Structure and energy properties of Fe_xCu_{1-x} nanoparticles

Morphology and size effects

J. Rojas-Nunez[1 4] , S.E. Baltazar[1 4] , R.I. González[2 4] , E.M. Bringa[3] and S. Allende[1 4]

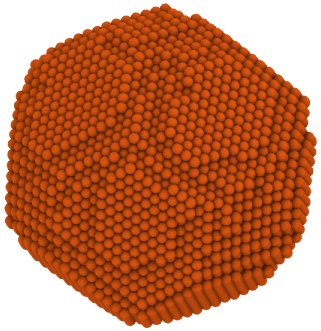
[1]Physics department, Universidad de Santiago de Chile, Santiago, Chile
[2]Centro de Genómica y Bioinformática, Facultad de Ciencias, Universidad Mayor, Santiago, Chile
[3]CONICET & Facultad de Ciencias Exactas y Naturales, Universidad Nacional de Cuyo, Mendoza, Argentina
[4]Center for the Development of Nanoscience and Nanotechnology (CEDENNA), Santiago, Chile

August 1, 2017

Bimetallic nanoparticles

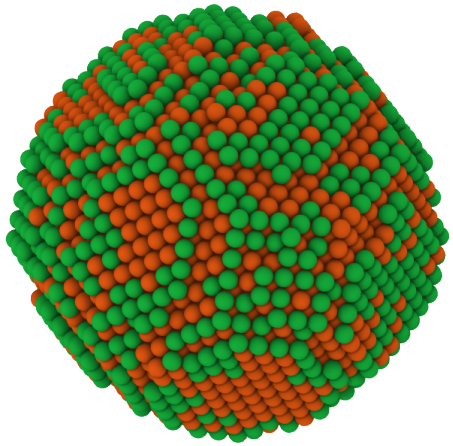
What are bimetallic nanoparticles?

Nanoparticles



Nanoparticle

Fe Cu



Bimetallic (Fe-Cu) nanoparticle

What are the special features about these nanoparticles?

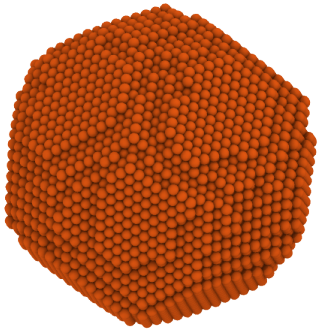
- More surface-volume ratio
- Different properties from their respective bulk materials

UdeSantiago de Chile

Bimetallic nanoparticles

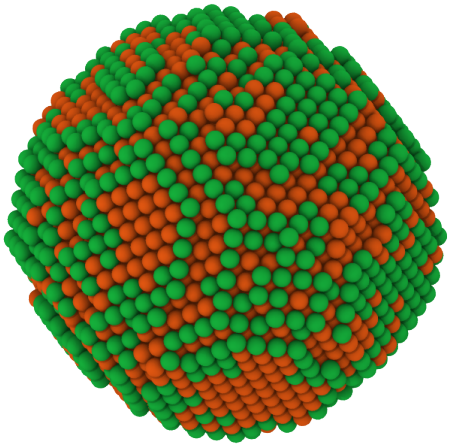
What are bimetallic nanoparticles?

Nanoparticles $1 \sim 100nm$



Nanoparticle

Fe Cu



Bimetallic (Fe-Cu) nanoparticle

What are the special features about these nanoparticles?

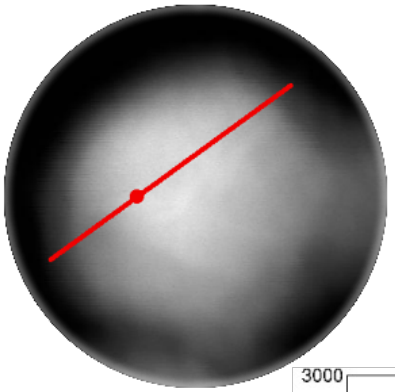
- More surface-volume ratio
- Different properties from their respective bulk materials

Bimetallic nanoparticles

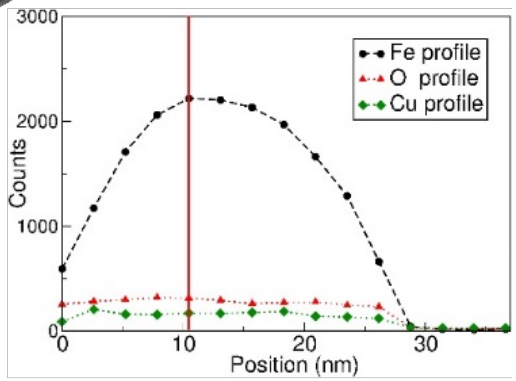
FeCu nanoparticles

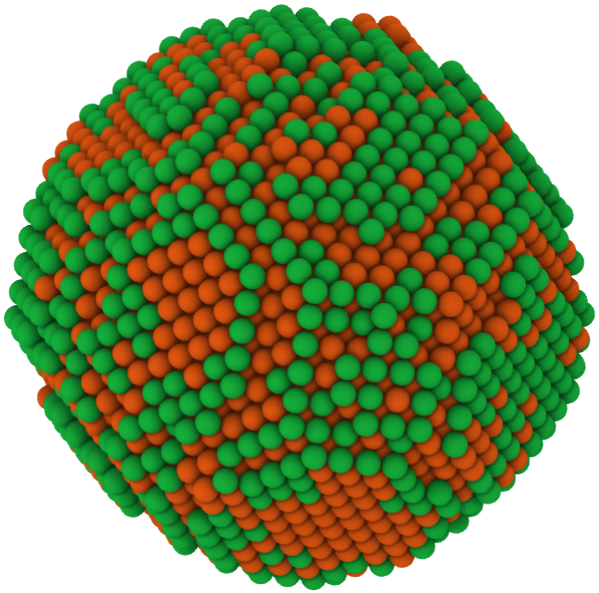
FeCu NP's

- Magnetic properties
- Arsenic adsorption



Linear mapping of FeCu NP*





* P. Sepulveda et al., submitted to ACS Appl. Mater. Interfaces (2017)

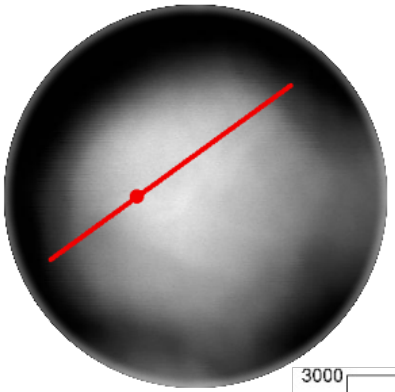
UdeSantiago de Chile

Bimetallic nanoparticles

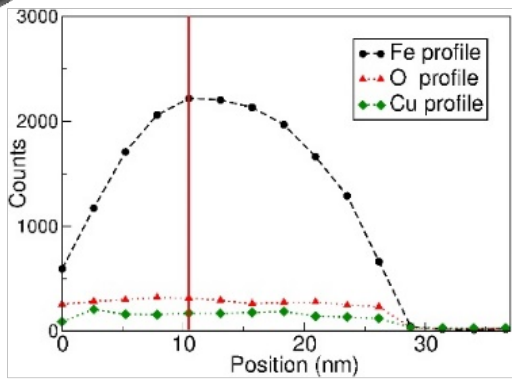
FeCu nanoparticles

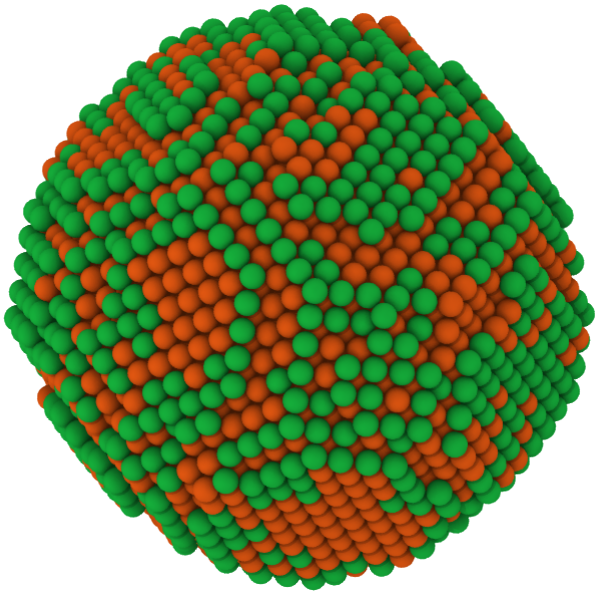
FeCu NP's

- Magnetic properties
- Arsenic adsorption



Linear mapping of FeCu NP*





* P. Sepulveda et al., submitted to ACS Appl. Mater. Interfaces (2017)

