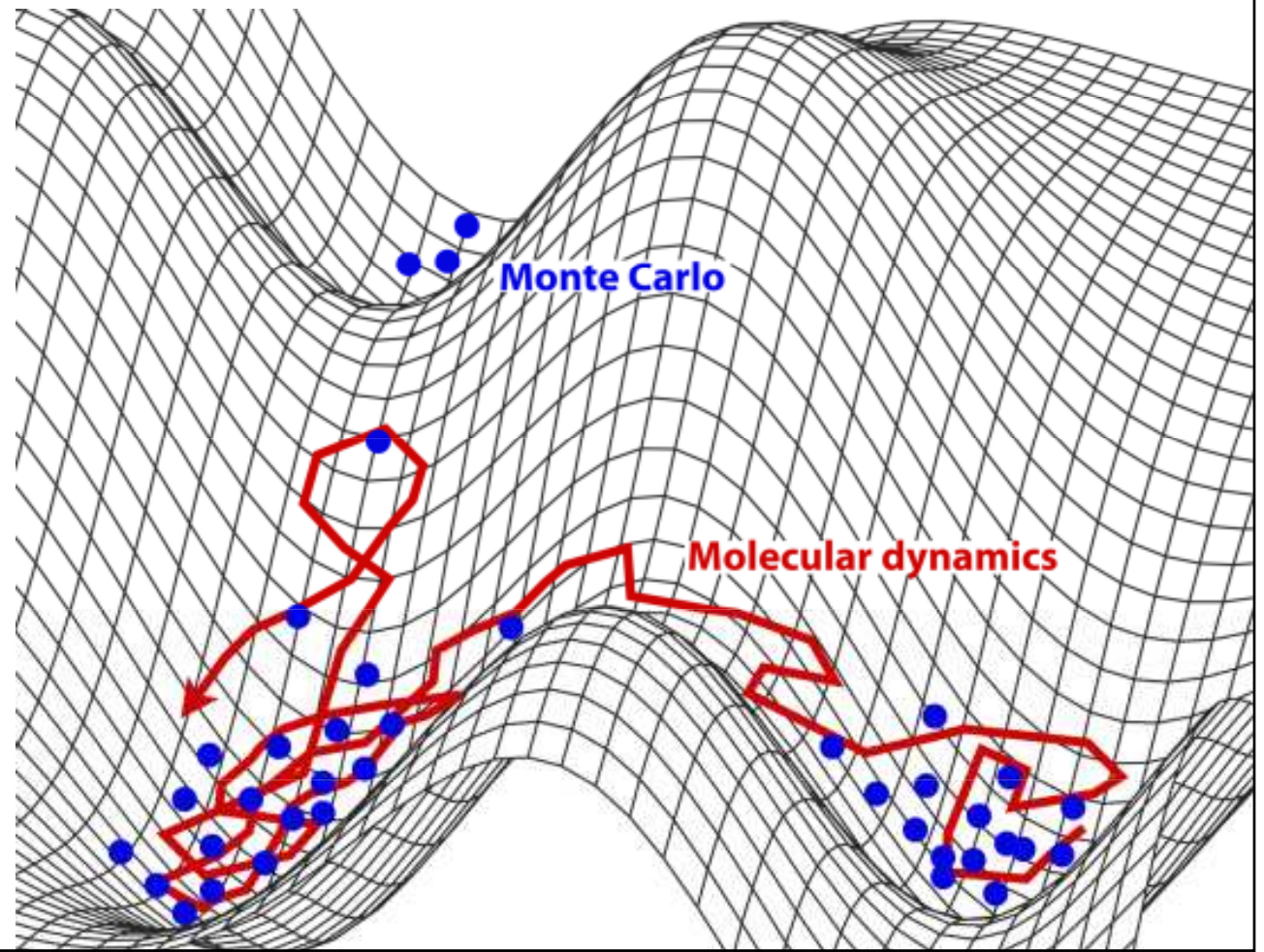


MD



MD – Monte Carlo

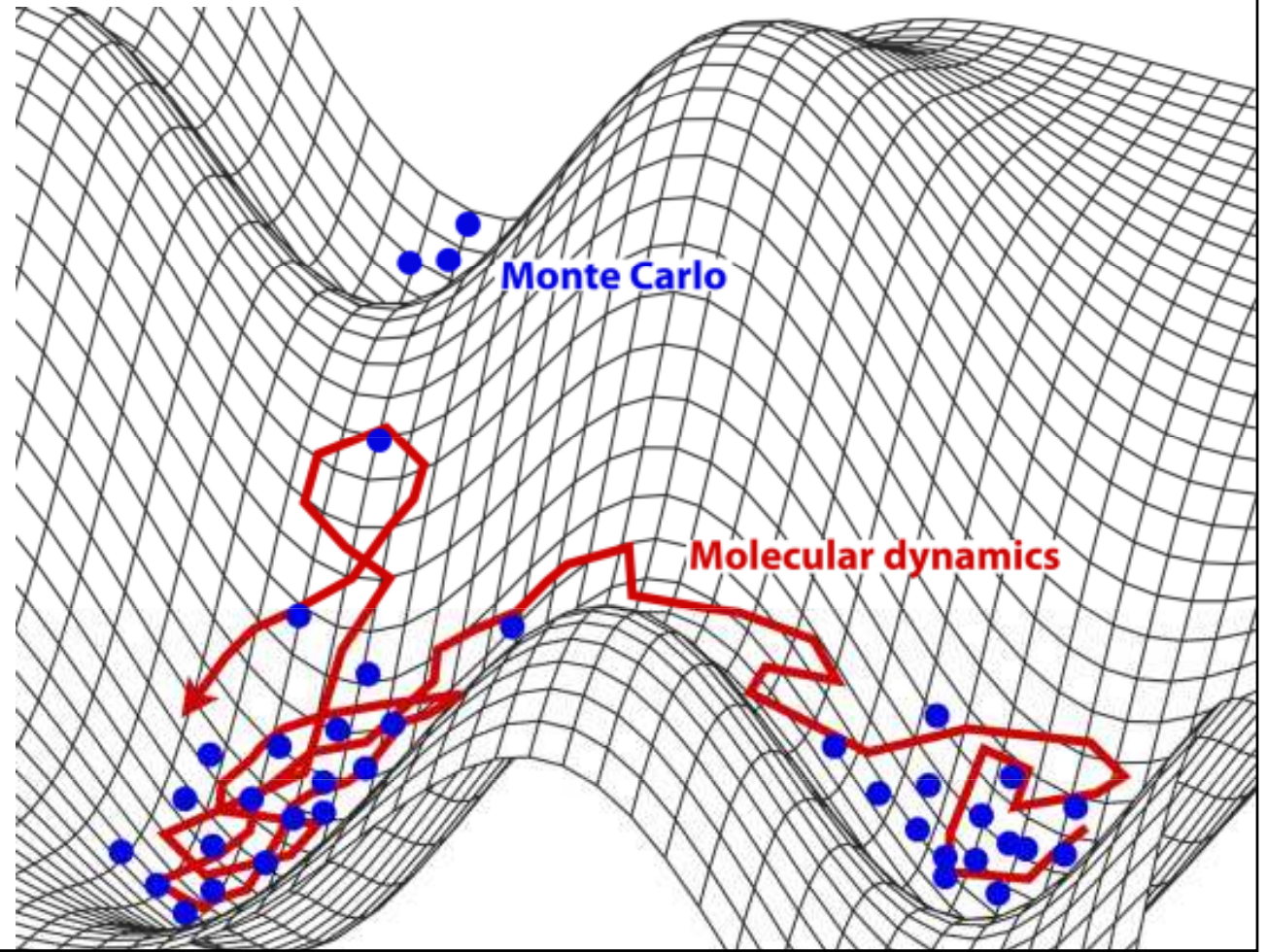
Boltzmanovo rozdělení



MD – Monte Carlo

Boltzmanovo rozdělení

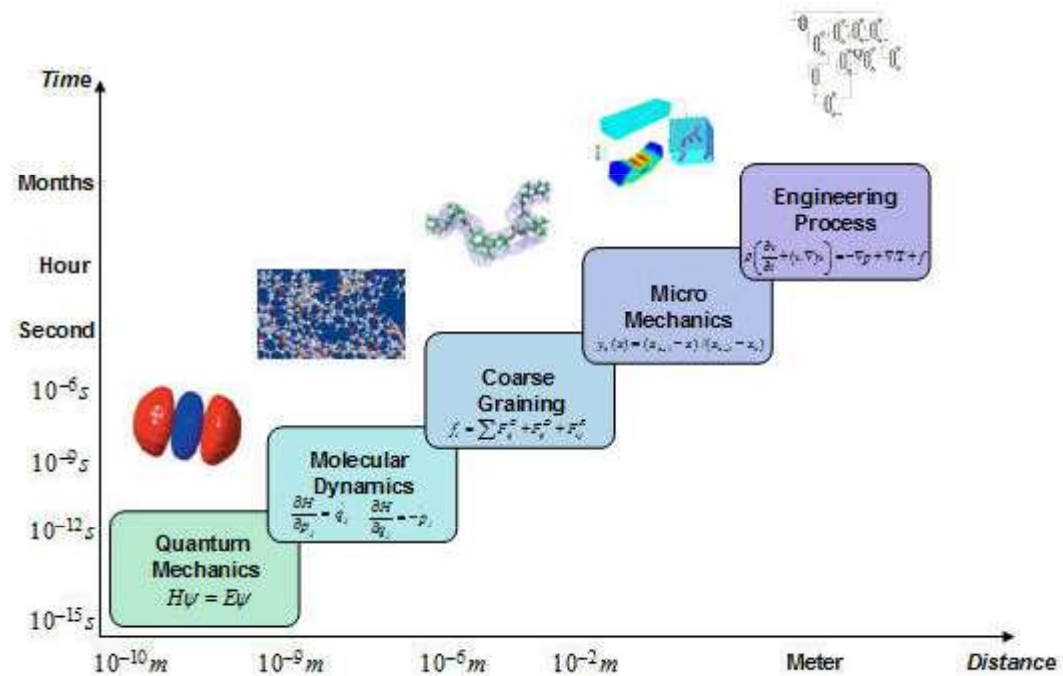
$$\frac{p_i}{p_j} = \exp\left(\frac{\varepsilon_j - \varepsilon_i}{kT}\right)$$



Výhody/nevýhody MD

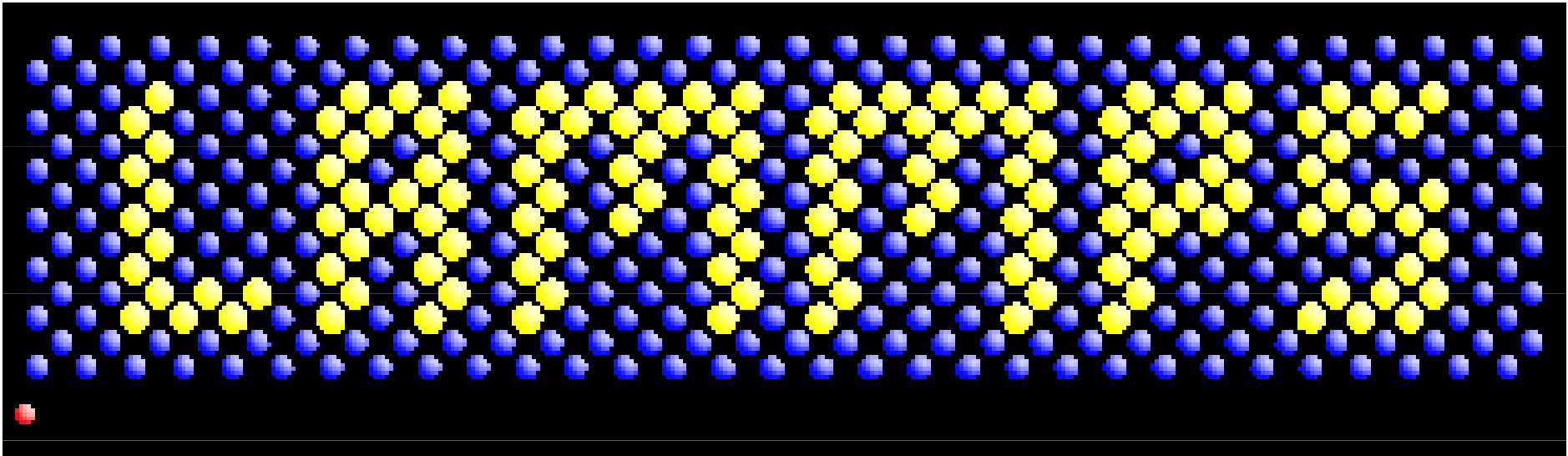
- Atomů 10^8
- Dynamika
- ns

- Tepelná aktivace
- Více dislokací
- Realistické rychlosti dislokací
- Difúze
- Potenciály? AI



