Special Topics on Basic EECS I
Design Technology Co-Optimization
Lecture 12

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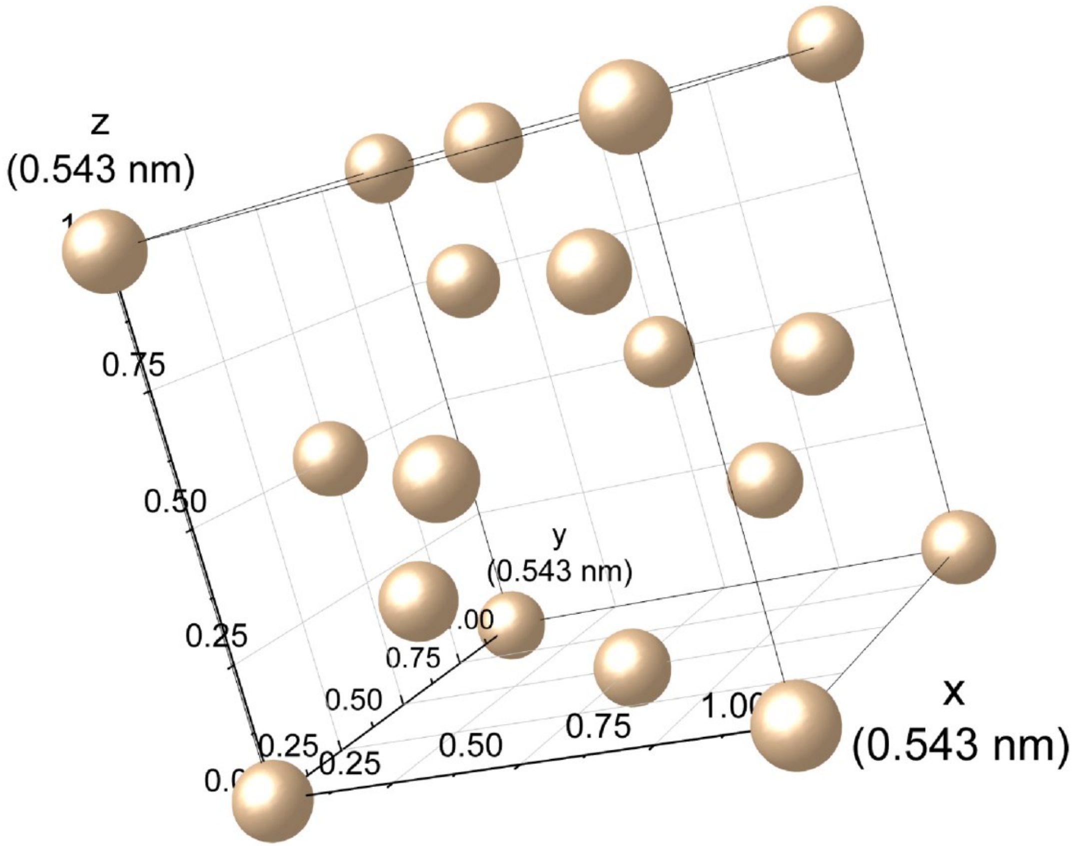
L12