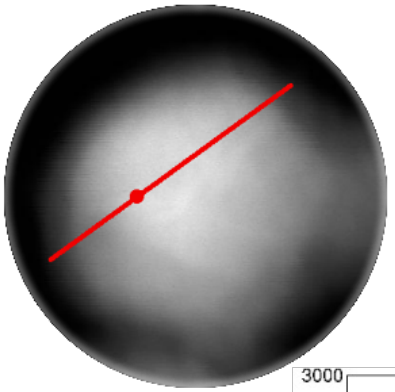
UdeSantiago de Chile

Bimetallic nanoparticles

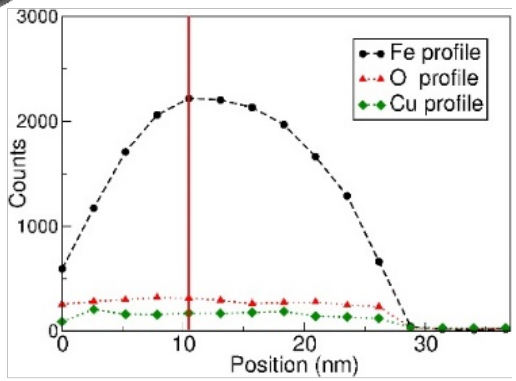
FeCu nanoparticles

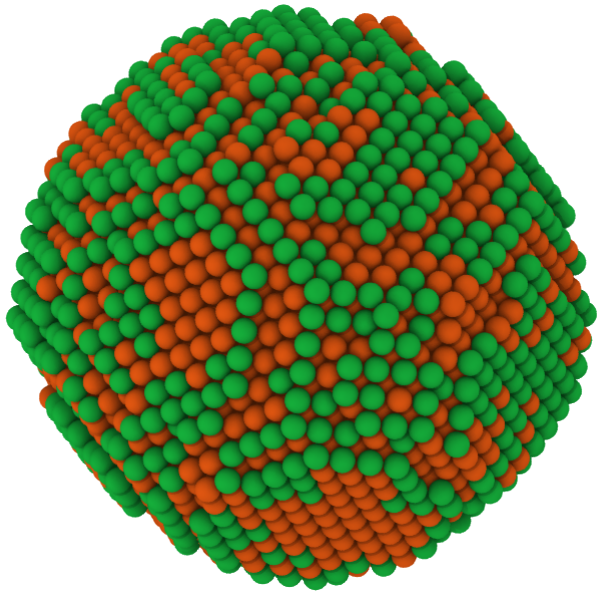
FeCu NP's

- Magnetic properties
- Arsenic adsorption



Linear mapping of FeCu NP*





What happens at different concentrations?

* P. Sepulveda et al., submitted to ACS Appl. Mater. Interfaces (2017)

UdeSantiago de Chile

Simulation method

Ensemble & interaction potential

Molecular dynamic simulations are performed using LAMMPS

Configurations

- Timestep: 1fs
- NVT ensemble
  - –Noose-Hover thermostat
  - –Apply temperature
- EAM interaction
  - –Parameters from Bonny et al. 2009

$$E_i = F_i\left(\sum_{j\neq i}\rho_j(r_{ij})\right) + \sum_{j\neq i}\phi_{ij}(r_{ij})$$

UdeSantiago de Chile

Simulation method

Ensemble & interaction potential

Molecular dynamic simulations are performed using LAMMPS

Configurations

- Timestep: 1fs
- NVT ensemble
  - –Noose-Hover thermostat
  - –Apply temperature
- EAM interaction
  - –Parameters from Bonny et al. 2009

$$E_i = F_i\left(\sum_{j\neq i}\rho_j(r_{ij})\right) + \sum_{j\neq i}\phi_{ij}(r_{ij})$$

Simulation method

Ensemble & interaction potential

Molecular dynamic simulations are performed using LAMMPS

Configurations

- Timestep: 1fs
- NVT ensemble
  - –Noose-Hover thermostat
  - –Apply temperature
- EAM interaction
  - –Parameters from Bonny et al. 2009

$$E_i = F_i\left(\sum_{j\neq i}\rho_j(r_{ij})\right) + \sum_{j\neq i}\phi_{ij}(r_{ij})$$

UdeSantiago de Chile

Simulation method

Ensemble & interaction potential

Molecular dynamic simulations are performed using LAMMPS

Configurations

- Timestep: 1fs
- NVT ensemble
  - –Noose-Hover thermostat
  - –Apply temperature
- EAM interaction
  - –Parameters from Bonny et al. 2009

Embedding function

$$\mathrm{E_i} = \mathrm{F_i}\left(\sum_{j\neq i}\rho_j(r_{ij})\right) + \sum_{j\neq i}\phi_{ij}(r_{ij})$$

UdeSantiago de Chile

Simulation method

Ensemble & interaction potential

Molecular dynamic simulations are performed using LAMMPS

Configurations

- Timestep: 1fs
- NVT ensemble
  - –Noose-Hover thermostat
  - –Apply temperature
- EAM interaction
  - –Parameters from Bonny et al. 2009

Embedding function

$$\mathrm{E_i} = \mathrm{F_i}\left(\sum_{j\neq i}\rho_j(r_{ij})\right) + \sum_{j\neq i}\phi_{ij}(r_{ij})$$

Pair interaction

Simulation method

Ensemble & interaction potential

Molecular dynamic simulations are performed using LAMMPS

Configurations

- Timestep: 1fs
- NVT ensemble
  - –Noose-Hover thermostat
  - –Apply temperature
- EAM interaction
  - –Parameters from Bonny et al. 2009

Embedding function

$$E_i = F_i\left(\sum_{j\neq i}\rho_j(r_{ij})\right) + \sum_{j\neq i}\phi_{ij}(r_{ij})$$

Pair interaction

No angular terms

UdeSantiago de Chile

Simulation method

Ensemble & interaction potential

Molecular dynamic simulations are performed using LAMMPS

Configurations

- Timestep: 1fs
- NVT ensemble
  –Noose-Hover thermostat
  –Apply temperature
- EAM interaction
  –Parameters from Bonny et al. 2009

Embedding function

$$\mathrm{E_i} = \mathrm{F_i}\left(\sum_{j\neq i}\rho_j(r_{ij})\right) + \sum_{j\neq i}\phi_{ij}(r_{ij})$$

Pair interaction

UdeSantiago de Chile

Simulation method

Ensemble & interaction potential

Molecular dynamic simulations are performed using LAMMPS

Configurations

- Timestep: 1fs
- NVT ensemble
  –Noose-Hover thermostat
  –Apply temperature
- EAM interaction
  –Parameters from Bonny et al. 2009

Embedding function

$$\mathrm{E_i} = \mathrm{F_i}\left(\sum_{j\neq i}\rho_j(r_{ij})\right) + \sum_{j\neq i}\phi_{ij}(r_{ij})$$

Pair interaction

UdeSantiago de Chile

Simulation method

Ensemble & interaction potential

Molecular dynamic simulations are performed using LAMMPS

Configurations

- Timestep: 1fs
- NVT ensemble
  –Noose-Hover thermostat
  –Apply temperature
- EAM interaction
  –Parameters from Bonny et al. 2009

Embedding function

$$\mathrm{E_i} = \mathrm{F_i}\left(\sum_{j\neq i}\rho_j(r_{ij})\right) + \sum_{j\neq i}\phi_{ij}(r_{ij})$$

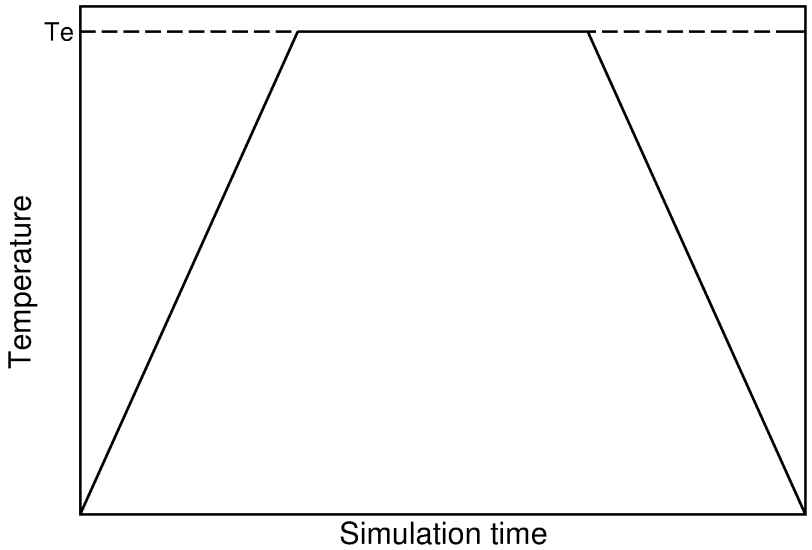
Pair interaction

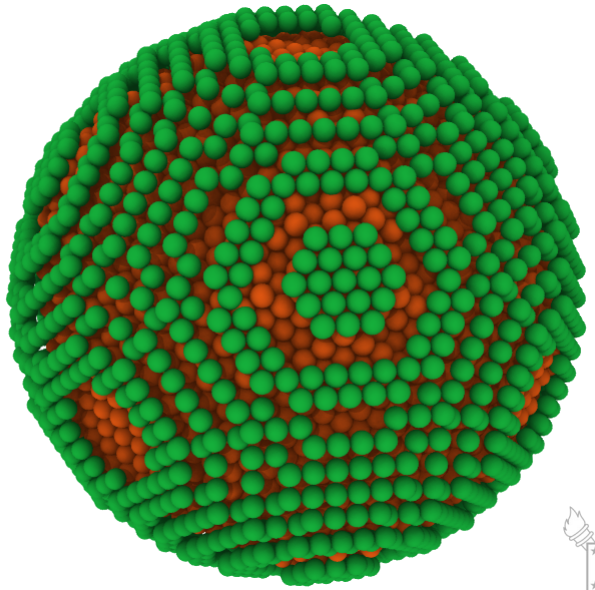
Simulation method

The annealing cycles

Searching process (The cycles)

Heating $\rightarrow$ Thermal equilibrium (Te) $\rightarrow$ Cooling $\rightarrow$ Minimization