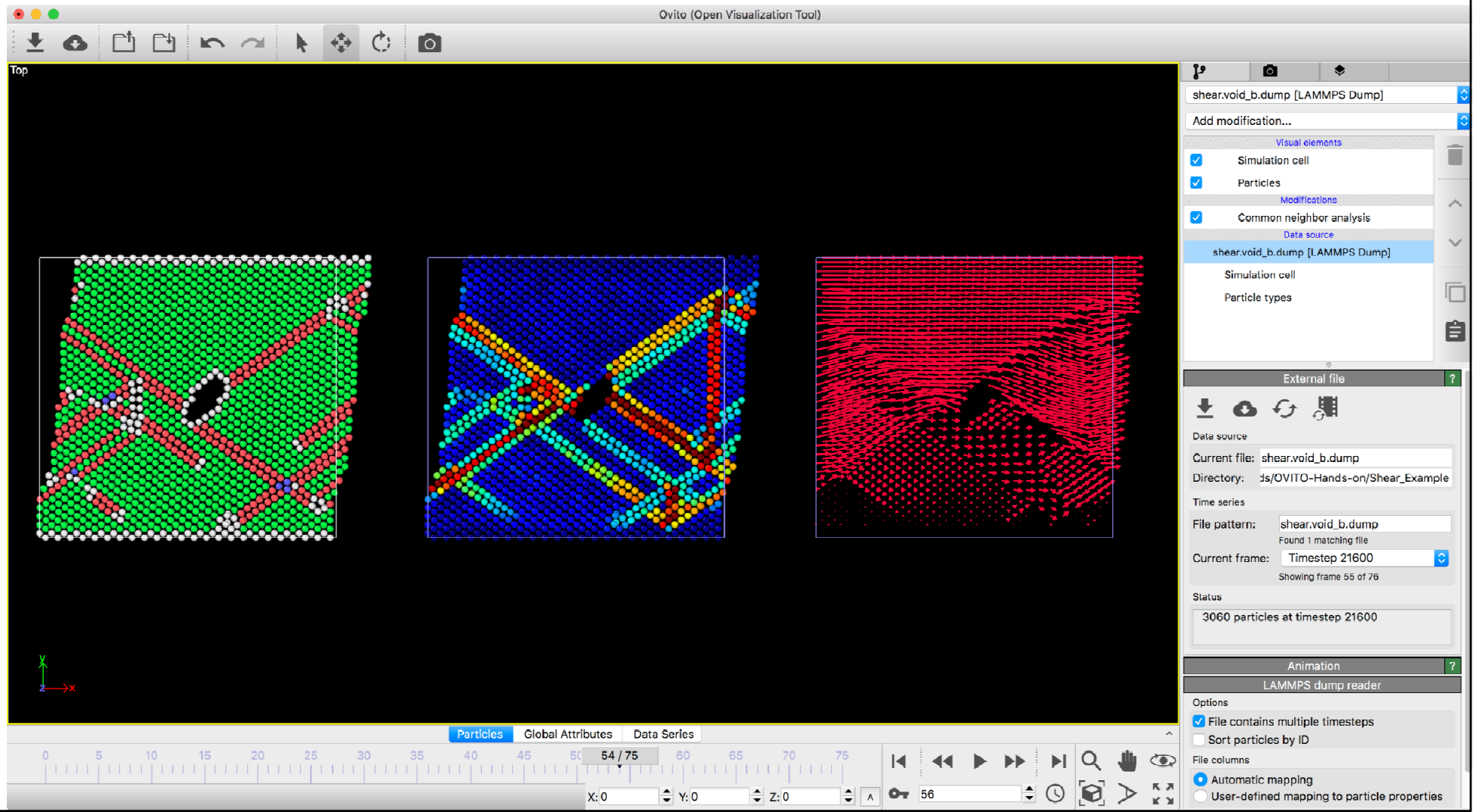
LAMMPS

- Large-scale Atomic/Molecular Massively Parallel Simulator
- Open source
- <https://lammps.org>