Kinetic lattice Monte Carlo simulation

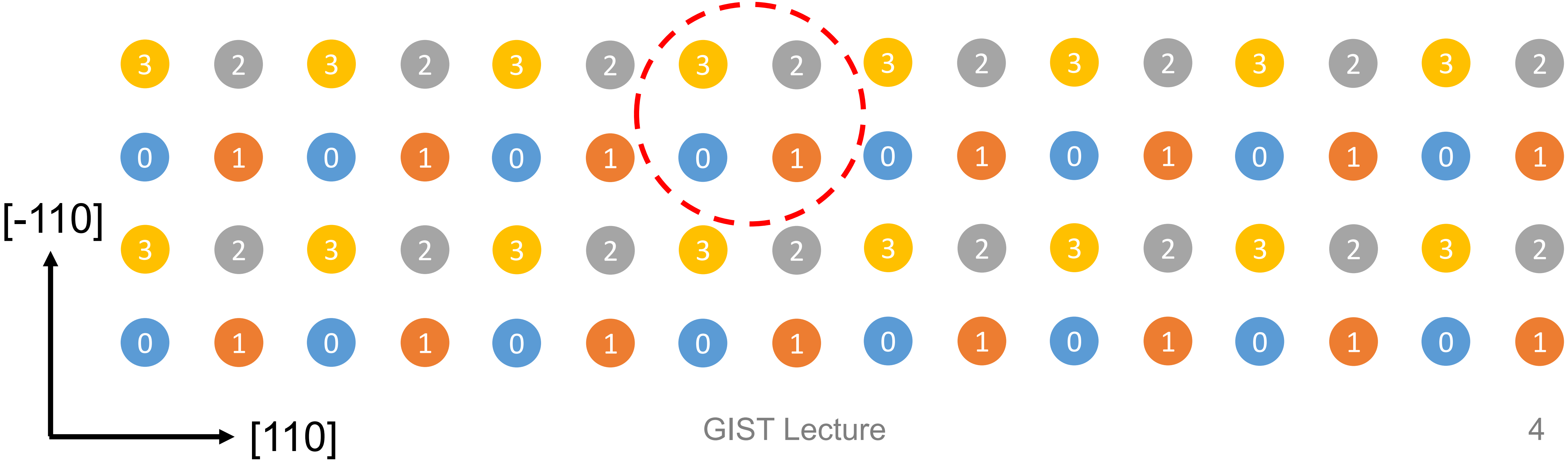
- Monte Carlo
  - Stochastic method for simulating discrete events over time
- Lattice
  - It assumes pre-defined atomic sites in a crystalline structure.
- Implementation
  - A prototype has been implemented in AngstromCraft.



Atomic structure of crystalline silicon

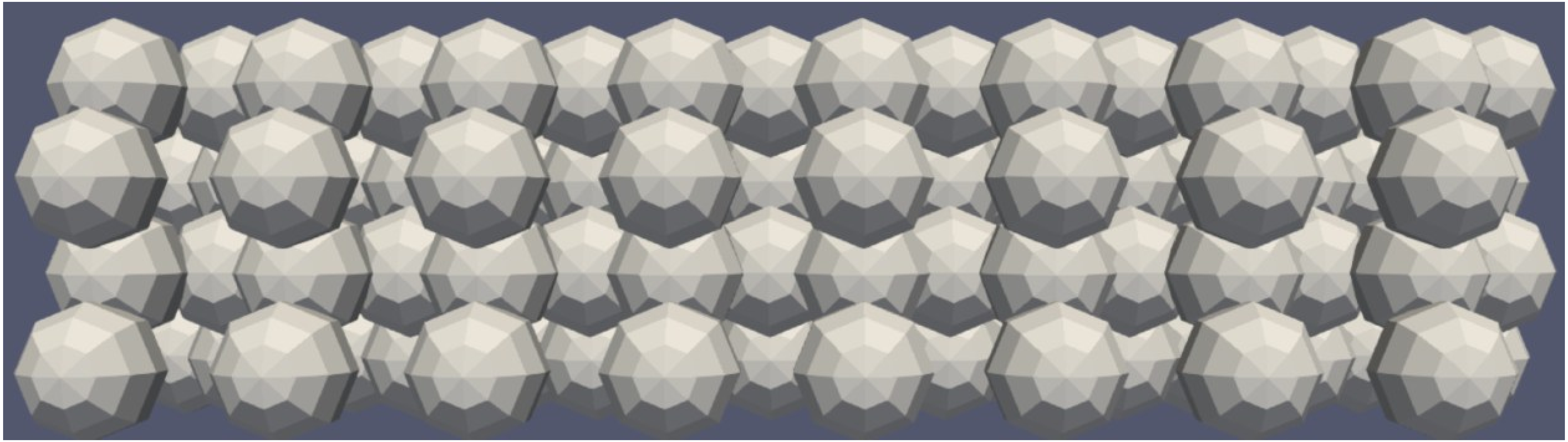
Atomic structure

- We assume (001) wafer and [110] channel direction.
  - Four layers are found.
  - Using triplet, (i, j, k), for a unit and an integer, a layer, we can uniquely determine the atomic position.