UdeSantiago de Chile

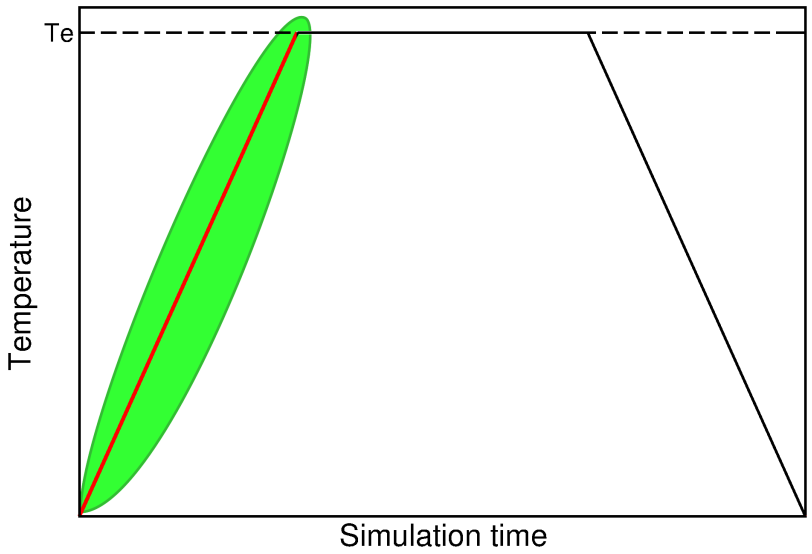
Simulation method

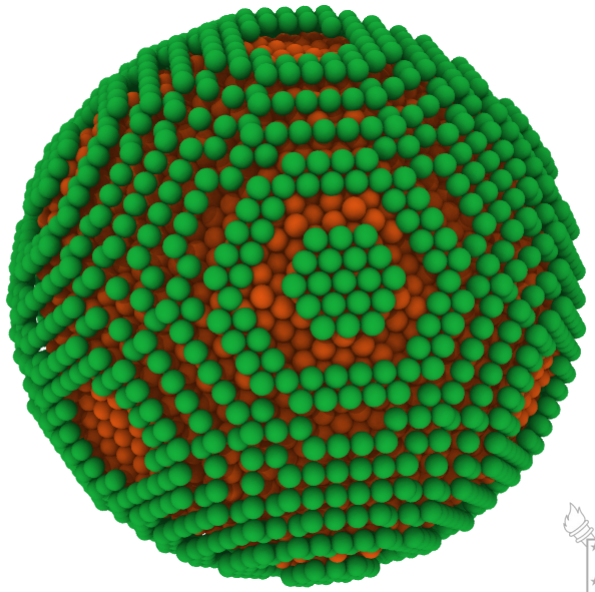
The annealing cycles

Searching process (The cycles)

Heating → Thermal equilibrium (Te) → Cooling → Minimization

Time: 5 ps





UdeSantiago de Chile

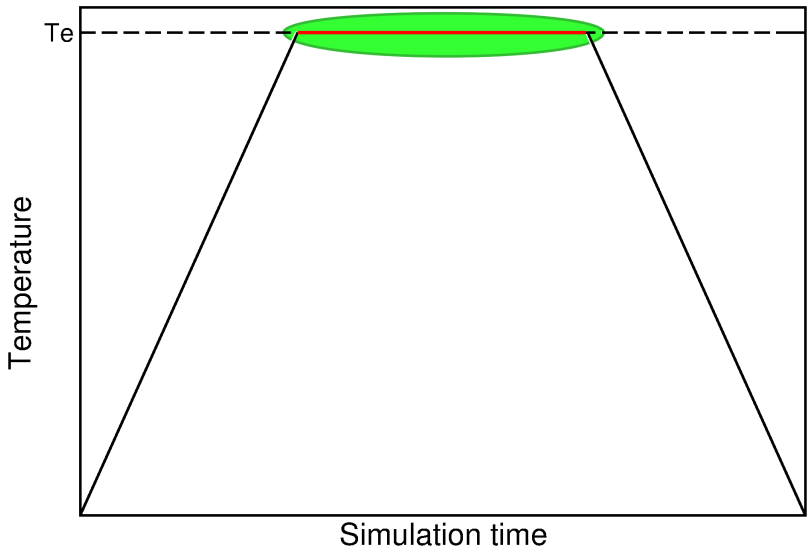
Simulation method

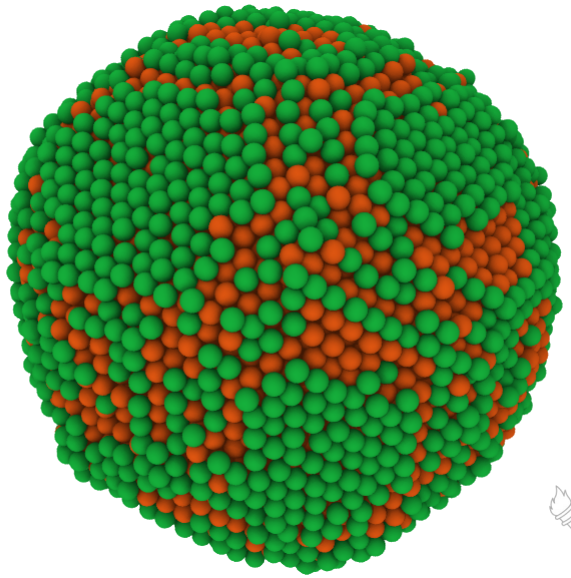
The annealing cycles

Searching process (The cycles)

Heating $\rightarrow$ Thermal equilibrium (Te) $\rightarrow$ Cooling $\rightarrow$ Minimization

Time: 3 ns (Hot-state is reached)





UdeSantiago de Chile

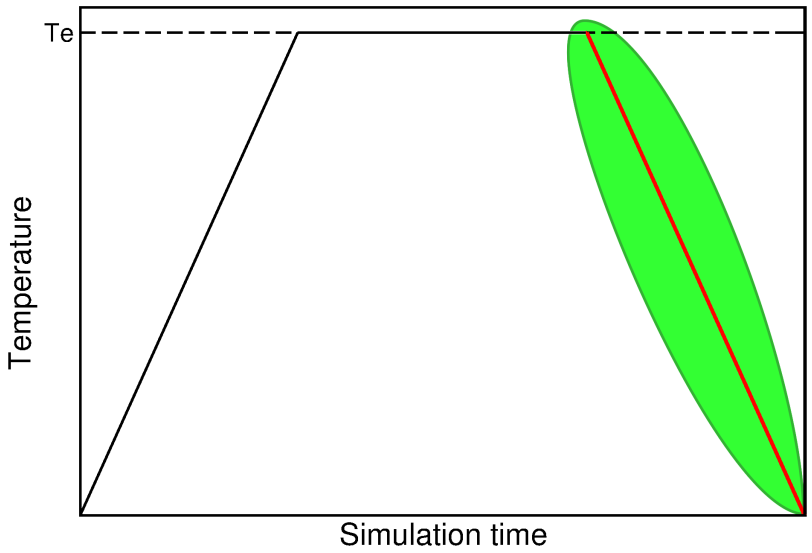
Simulation method

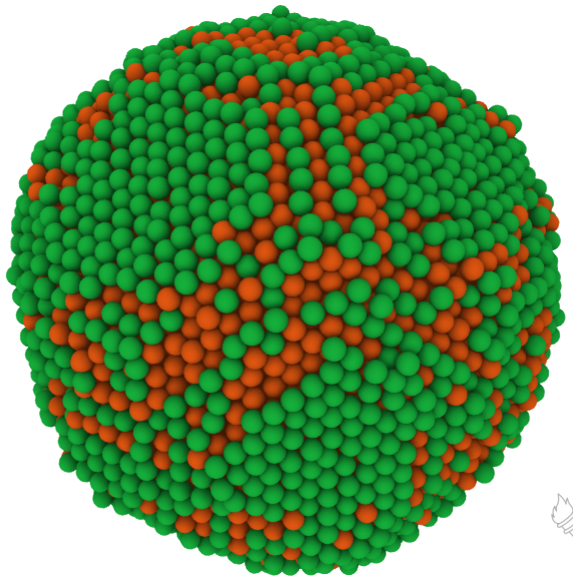
The annealing cycles

Searching process (The cycles)

Heating $\rightarrow$ Thermal equilibrium (Te) $\rightarrow$ Cooling $\rightarrow$ Minimization

Time: 5 ps





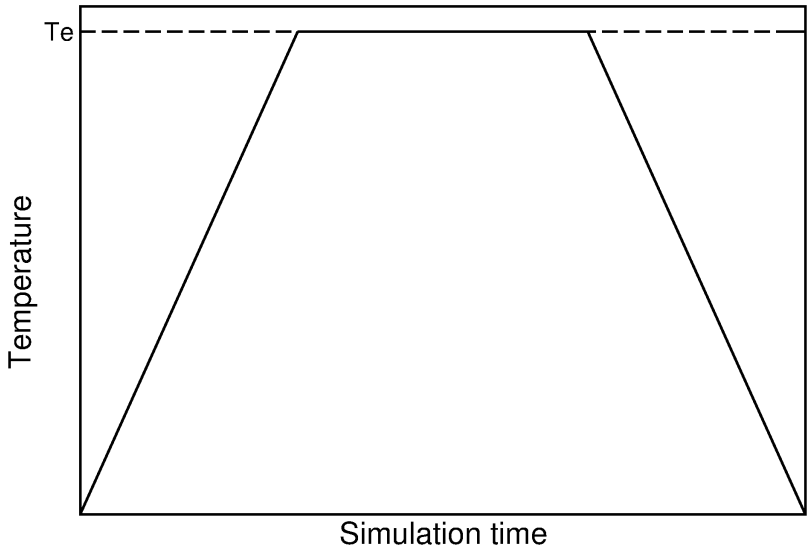
UdeSantiago de Chile

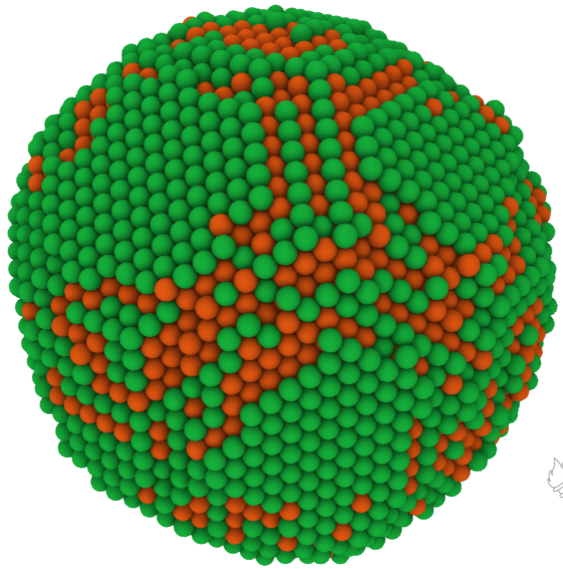
Simulation method

The annealing cycles

Searching process (The cycles)