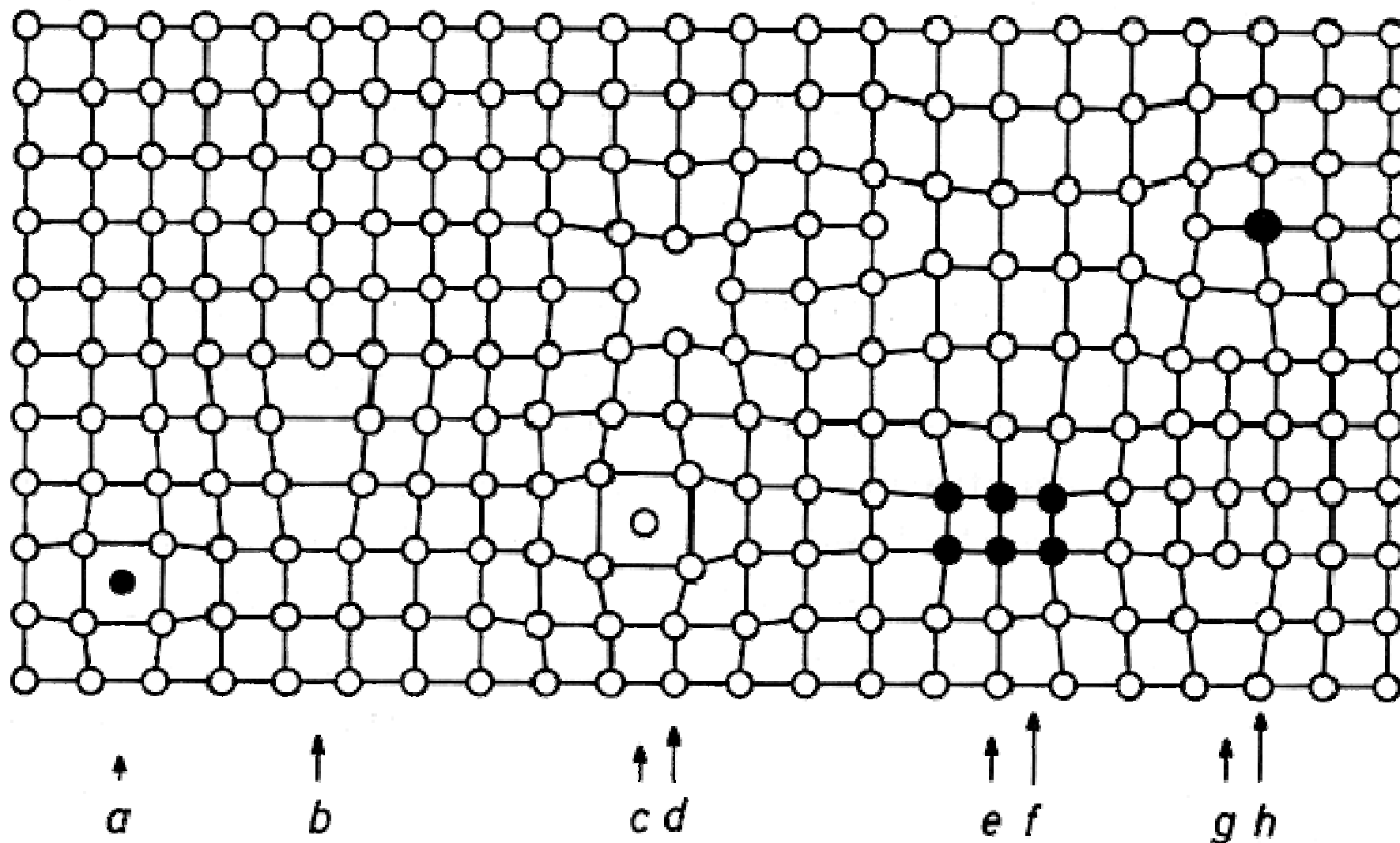


OVITO

- Zobrazuje atomy, molekuly; Basic – free, PRO \$\$\$; <https://ovito.org>



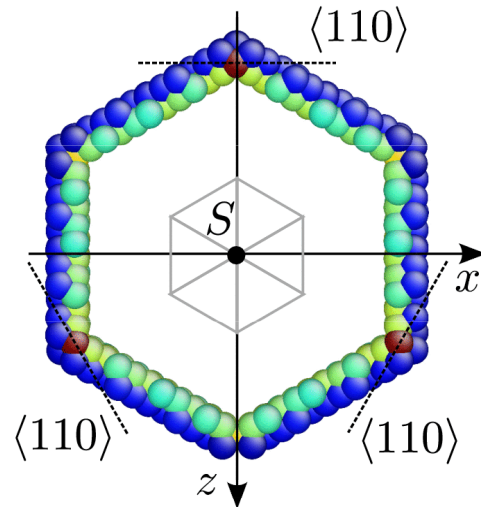
Bodové a lineární poruchy



Prizmatické dislokační smyčky

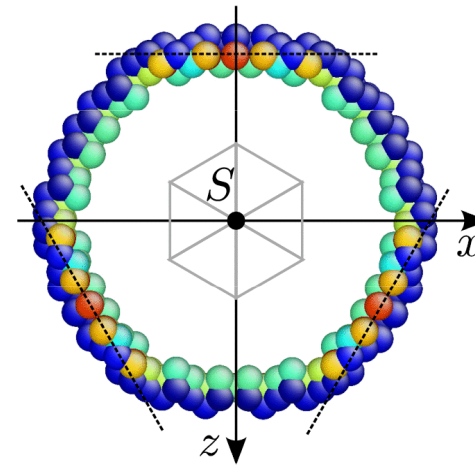
(a) symmetric hexagonal

$$N_{int} = 397$$



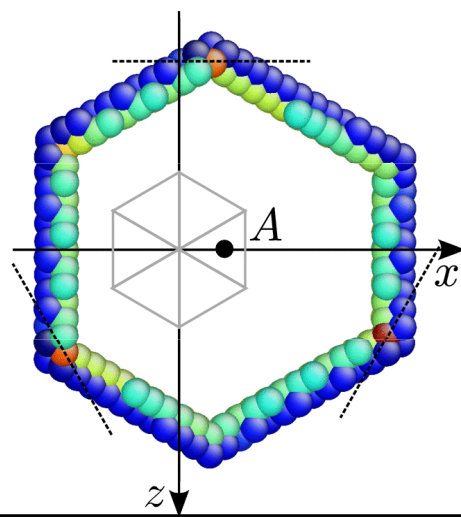
(b) symmetric circular

$$N_{int} = 397$$



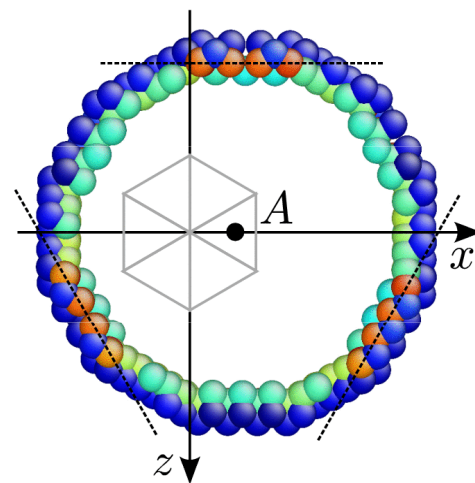
(c) asymmetric hexagonal

$$N_{int} = 396$$

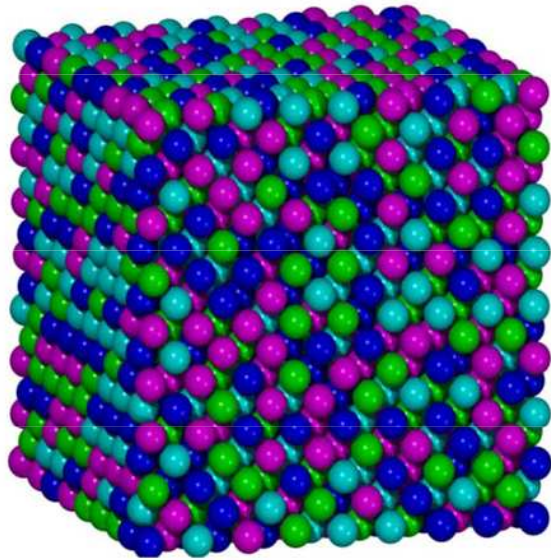


(d) asymmetric circular

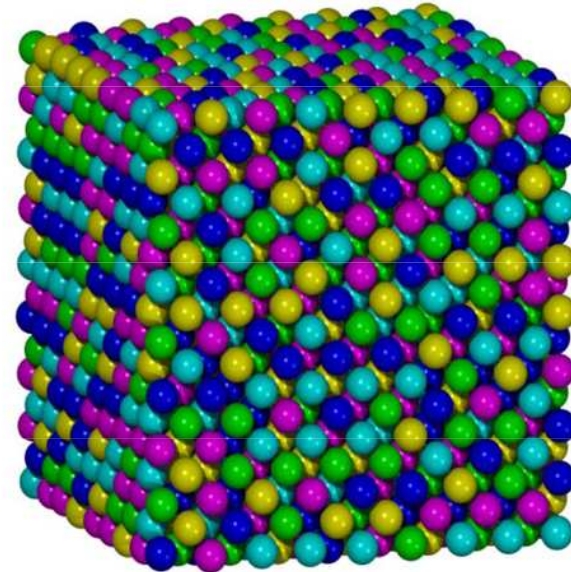
$$N_{int} = 396$$