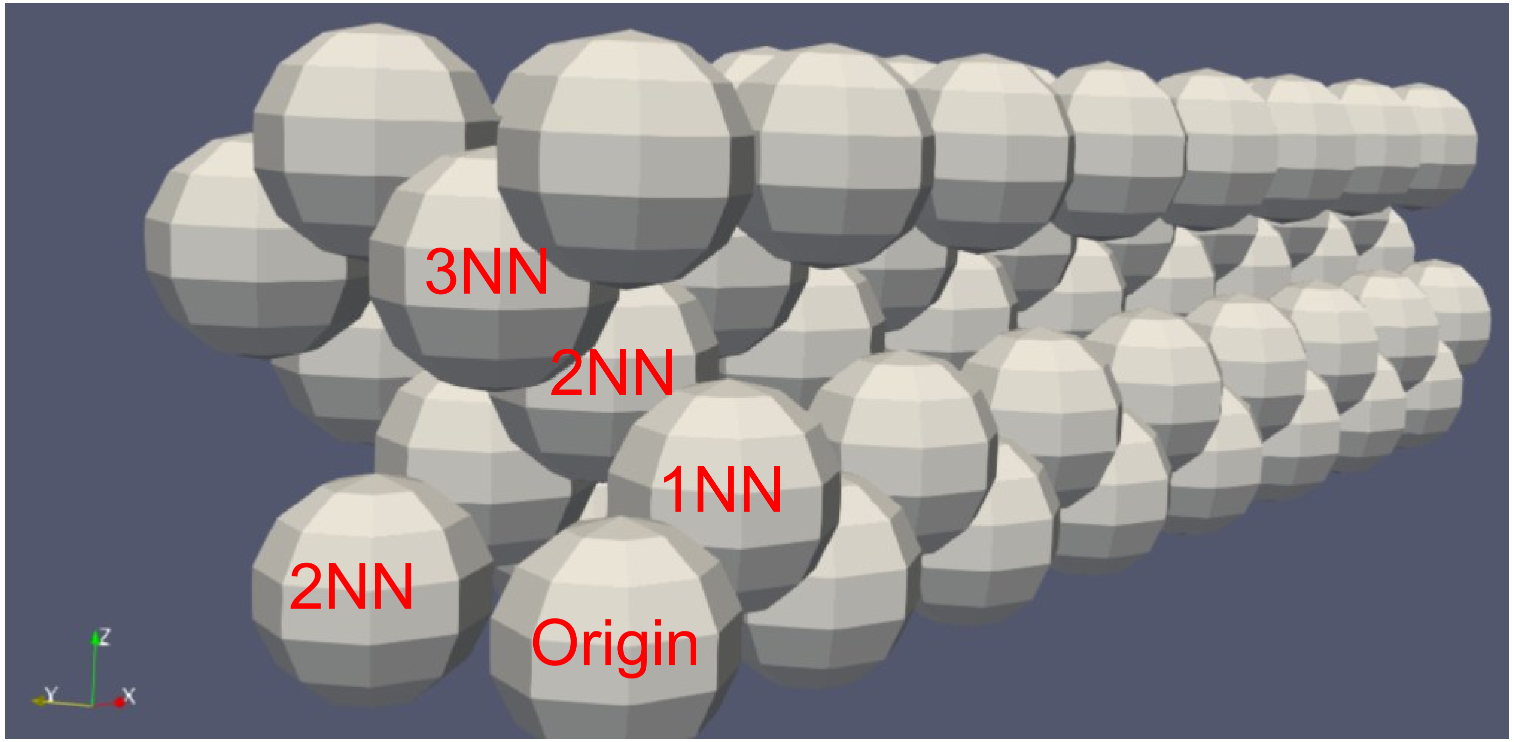
Visualization in Paraview

- In this example, a 9×2 array of atoms in the (001) plane
  - Four layers are found.