Heating $\rightarrow$ Thermal equilibrium (Te) $\rightarrow$ Cooling $\rightarrow$ Minimization





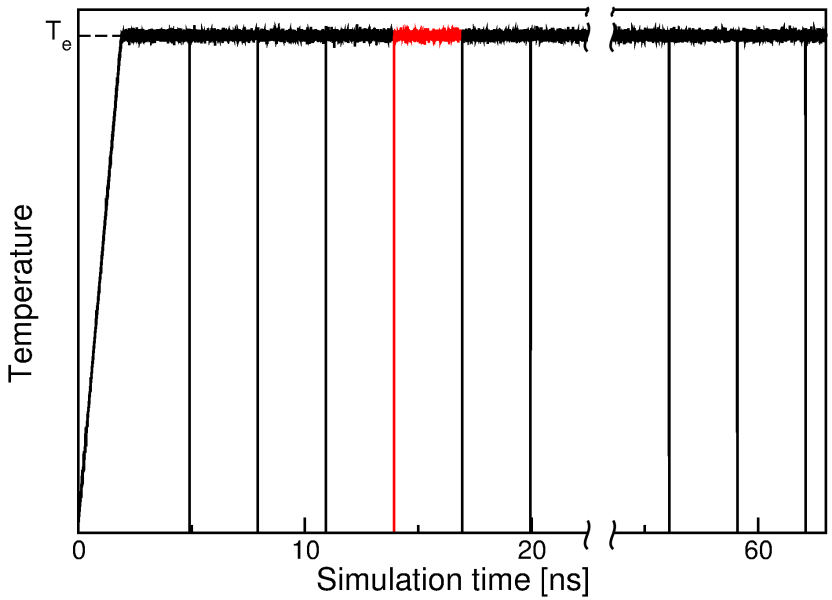
UdeSantiago de Chile

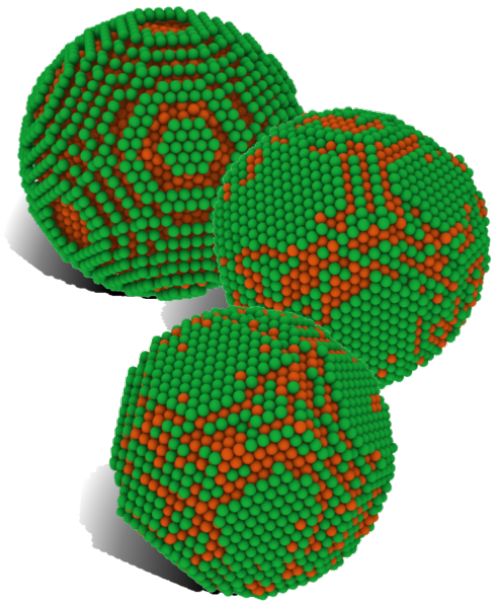
Simulation method

The annealing cycles

Searching process (The cycles)

Heating $\rightarrow$ Thermal equilibrium (Te) $\rightarrow$ Cooling $\rightarrow$ Minimization





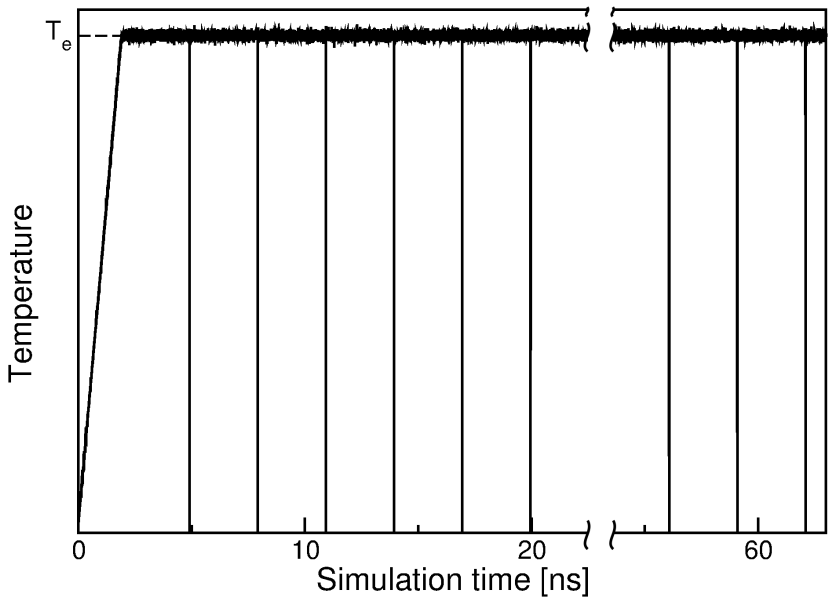
UdeSantiago de Chile

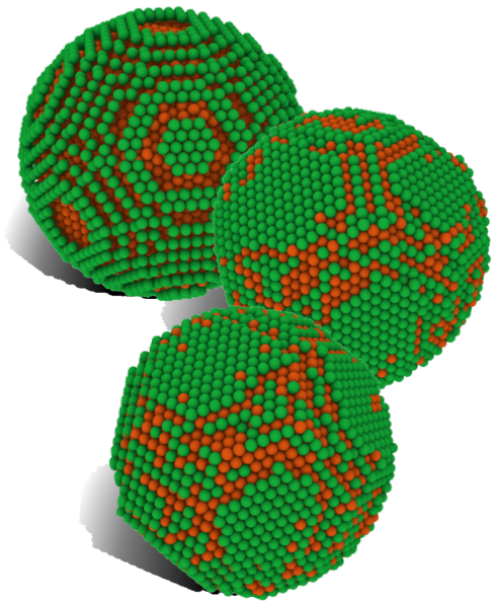
Simulation method

The annealing cycles

Searching process (The cycles)

Heating $\rightarrow$ Thermal equilibrium (Te) $\rightarrow$ Cooling $\rightarrow$ Minimization





Repeat until a convergence criteria is reached

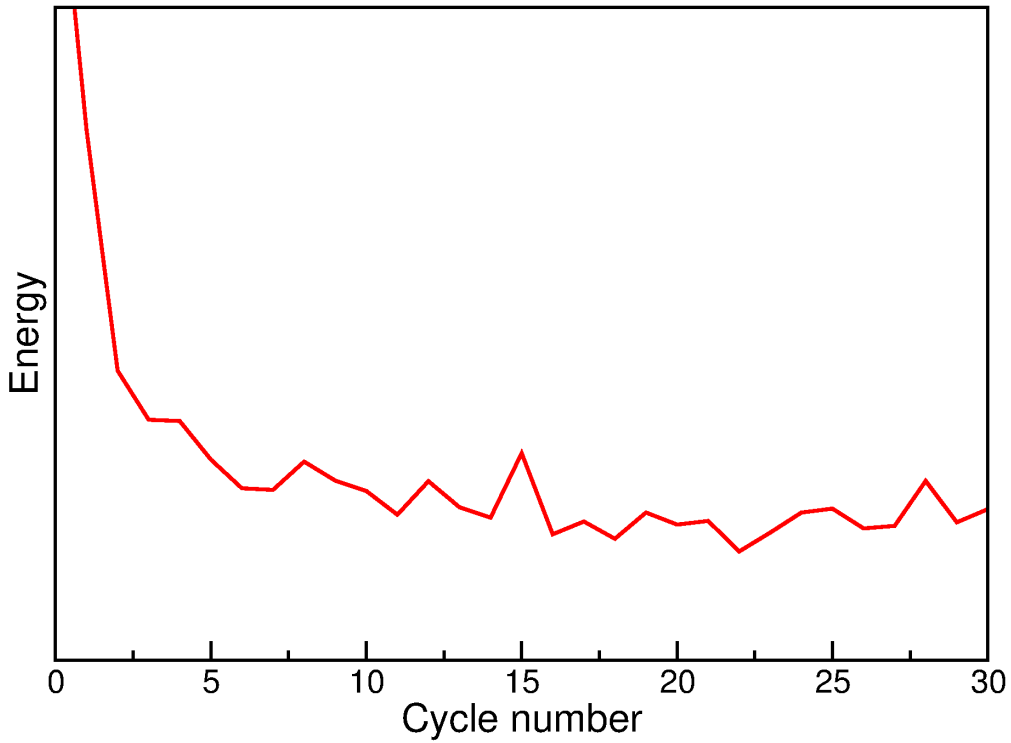
UdeSantiago de Chile

Simulation method

Final cooldown

Final cooldown steps

Reached criteria $\rightarrow$ Cooling $\rightarrow$ Thermal equilibrium $\rightarrow$ Minimization