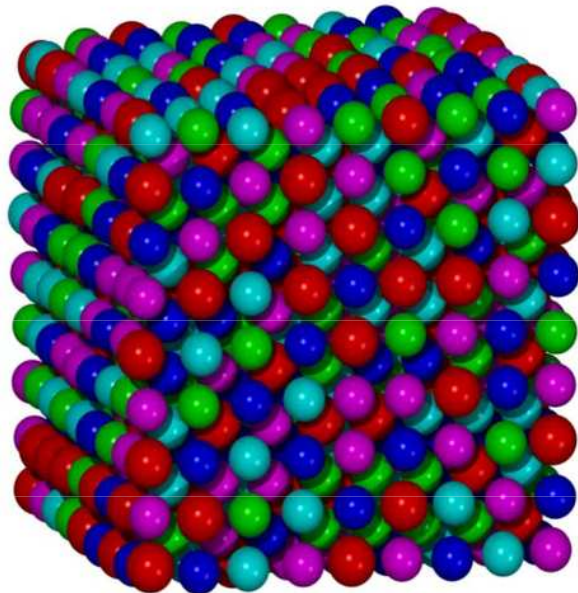
HEA



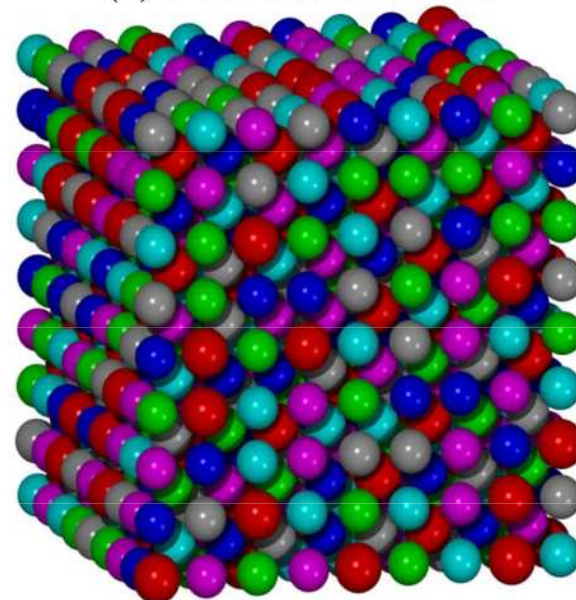
(a) FCC FeCoCrNi



(b) FCC CoCrFeMnNi



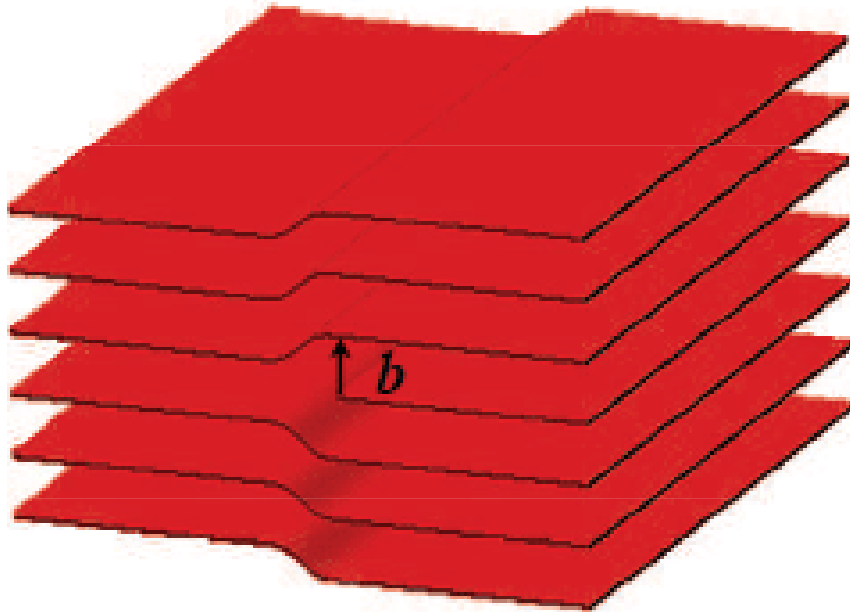
(c) BCC AlCoCrFeNi



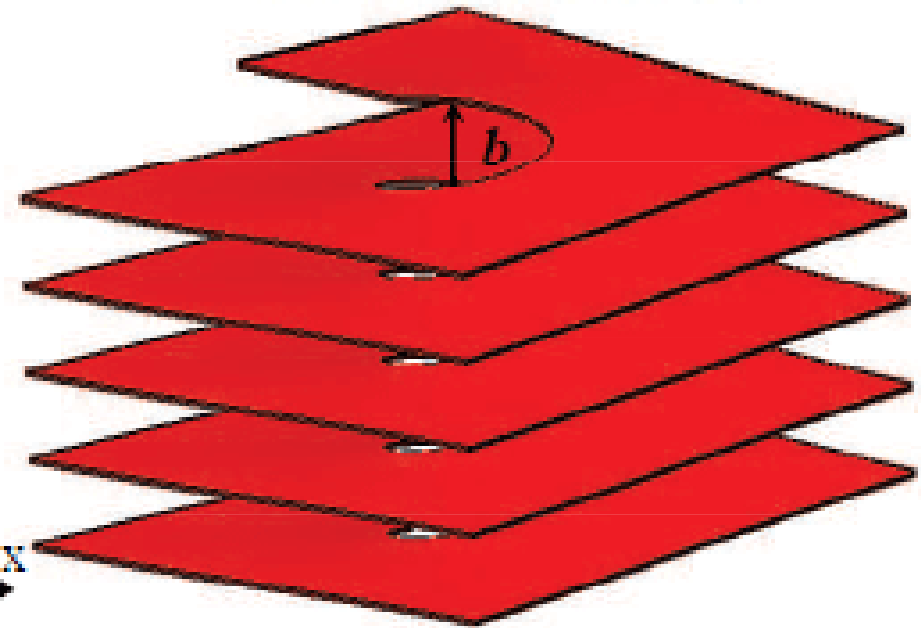
(d) BCC AlCoCrCuFeNi

Dislokace

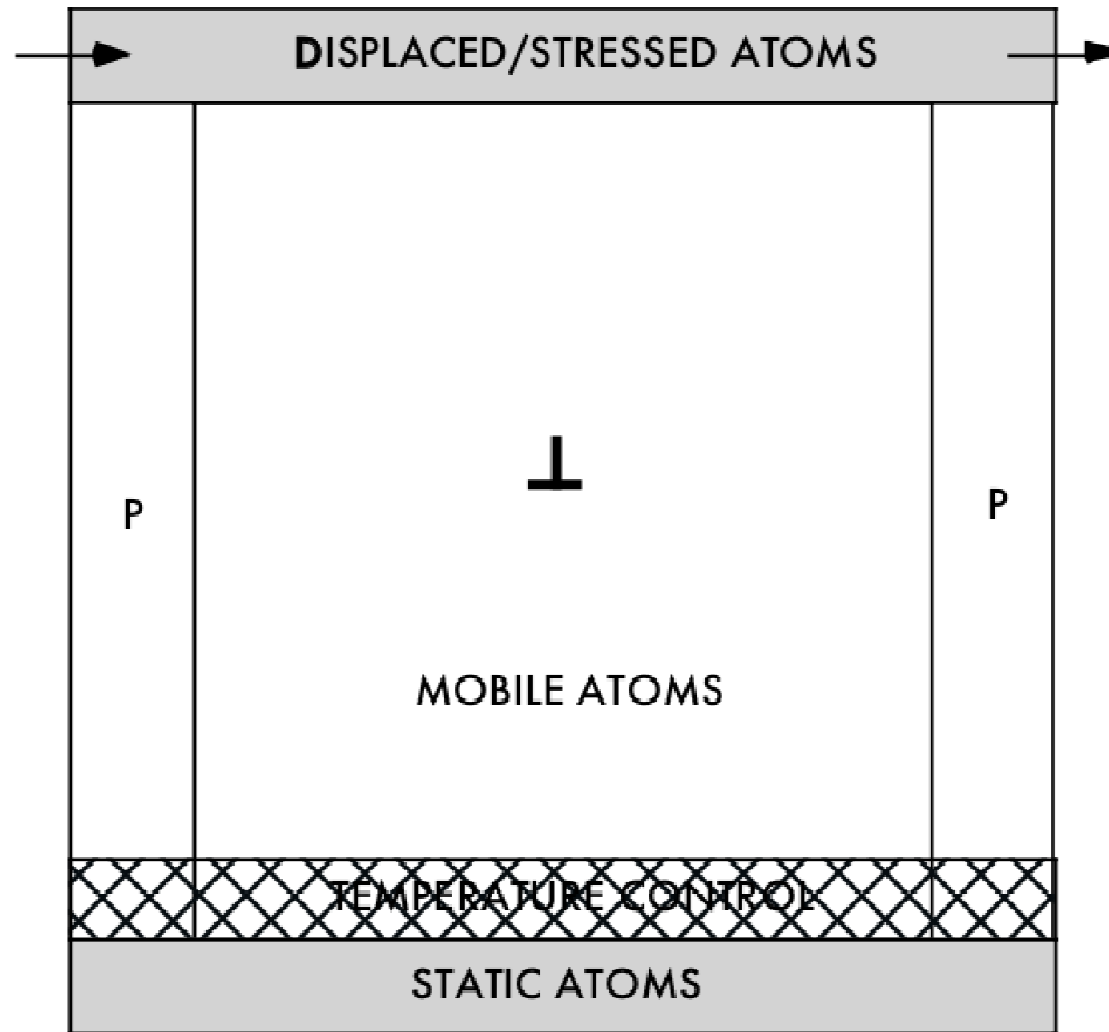
Edge dislocation



Screw dislocation

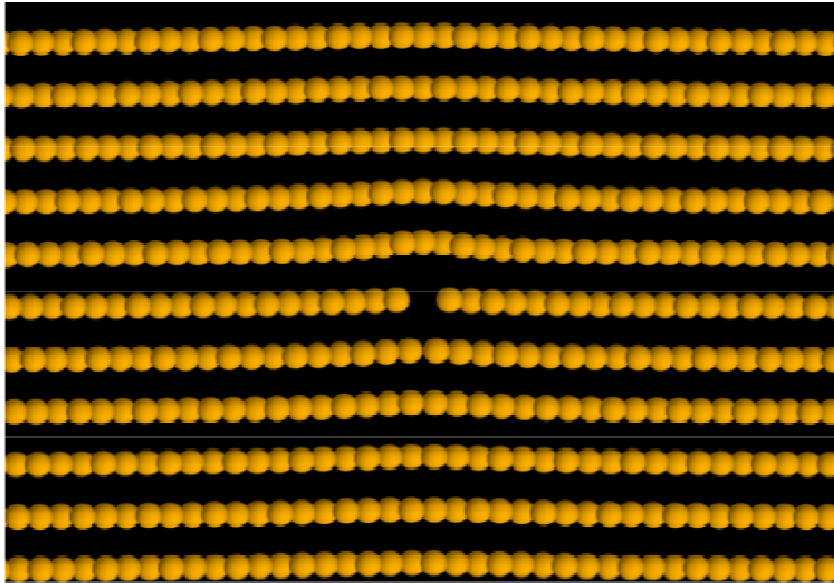


Dislokace

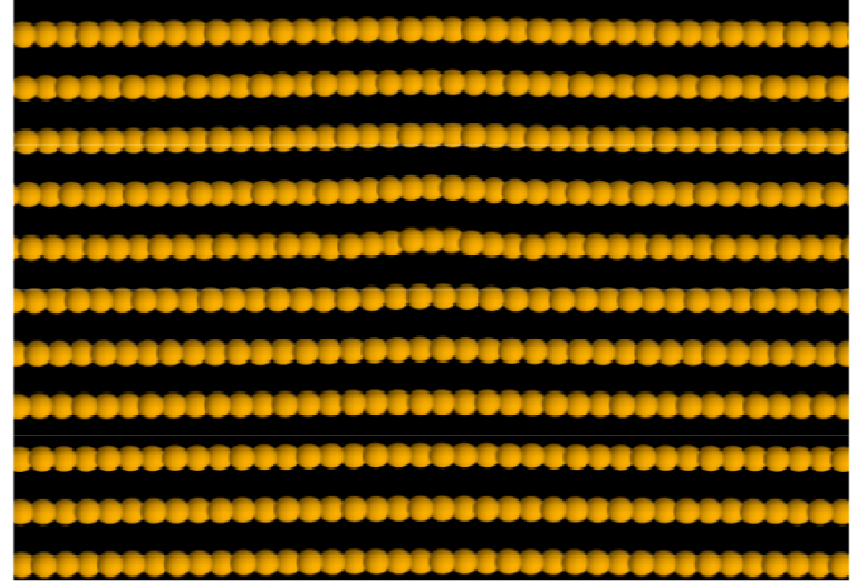


Hranová $\frac{1}{2}\langle 111 \rangle$

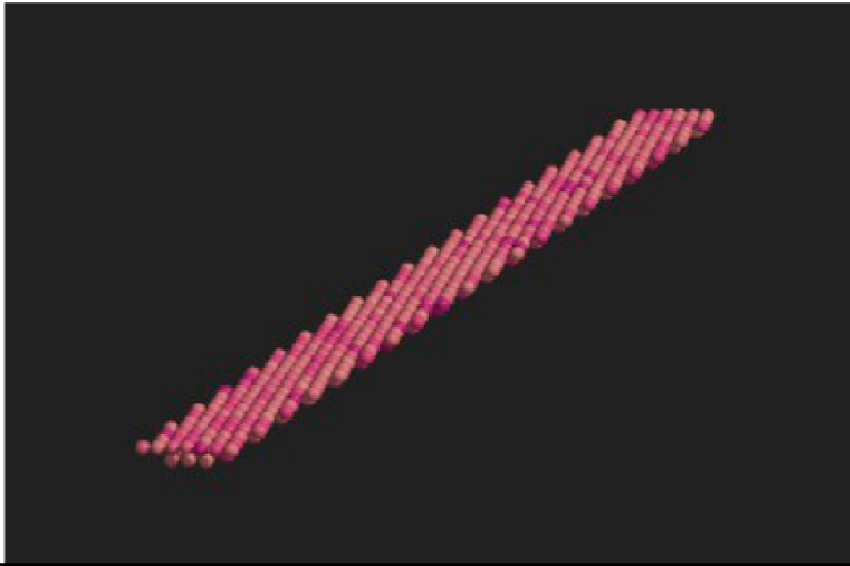
View along $\langle 112 \rangle$



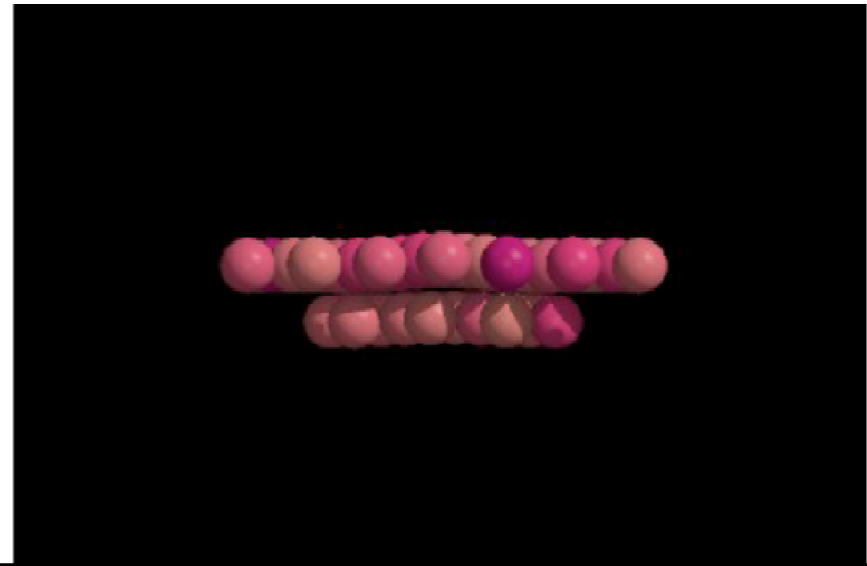
View along $\langle 112 \rangle$ relaxed by MD