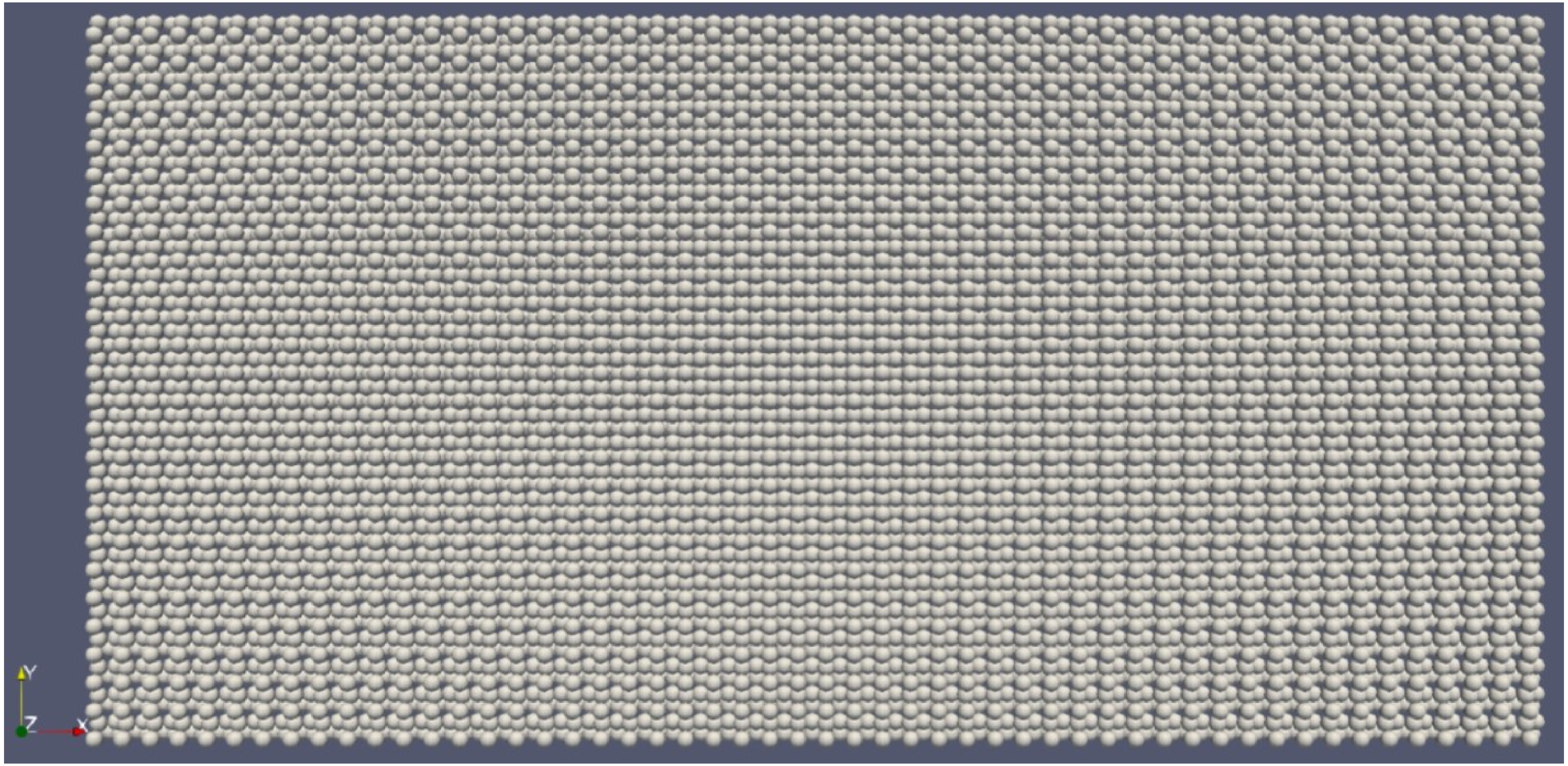
Nearest neighbors

- First, second, third
  - 4 first NNs, their distance is $\frac{\sqrt{3}}{4}a$. 12 second NNs, their distance is $\frac{\sqrt{2}}{2}a$. 12 third NNs, their distance is $\frac{\sqrt{11}}{4}a$.