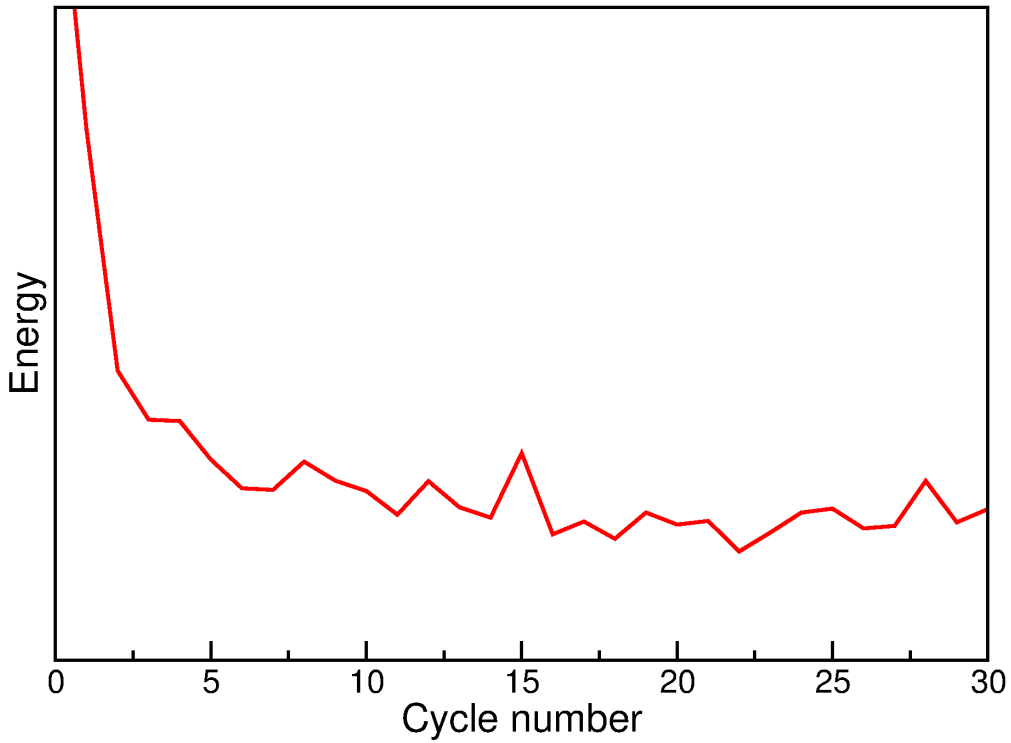
Simulation method

Final cooldown

Final cooldown steps

Reached criteria $\rightarrow$ Cooling $\rightarrow$ Thermal equilibrium $\rightarrow$ Minimization

$$\text{Deviation} < \text{Threshold}$$



UdeSantiago de Chile

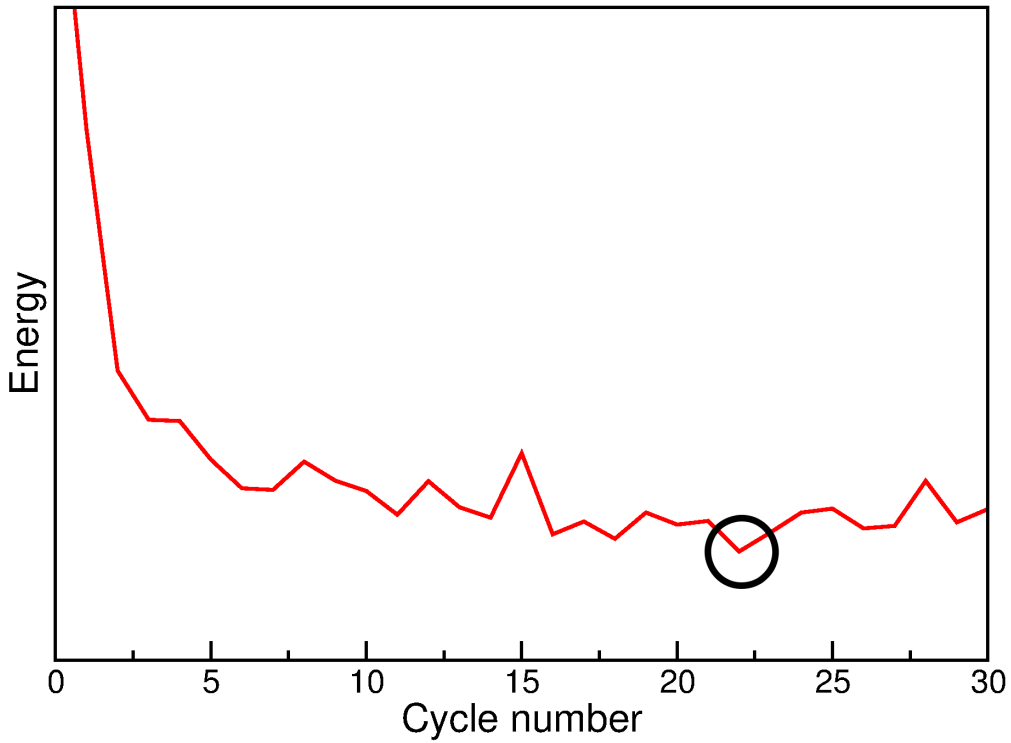
Simulation method

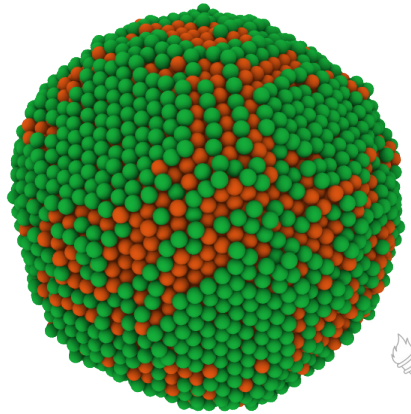
Final cooldown

Final cooldown steps

Reached criteria $\rightarrow$ Cooling $\rightarrow$ Thermal equilibrium $\rightarrow$ Minimization

Take most stable configuration's hot-state





UdeSantiago de Chile

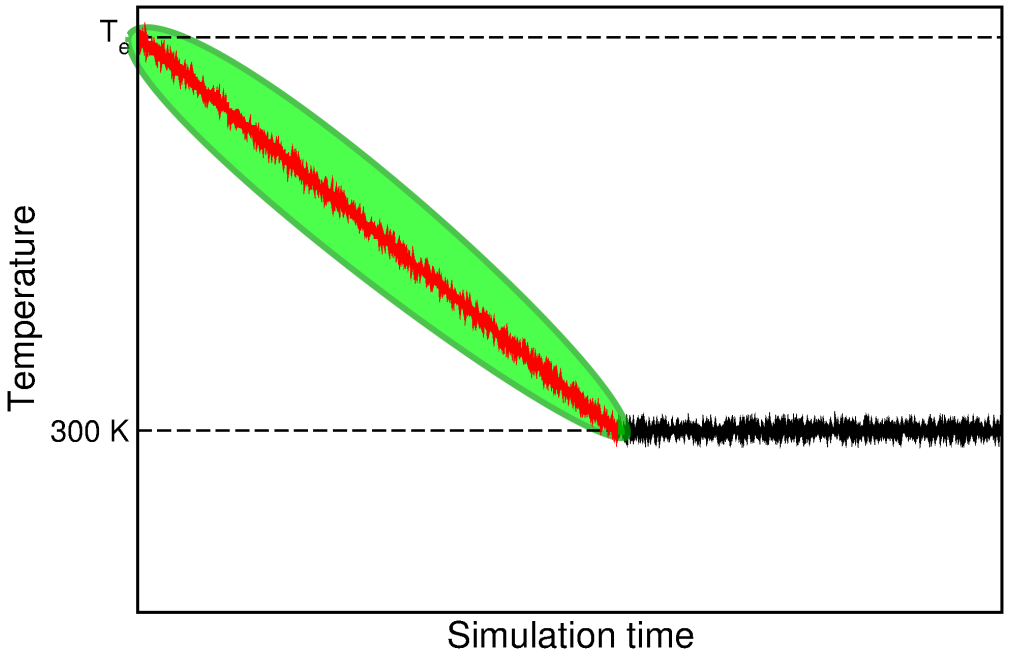
Simulation method

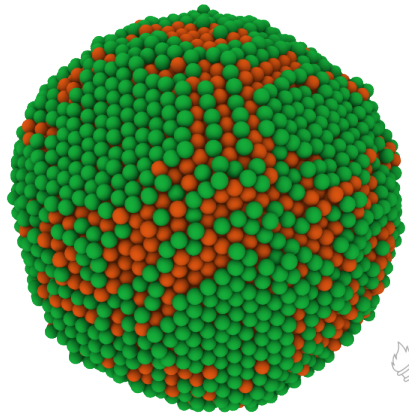
Final cooldown

Final cooldown steps

Reached criteria $\rightarrow$ Cooling $\rightarrow$ Thermal equilibrium $\rightarrow$ Minimization