High Ep atoms

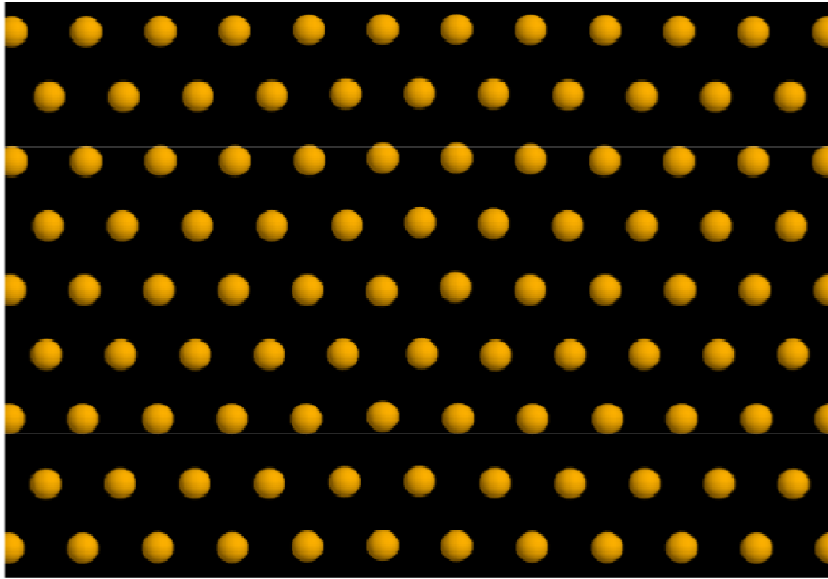


View along $\langle 112 \rangle$, high Ep atoms

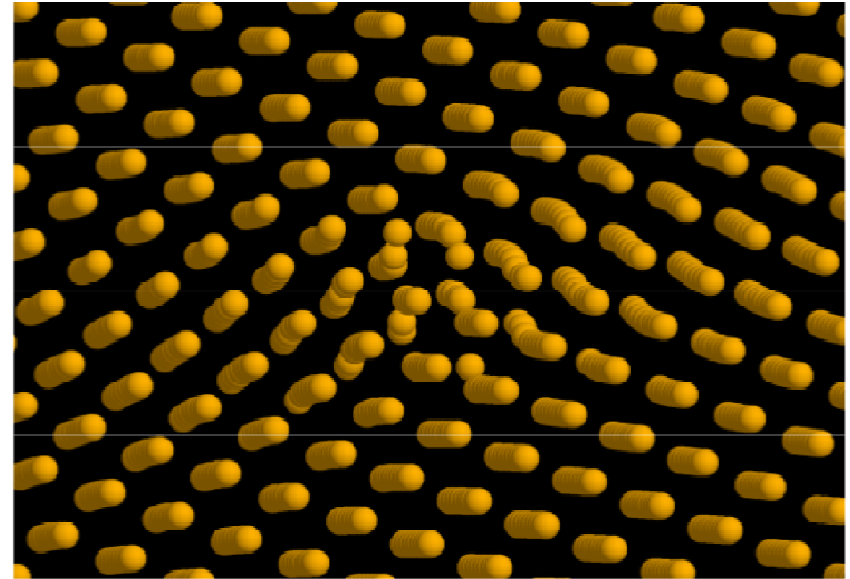


Šroubová $\frac{1}{2}\langle 111 \rangle$

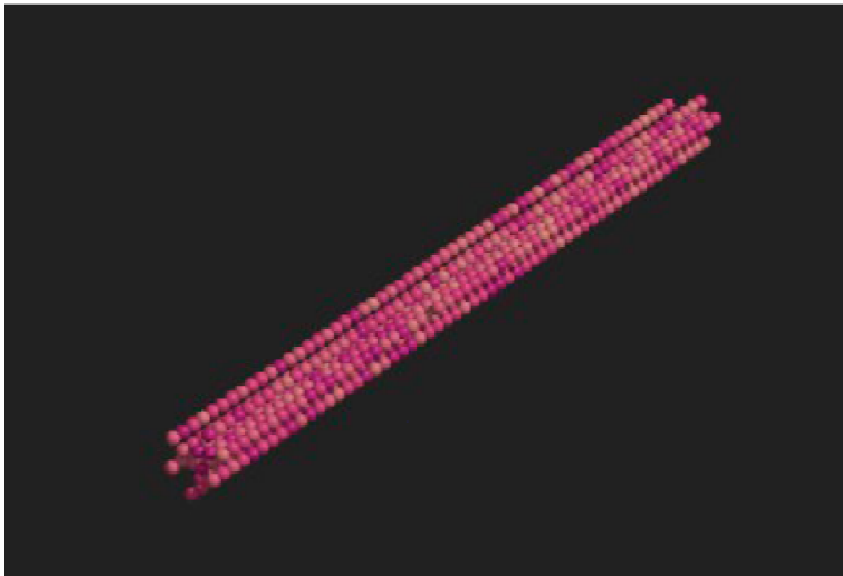
View along $\langle 111 \rangle$



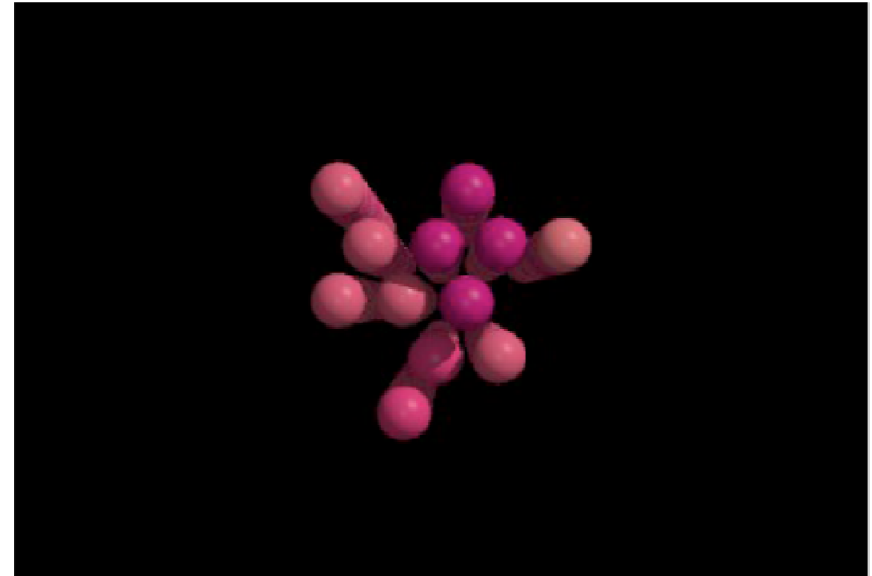
View away from $\langle 111 \rangle$



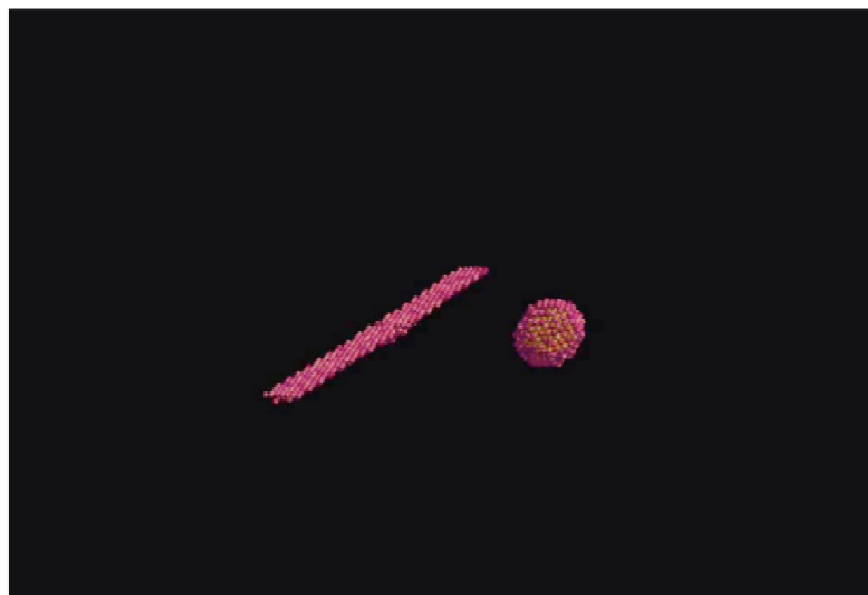
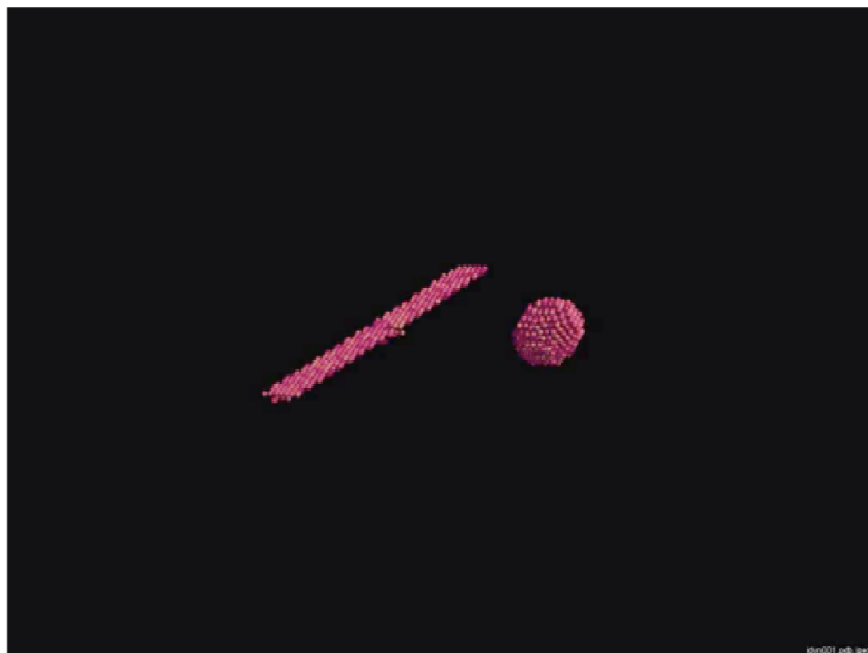
High Ep atoms



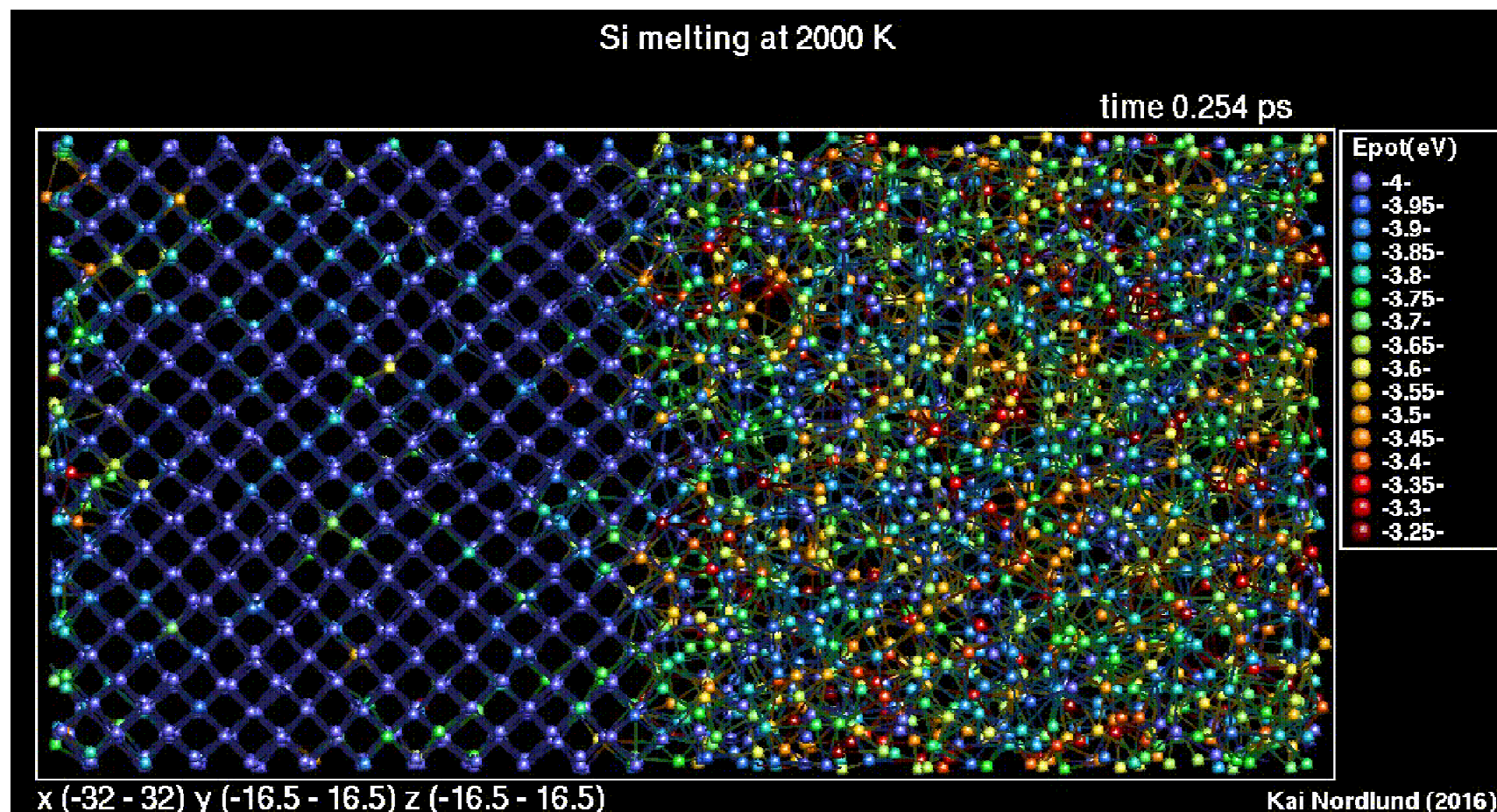
View along $\langle 111 \rangle$, high Ep atoms