A 20-by-10 nm^2 rectangle

- A 52×26 array of atoms in the (001) plane
  - Periodic boundary condition



Adsorption rate

- Following R. Chen et al., the adsorption rate is calculated as

$$\nu_{ads} \propto \exp\left(\frac{E_b}{k_B T}\right)$$

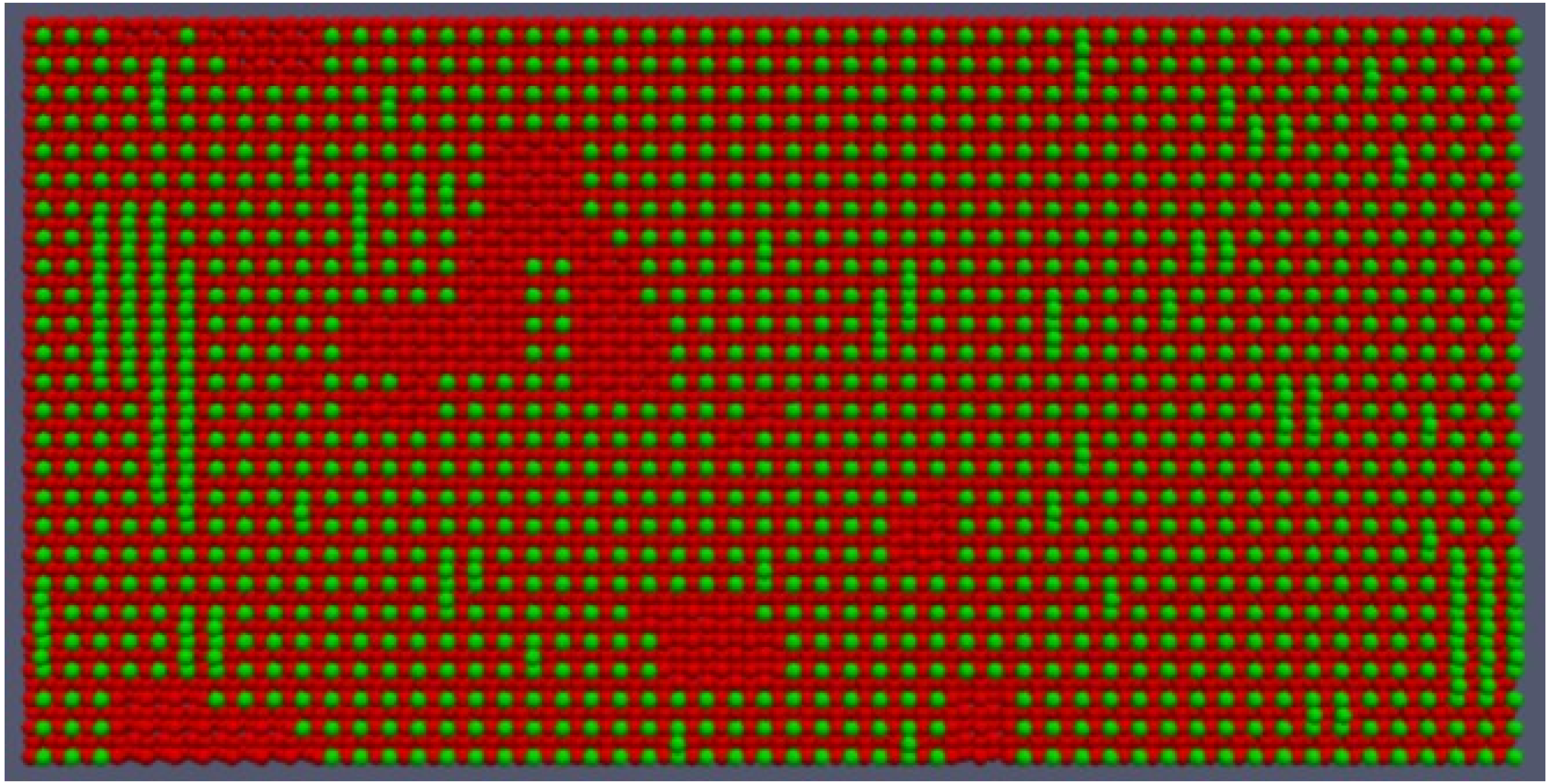
  - The total binding energy is calculated as

$$E_b = E_b^{1NN}(n_1) + n_2 E_b^{2NN} + n_3 E_b^{3NN}$$

  - R. Chen's parameters are $E_b^{2NN} = 0.15\ \mathrm{eV}$ and $E_b^{3NN} = 0.12\ \mathrm{eV}$.
  - For each site, the adsorption rate is calculated.
  - On a clean (001) surface, we have $n_1 = 2$, $n_2 = 4$, and $n_3 = 6$.
  - When another atom is added next to that atom, we have $n_1 = 2$, $n_2 = 5$, and $n_3 = 6$.
  - At 600 ℃, 0.15 eV yields 7.3 times higher adsorption rate.