Ramp: 0.25 K/ps





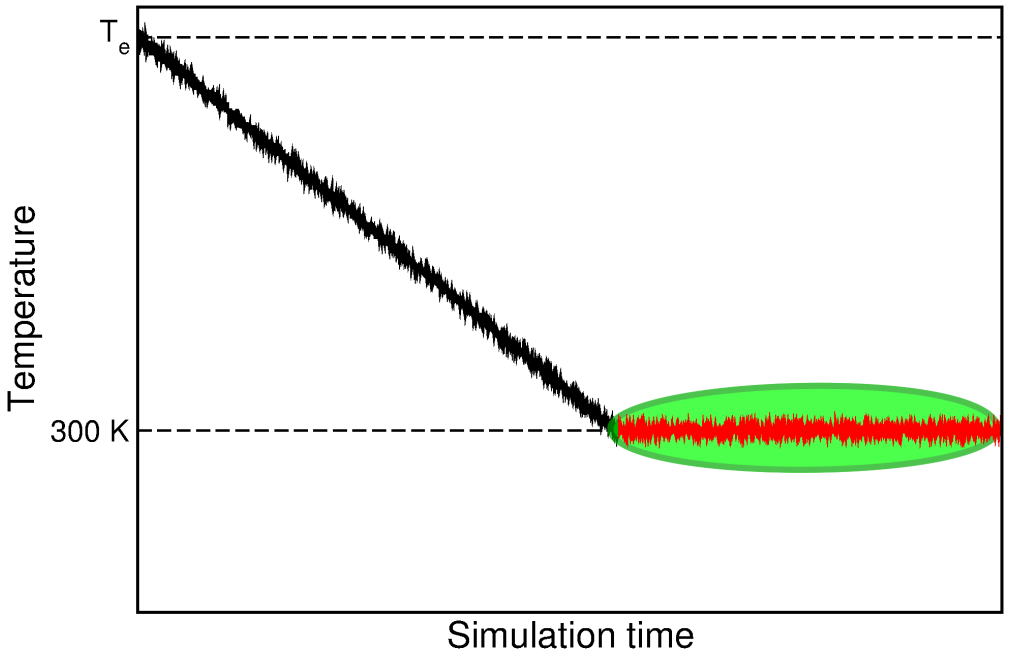
Simulation method

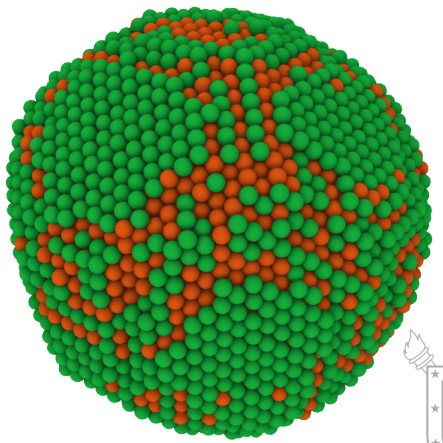
Final cooldown

Final cooldown steps

Reached criteria → Cooling → Thermal equilibrium → Minimization

Time: 3.1 ns



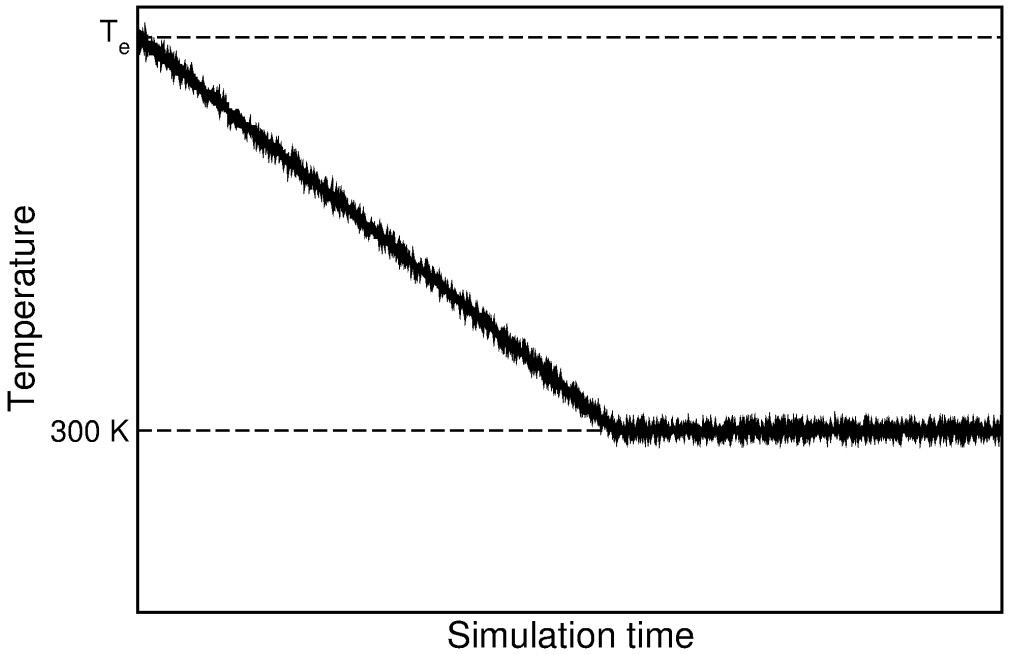


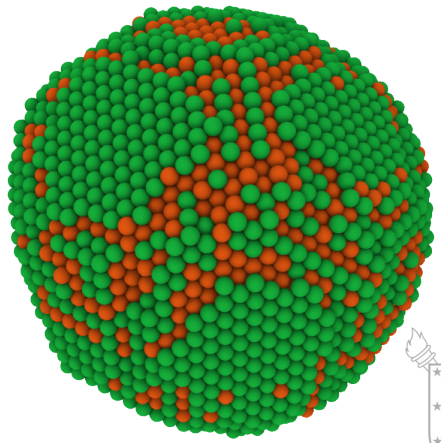
Simulation method

Final cooldown

Final cooldown steps

Reached criteria → Cooling → Thermal equilibrium → Minimization





Simulation method

Initial configurations

Applying the search process to bimetallic clusters.
Mobilities are different between elements $\rightarrow$ separated treatment.

Cooking initial structures

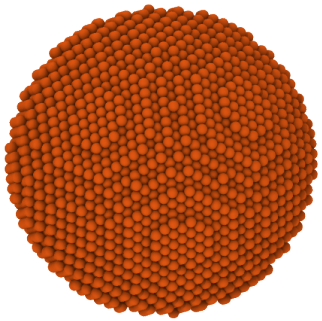
- Apply the search routine to the monoatomic clusters

Core-Shell

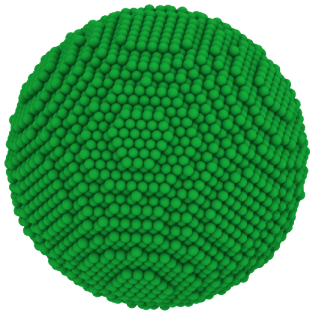
- Wrap the Fe core with a spherical Cu shell

Janus

- Locate the Cu cluster next to the Fe one



Fe Cu



UdeSantiago de Chile

Simulation method

Initial configurations

Applying the search process to bimetallic clusters.
Mobilities are different between elements $\rightarrow$ separated treatment.

Cooking initial structures

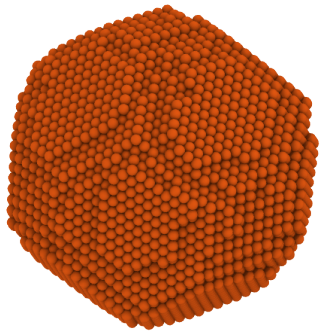
- Apply the search routine to the monoatomic clusters

Core-Shell

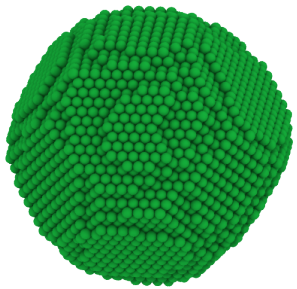
- Wrap the Fe core with a spherical Cu shell

Janus

- Locate the Cu cluster next to the Fe one



Fe Cu



UdeSantiago de Chile

Simulation method

Initial configurations

Applying the search process to bimetallic clusters.
Mobilities are different between elements $\rightarrow$ separated treatment.

Cooking initial structures

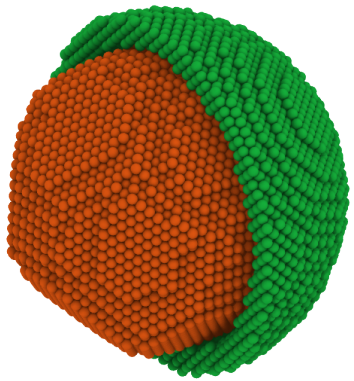
- Apply the search routine to the monoatomic clusters

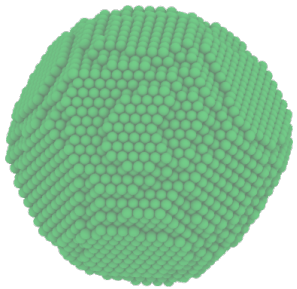
Core-Shell

- Wrap the Fe core with a spherical Cu shell

Janus

- Locate the Cu cluster next to the Fe one





UdeSantiago de Chile

Simulation method

Initial configurations

Applying the search process to bimetallic clusters.
Mobilities are different between elements $\rightarrow$ separated treatment.

Cooking initial structures

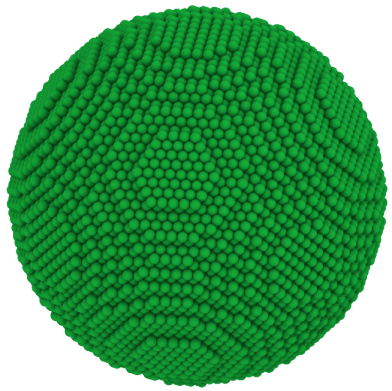
- Apply the search routine to the monoatomic clusters

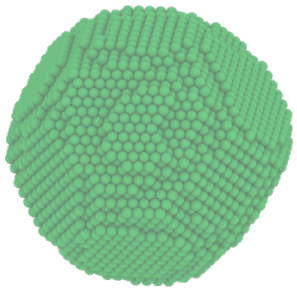
Core-Shell

- Wrap the Fe core with a spherical Cu shell

Janus

- Locate the Cu cluster next to the Fe one





UdeSantiago de Chile

Simulation method

Initial configurations

Applying the search process to bimetallic clusters.
Mobilities are different between elements $\rightarrow$ separated treatment.