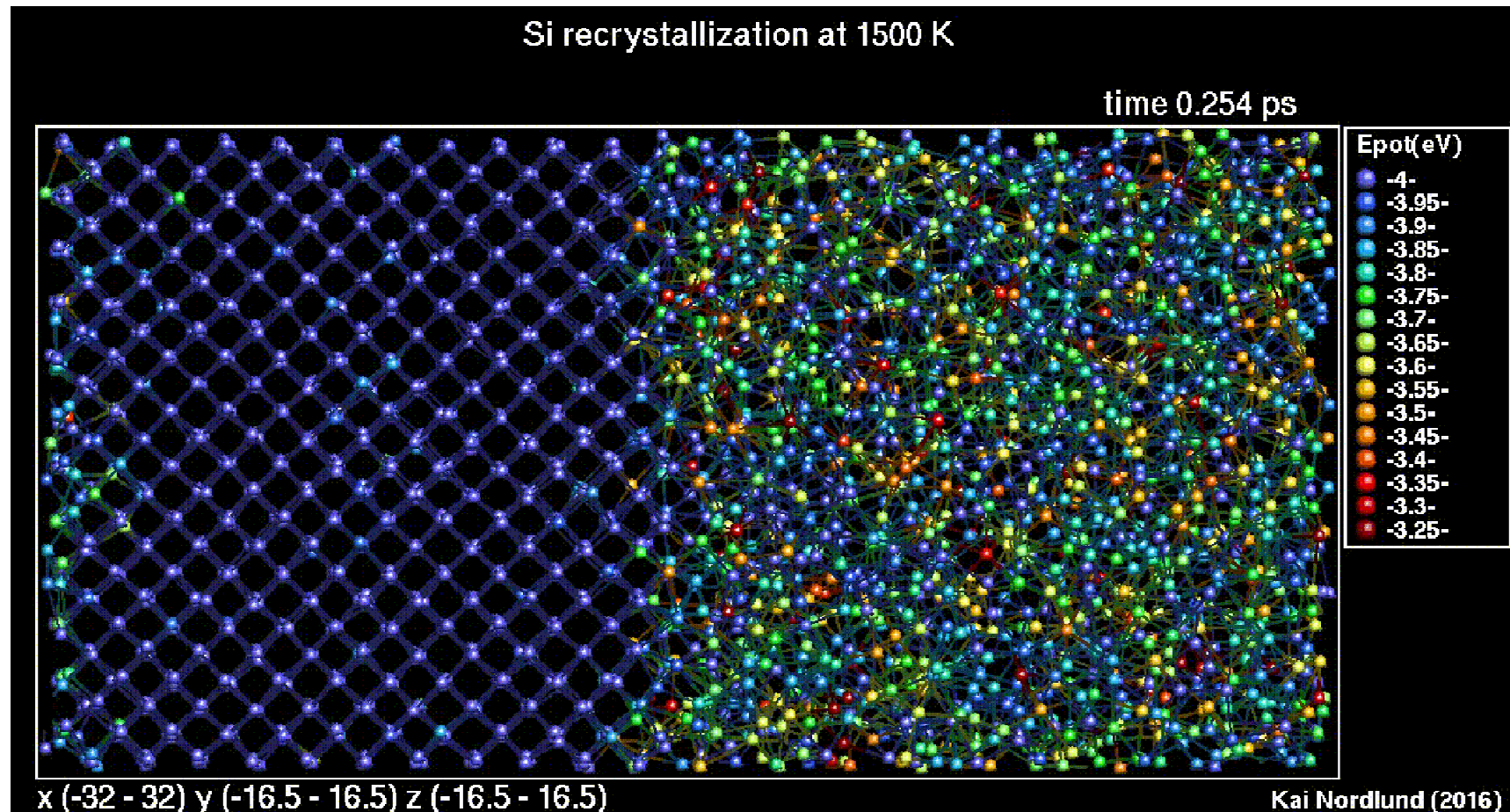
Hranová $\frac{1}{2}\langle 111 \rangle$ a bublina



Teplota tání



Teplota tání



NiTi sváření

10ns

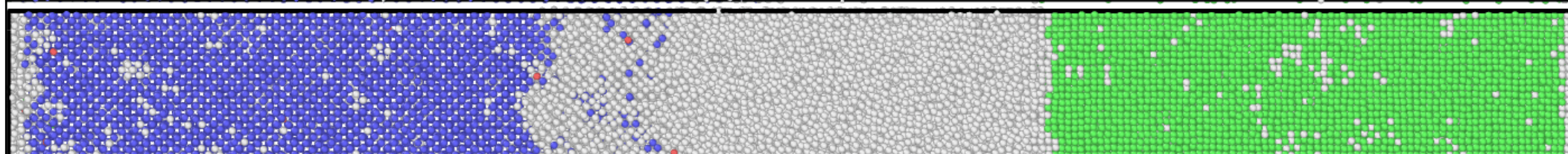
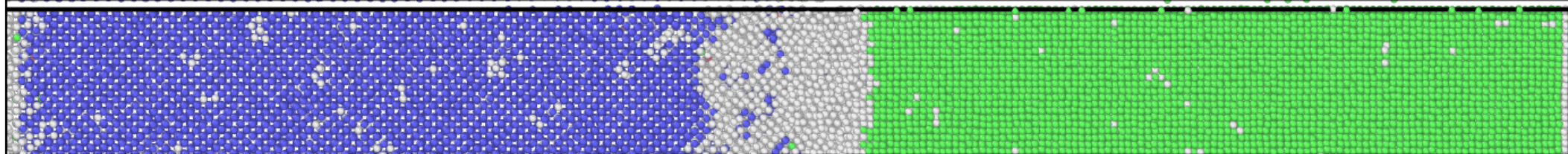
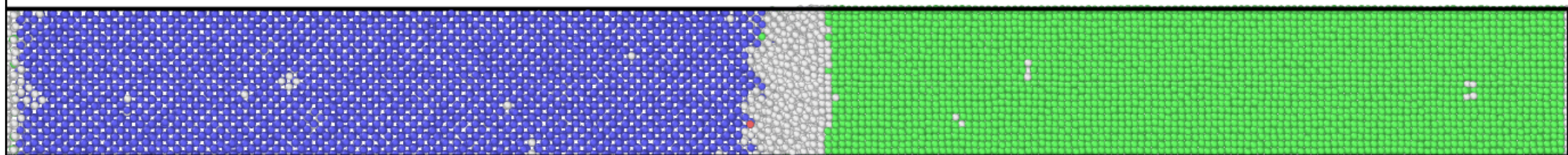
800K