Adding some atoms randomly

- 676 (= 52 X 26) atoms
  - It is simulated at 600 ℃.
  - The surface is not uniform.

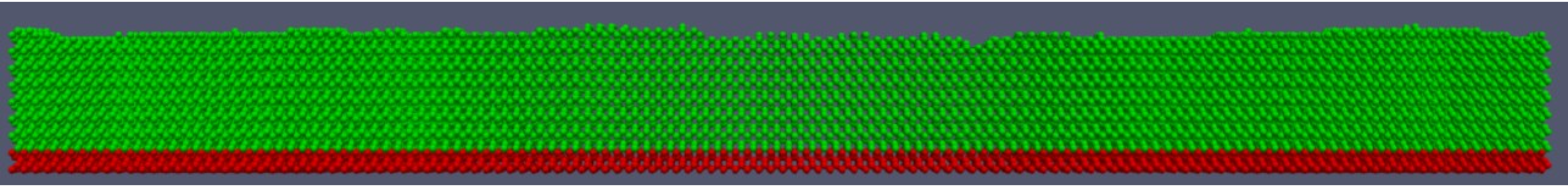


Introducing "hard walls"

- These walls do not provide the nearest neighbors.
  - Reduction of NNs
  - For a clean (001) surface, there are 2 1st NNs, 4 2nd NNs, and 6 3rd NNs.
  - When a hard wall exists, there may be various cases.
  - $n_1 = 2$, $n_2 = 2$, and $n_3 = 3$ ➔ 0.66 eV reduction
  - $n_1 = 2$, $n_2 = 4$, and $n_3 = 6$ ➔ No reduction
  - $n_1 = 2$, $n_2 = 4$, and $n_3 = 4$ ➔ 0.24 eV reduction
  - $n_1 = 1$, $n_2 = 2$, and $n_3 = 4$ ➔ 0.64 eV reduction
  - Therefore, hard walls significantly slow down the growth.

With/without hard walls

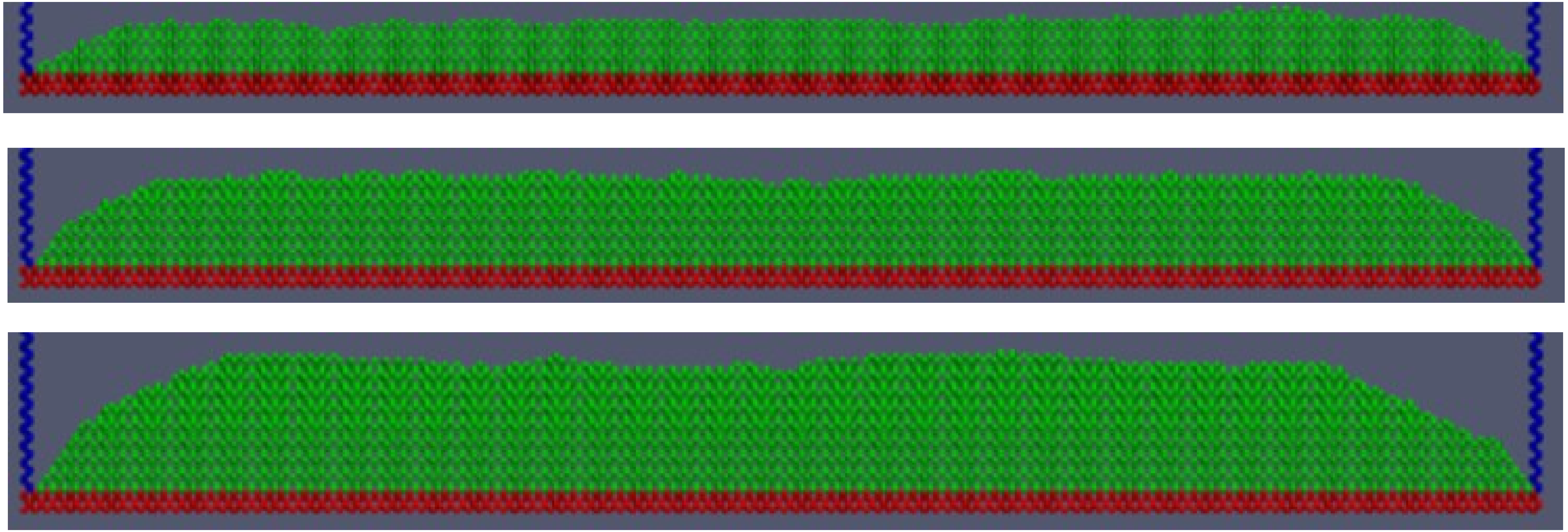
- 50-nm-long structure
  - Along the y-direction, only three units are assigned.
  - When 28 layers (~ 3.8 nm) are deposited without hard walls, we has an almost uniform profile.