Cooking initial structures

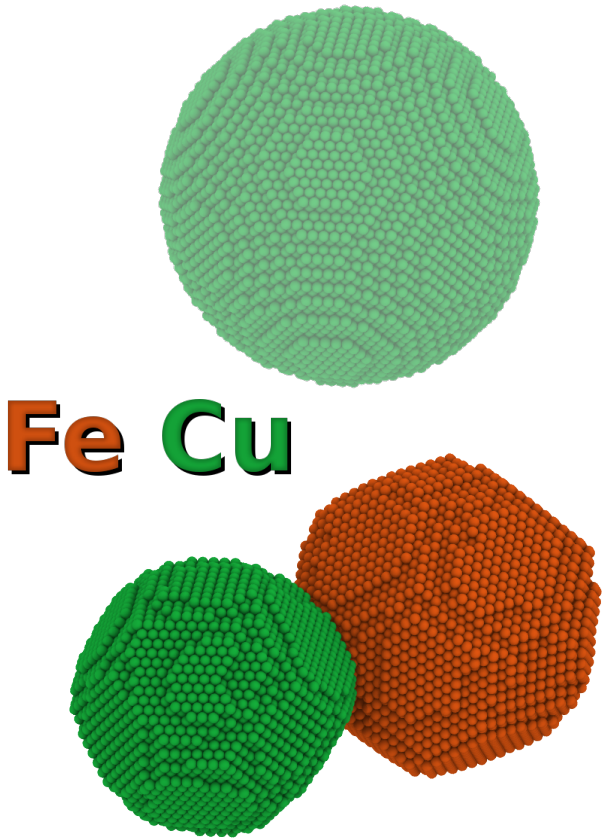
- Apply the search routine to the monoatomic clusters

Core-Shell

- Wrap the Fe core with a spherical Cu shell

Janus

- Locate the Cu cluster next to the Fe one



UdeSantiago de Chile

Simulation method

Initial configurations

Applying the search process to bimetallic clusters.
Mobilities are different between elements $\rightarrow$ separated treatment.

Cooking initial structures

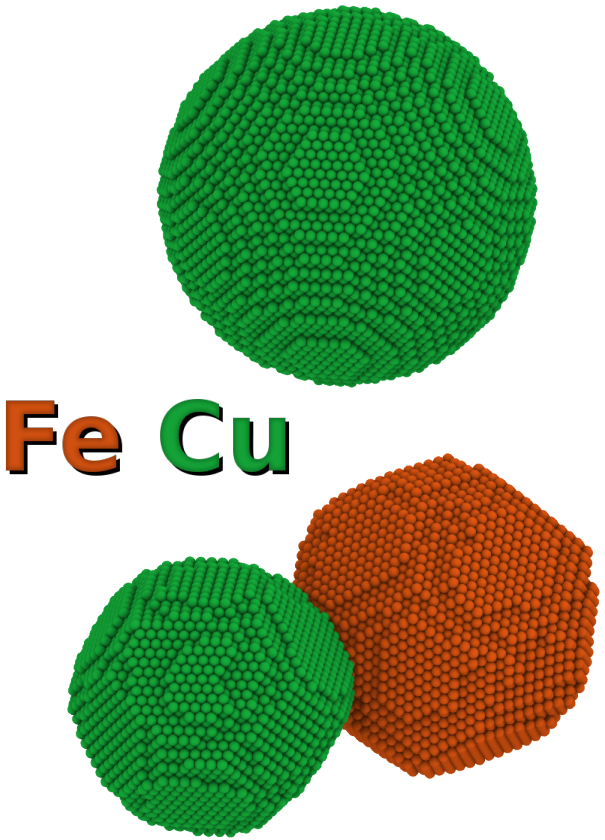
- Apply the search routine to the monoatomic clusters

Core-Shell

- Wrap the Fe core with a spherical Cu shell

Janus

- Locate the Cu cluster next to the Fe one



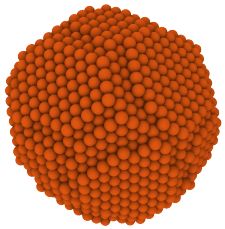
UdeSantiago de Chile

We're ready to go!

Results

Energy and configuration at different sizes and cooper concentrations

Three different "sizes" of Fe were used.



Sizes

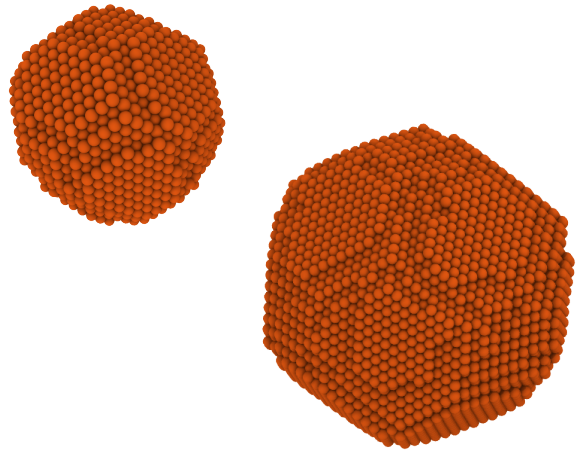
- Small ($\sim 5nm$)
- Medium ($\sim 7nm$)
- Big ($\sim 9nm$)

UdeSantiago de Chile

Results

Energy and configuration at different sizes and cooper concentrations

Three different "sizes" of Fe were used.



Sizes

- Small ($\sim 5nm$)
- Medium ($\sim 7nm$)
- Big ($\sim 9nm$)

UdeSantiago de Chile

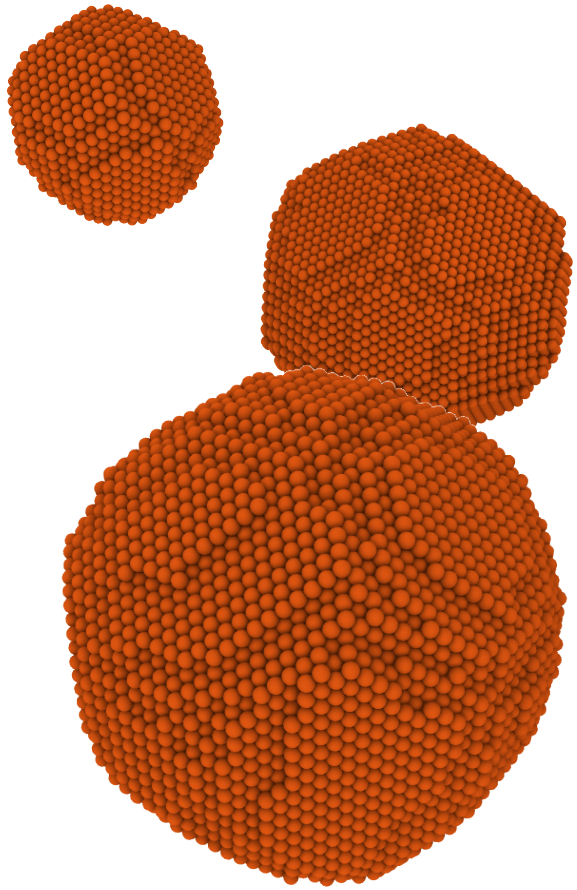
Results

Energy and configuration at different sizes and cooper concentrations

Three different "sizes" of Fe were used.

Sizes

- Small ($\sim 5nm$)
- Medium ($\sim 7nm$)
- Big ($\sim 9nm$)

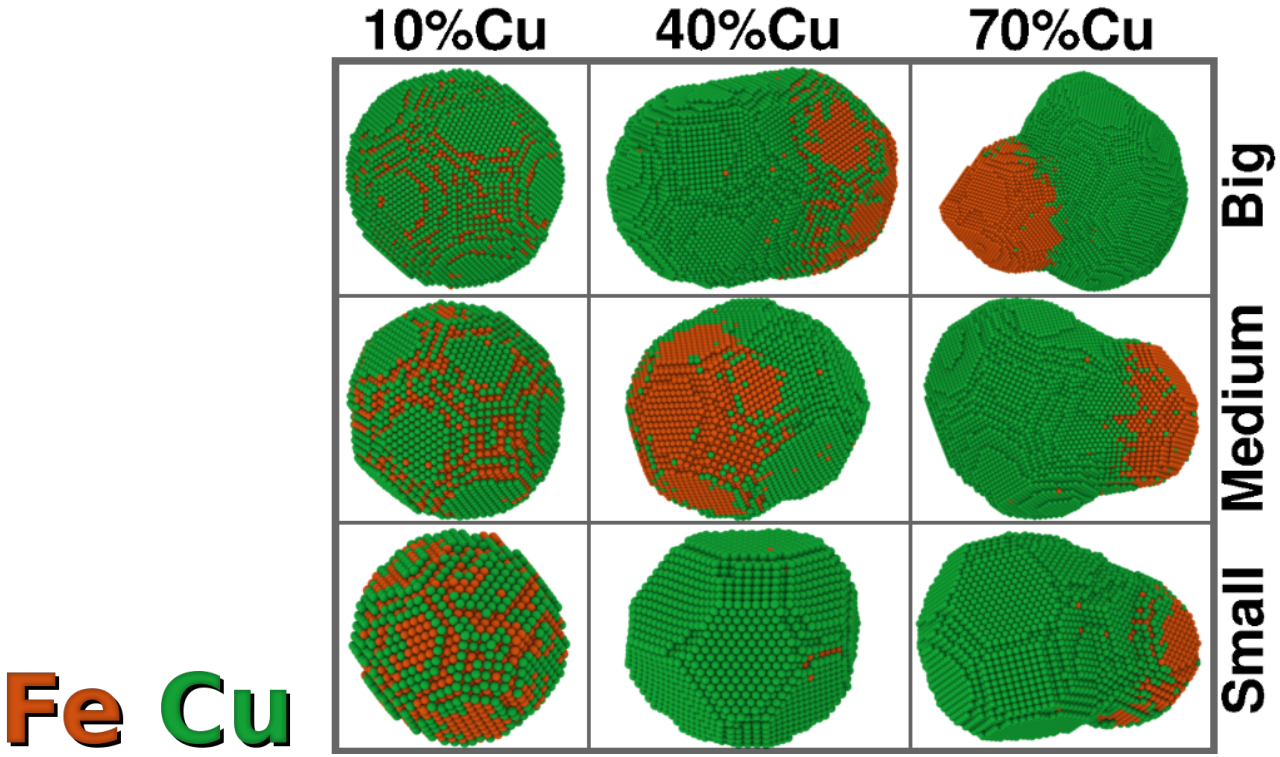


UdeSantiago de Chile

Results

Energy and configuration at different sizes and cooper concentrations

Final configurations were found for different sizes and concentrations (Full)