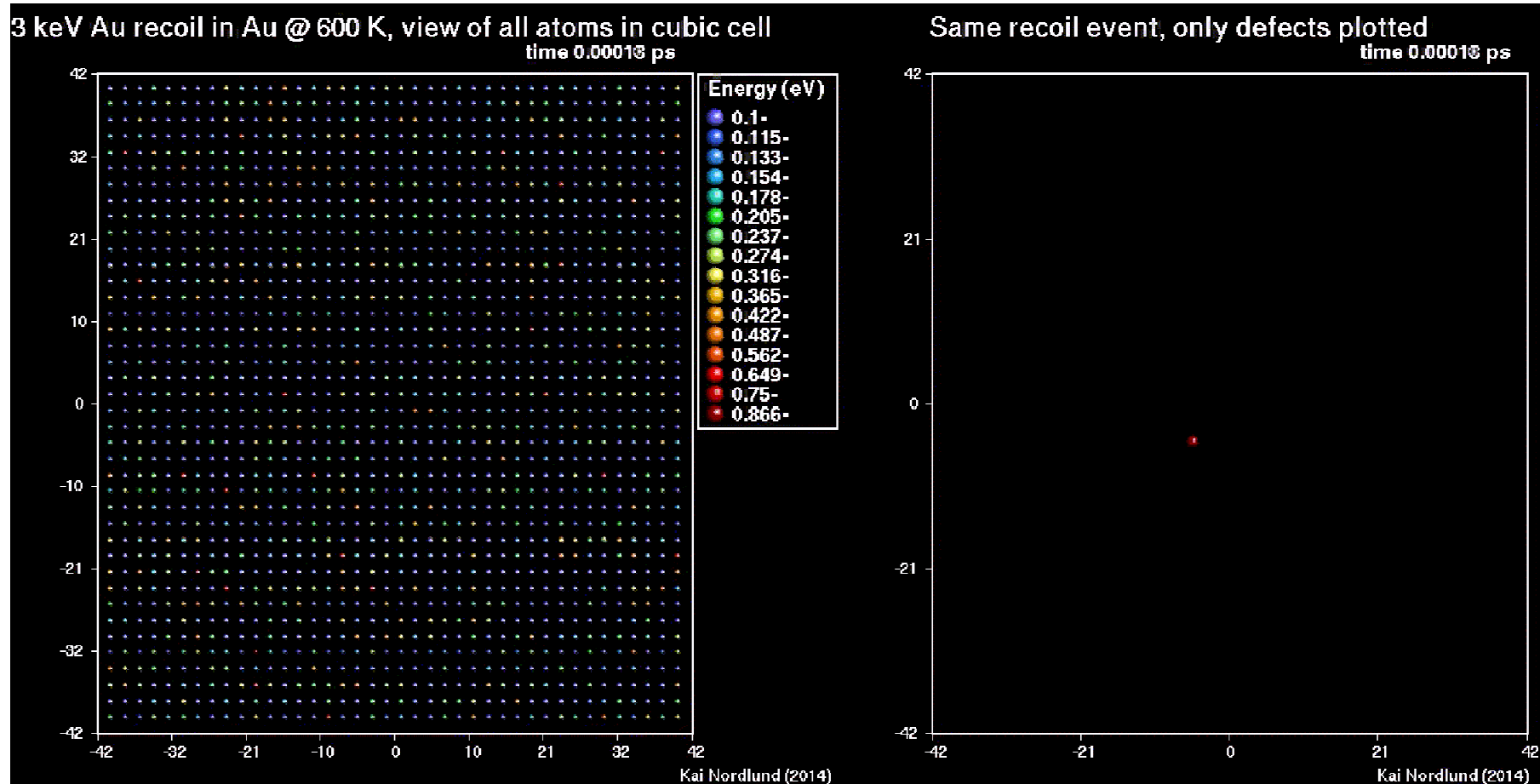
1000K



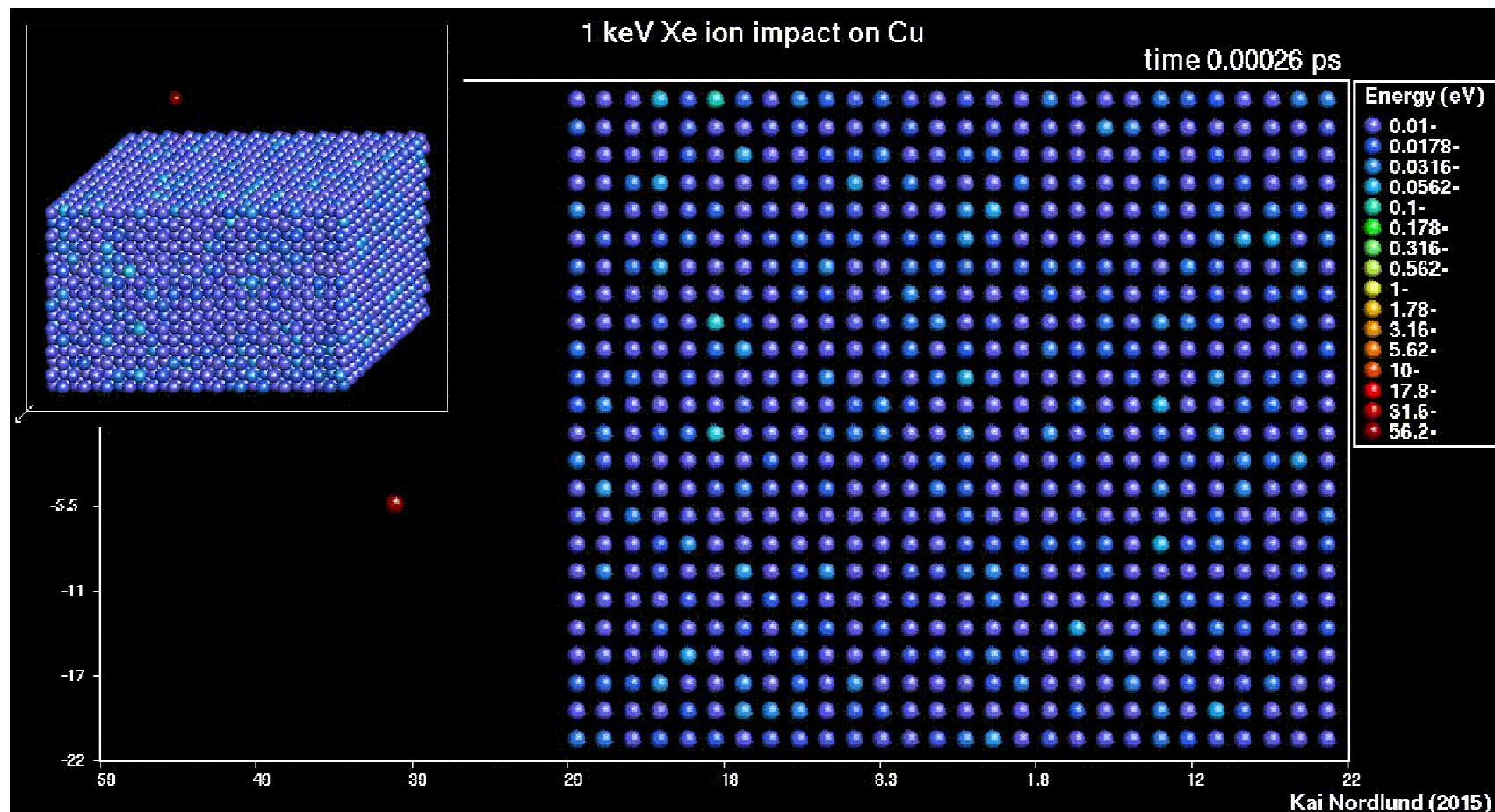
1200K



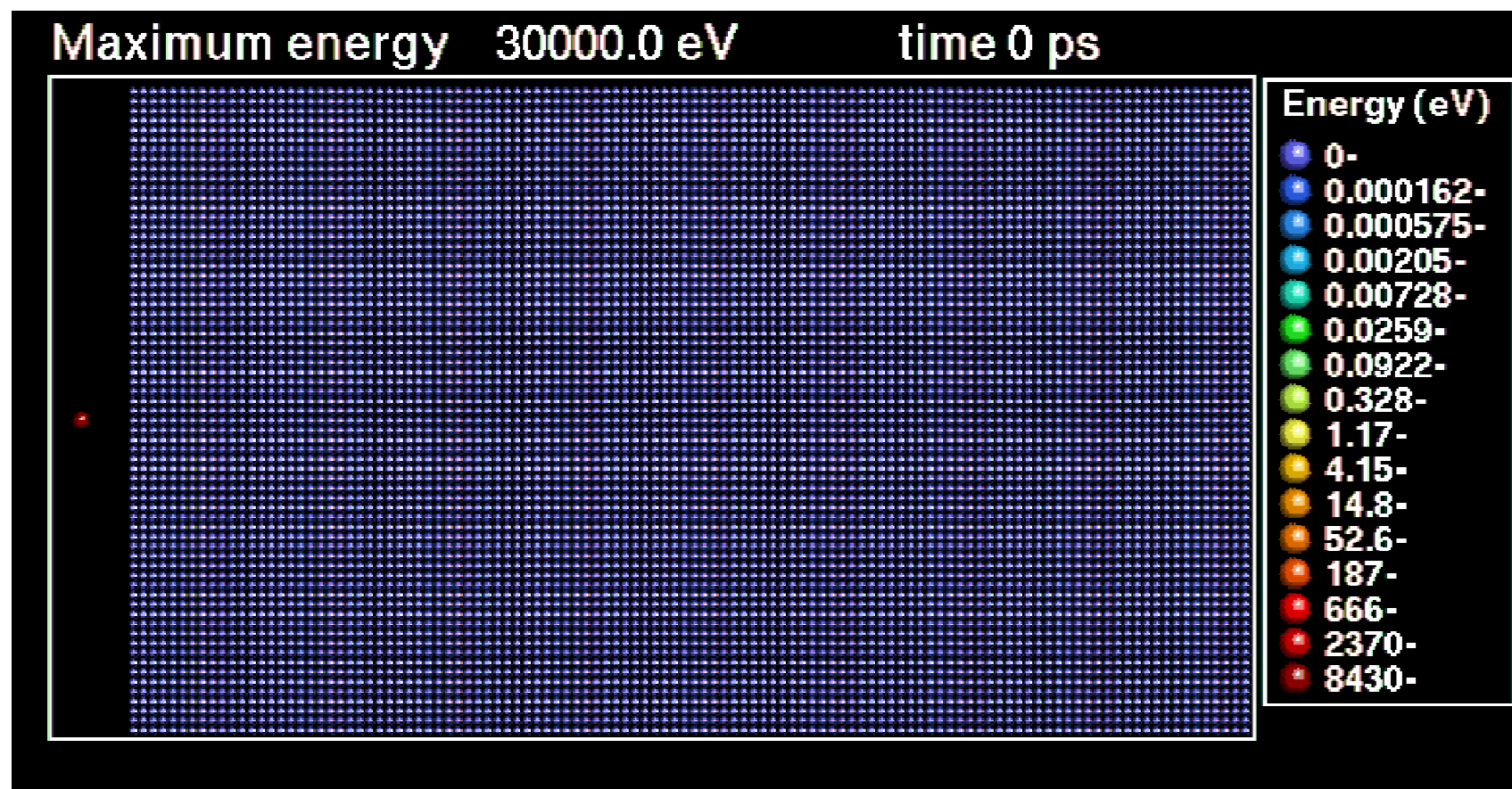
Radiační poškození neutron



Radiční poškození iont

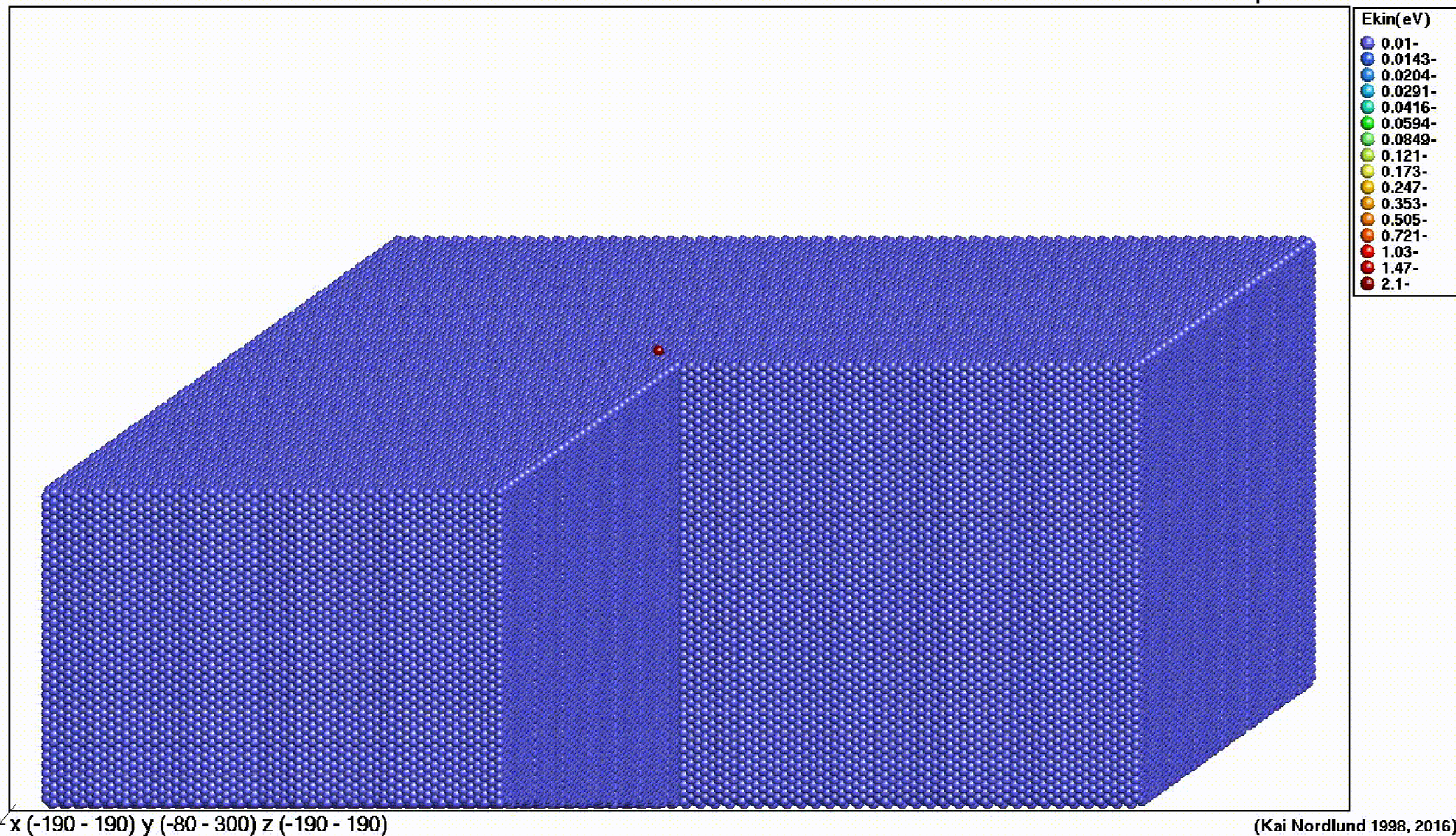


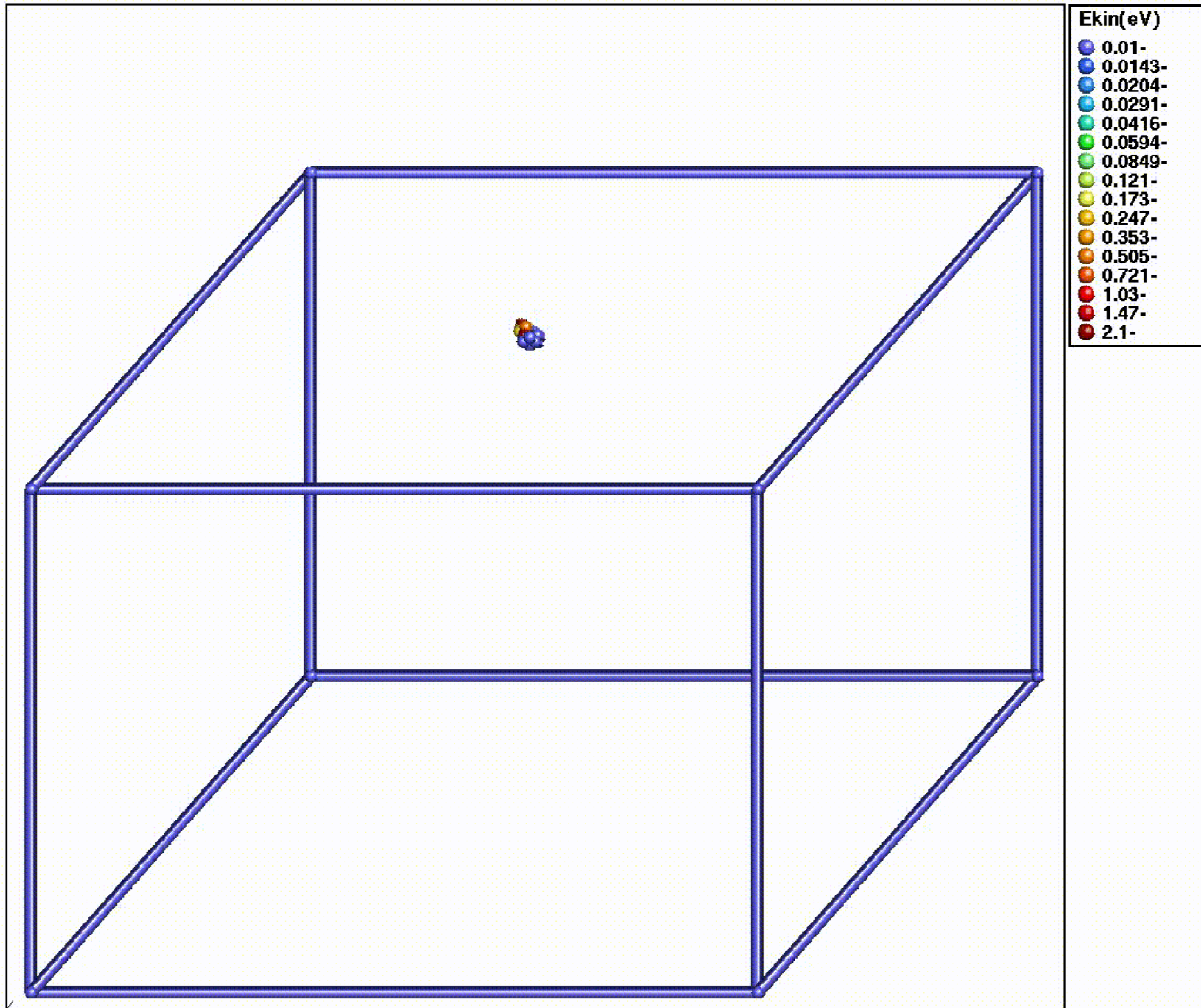
Radiční poškození iont



50 keV Xe impact on Au

time 0 ps