  - Hard walls (blue atoms)

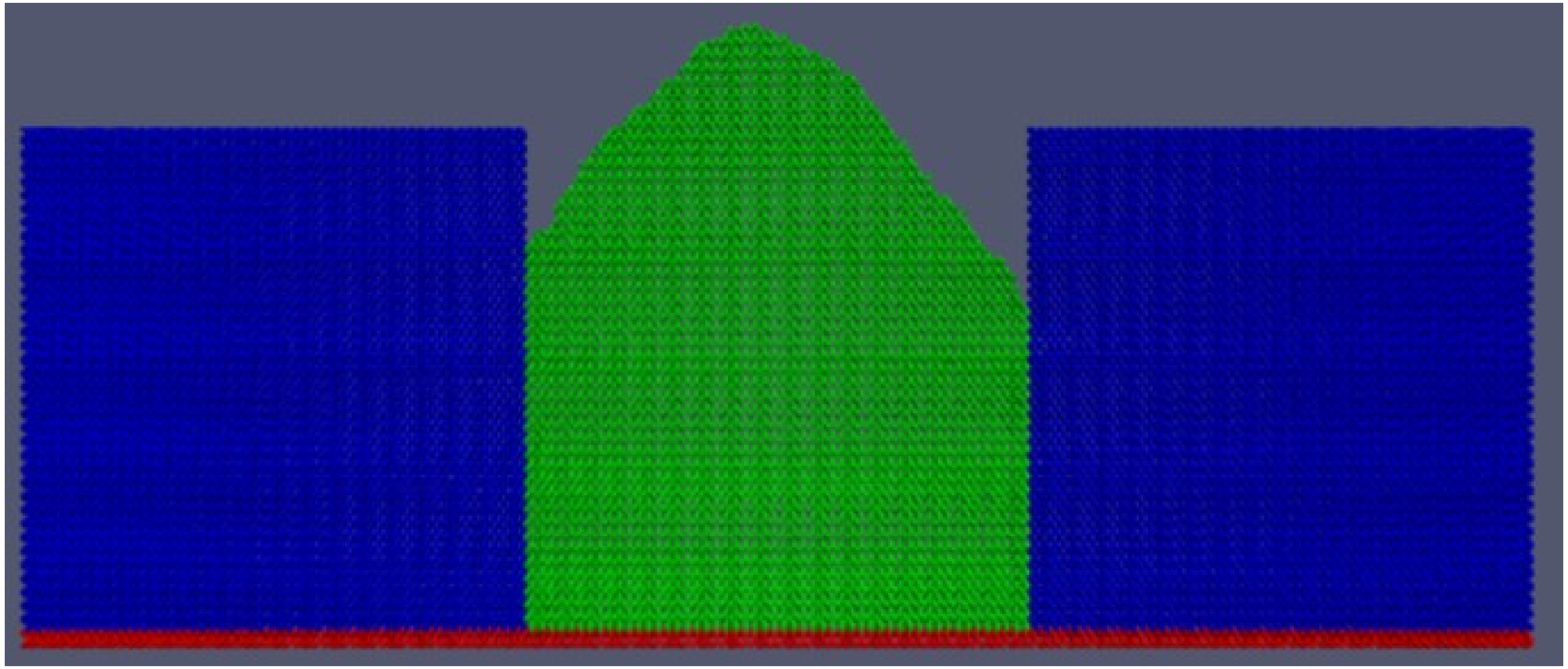
12, 20, and 28 layers

- {311} surfaces and {111} surfaces



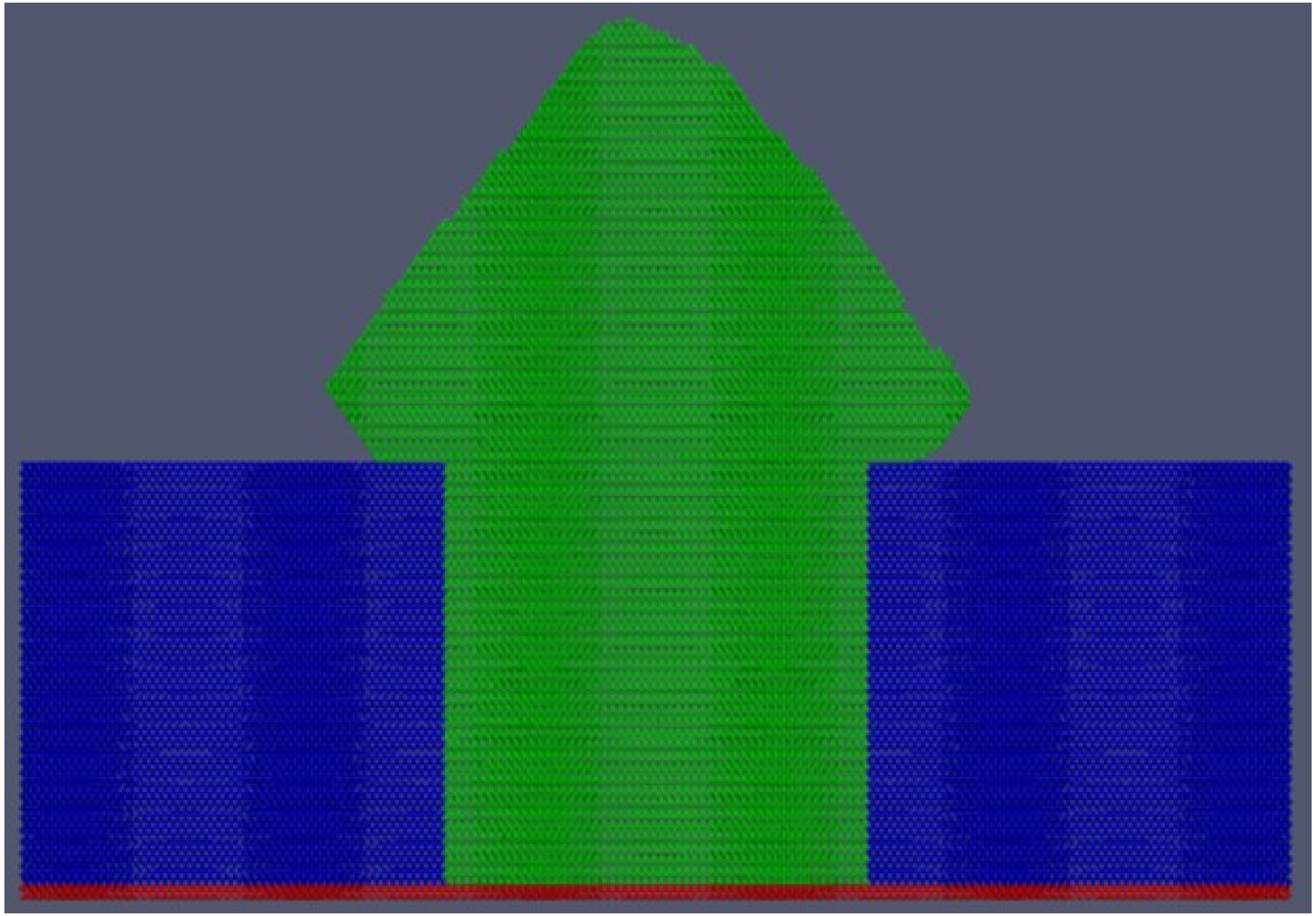
Another example, a 20-nm-thick fin

- 147 layers (~ 20 nm, when uniformly distributed)
  - {111} surfaces become dominant.



294 layers

- A diamond-like shape is clearly observed.



Thank you!