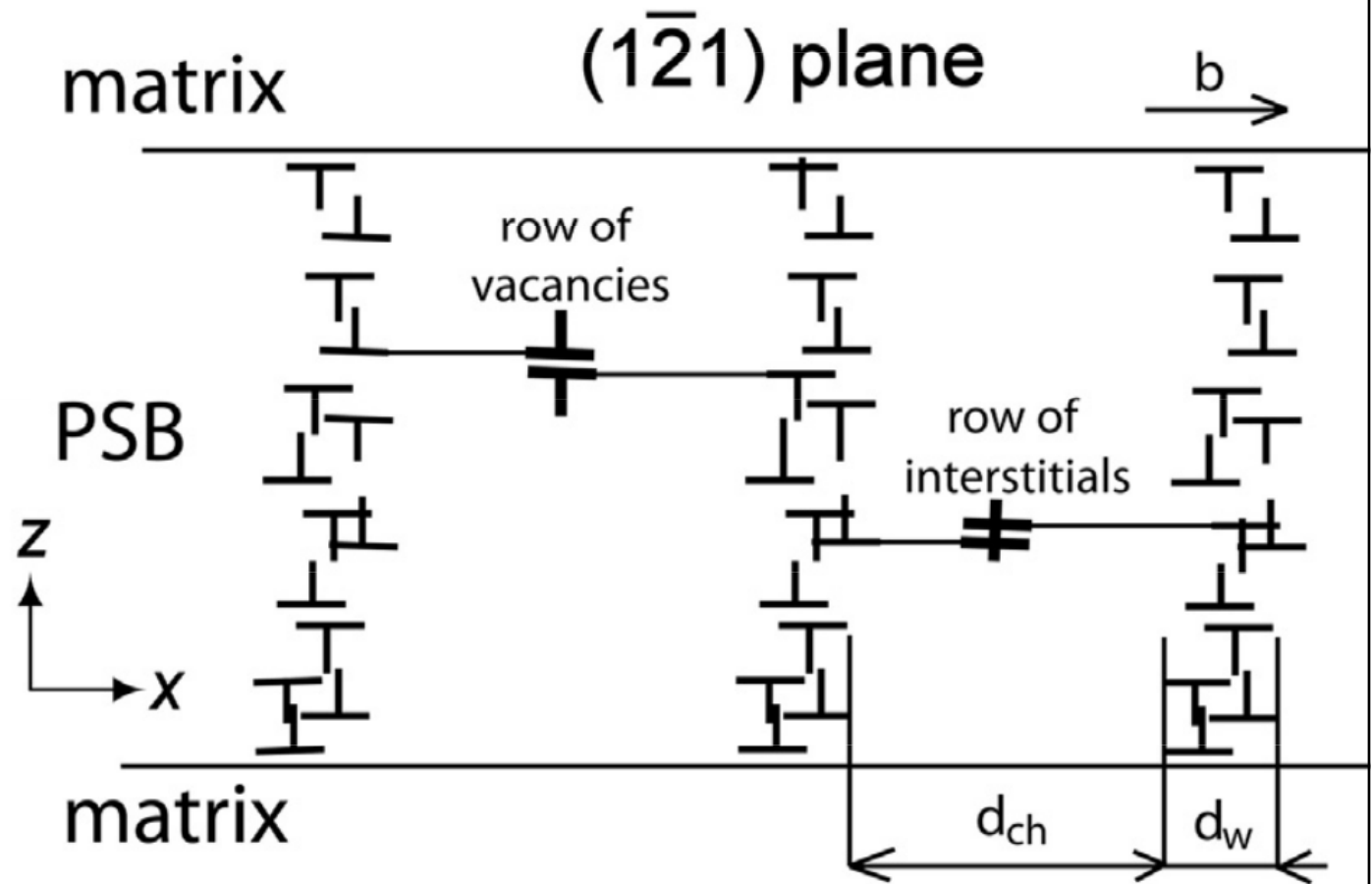
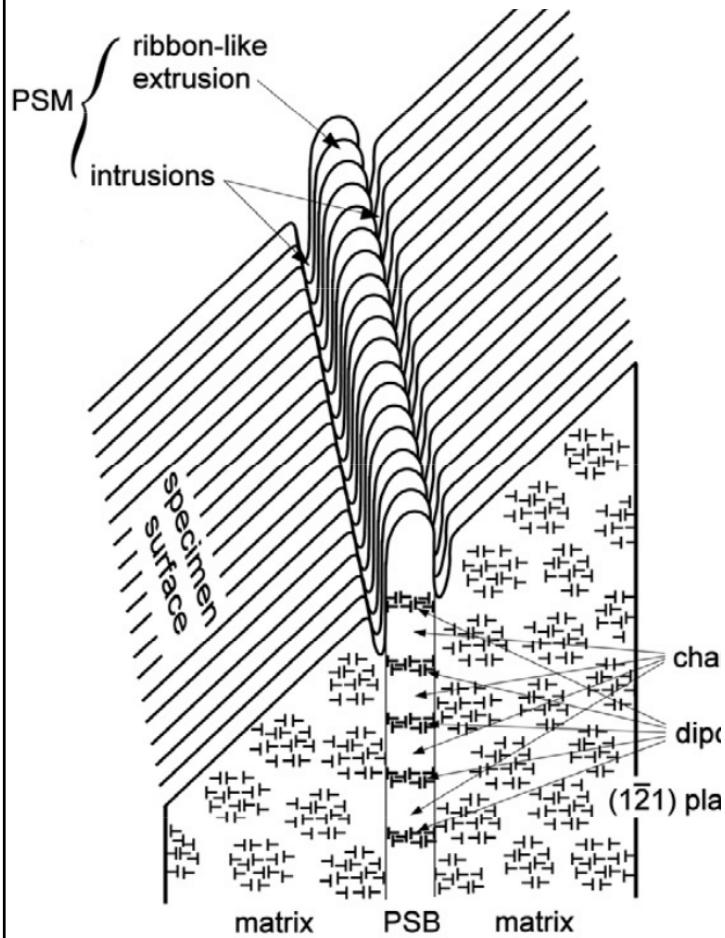




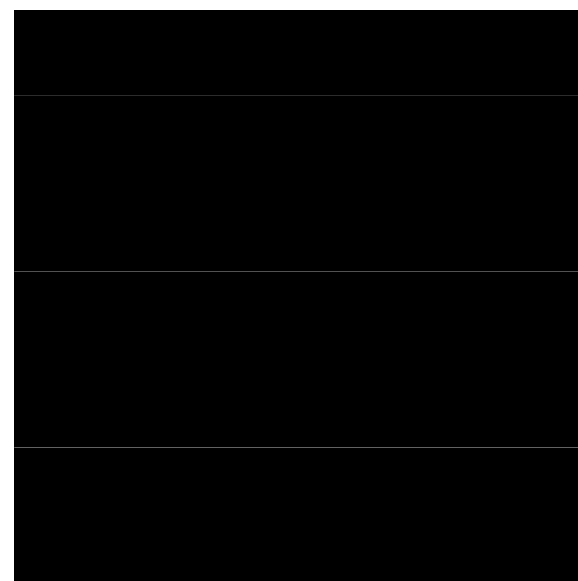
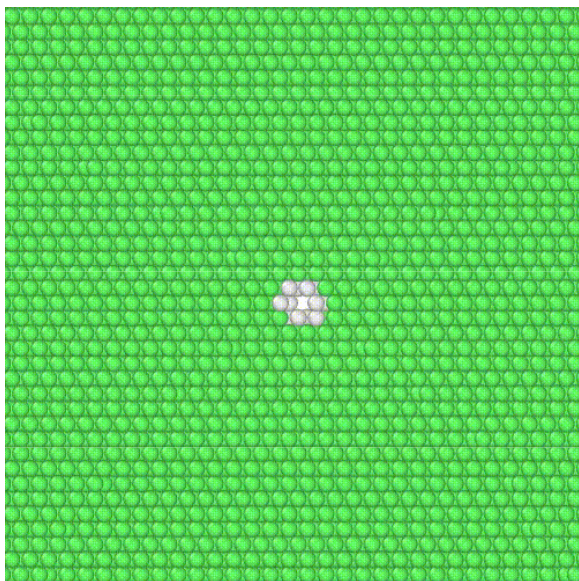
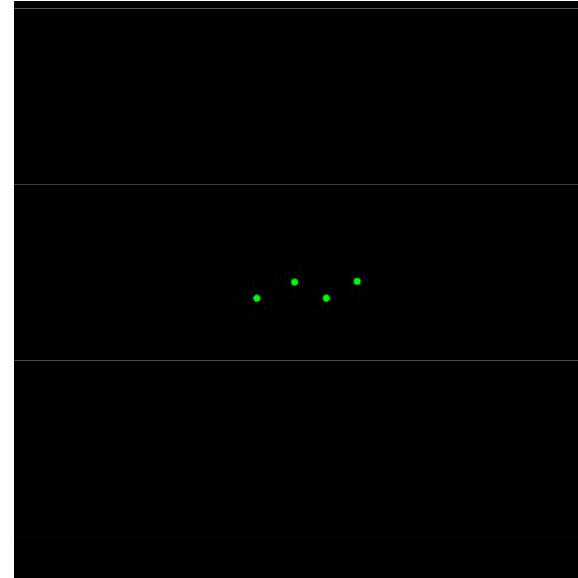
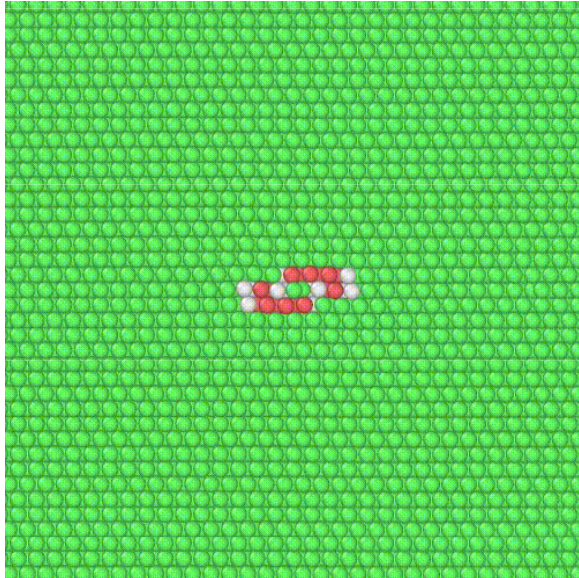
x (-190 - 190) y (-220 - 300) z (-190 - 190)

(Kai Nordlund 1998, 2016)

Únava Cu



Únava Cu



Únava Cu