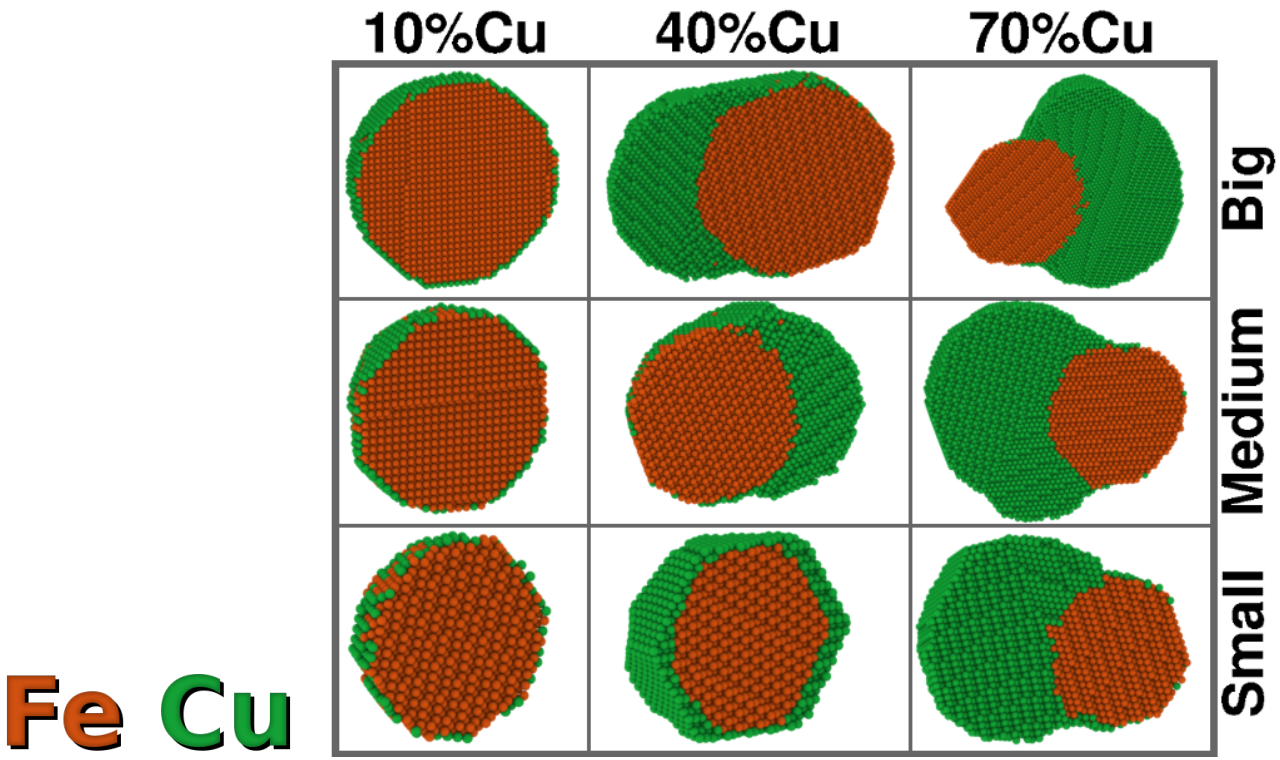
J. Rojas-Nunez et al., to be submitted

UdeSantiago de Chile

Results

Energy and configuration at different sizes and cooper concentrations

Final configurations were found for different sizes and concentrations (Cross-section)



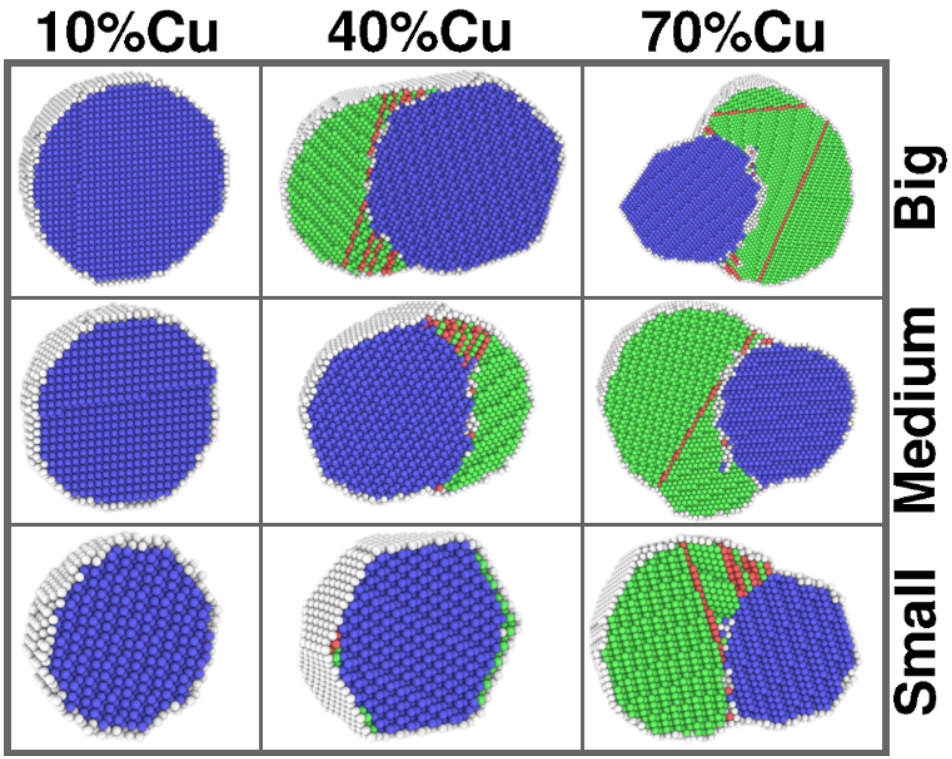
J. Rojas-Nunez et al., to be submitted

UdeSantiago de Chile

Results

Energy and configuration at different sizes and cooper concentrations

Structural analysis has been performed (Common neighbor analysis)



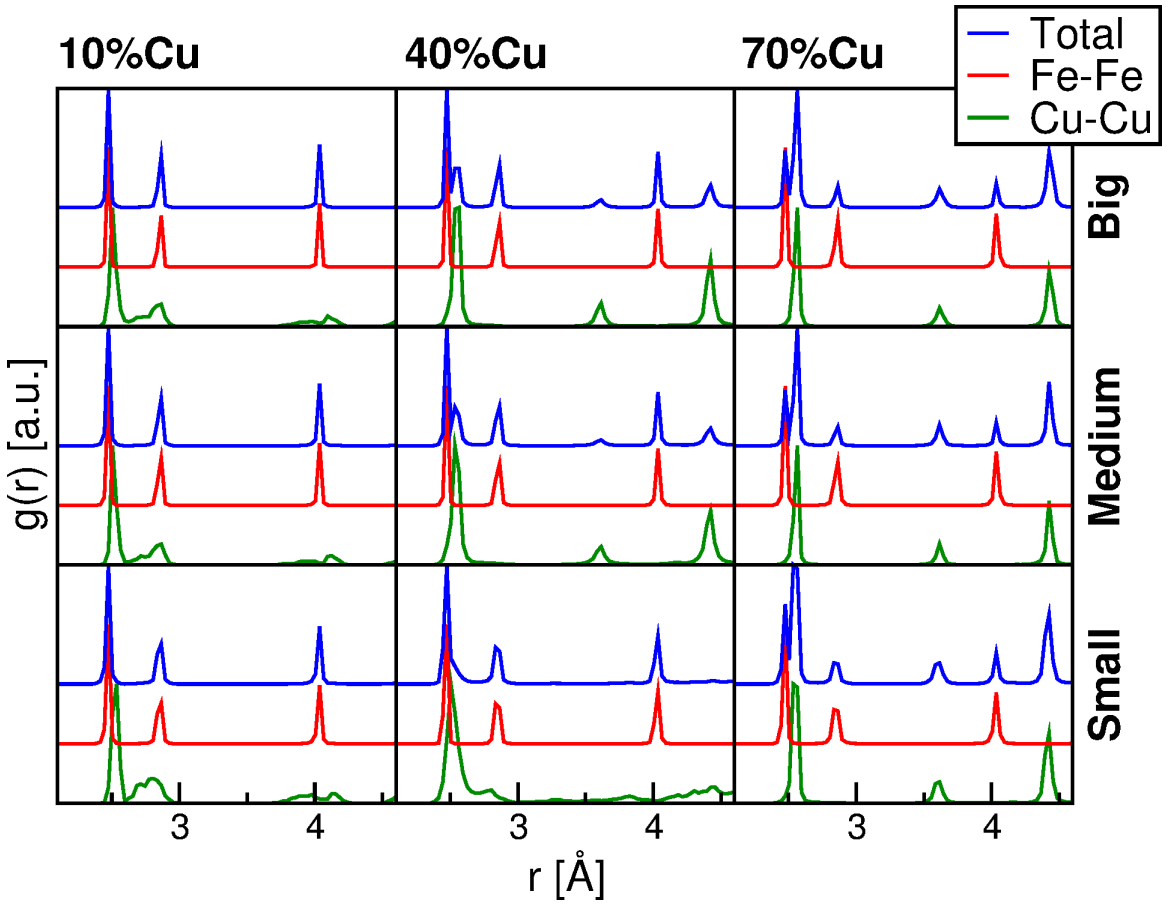
J. Rojas-Nunez et al., to be submitted

UdeSantiago de Chile

Results

Energy and configuration at different sizes and cooper concentrations

Structural analysis has been performed (Pair correlation function)

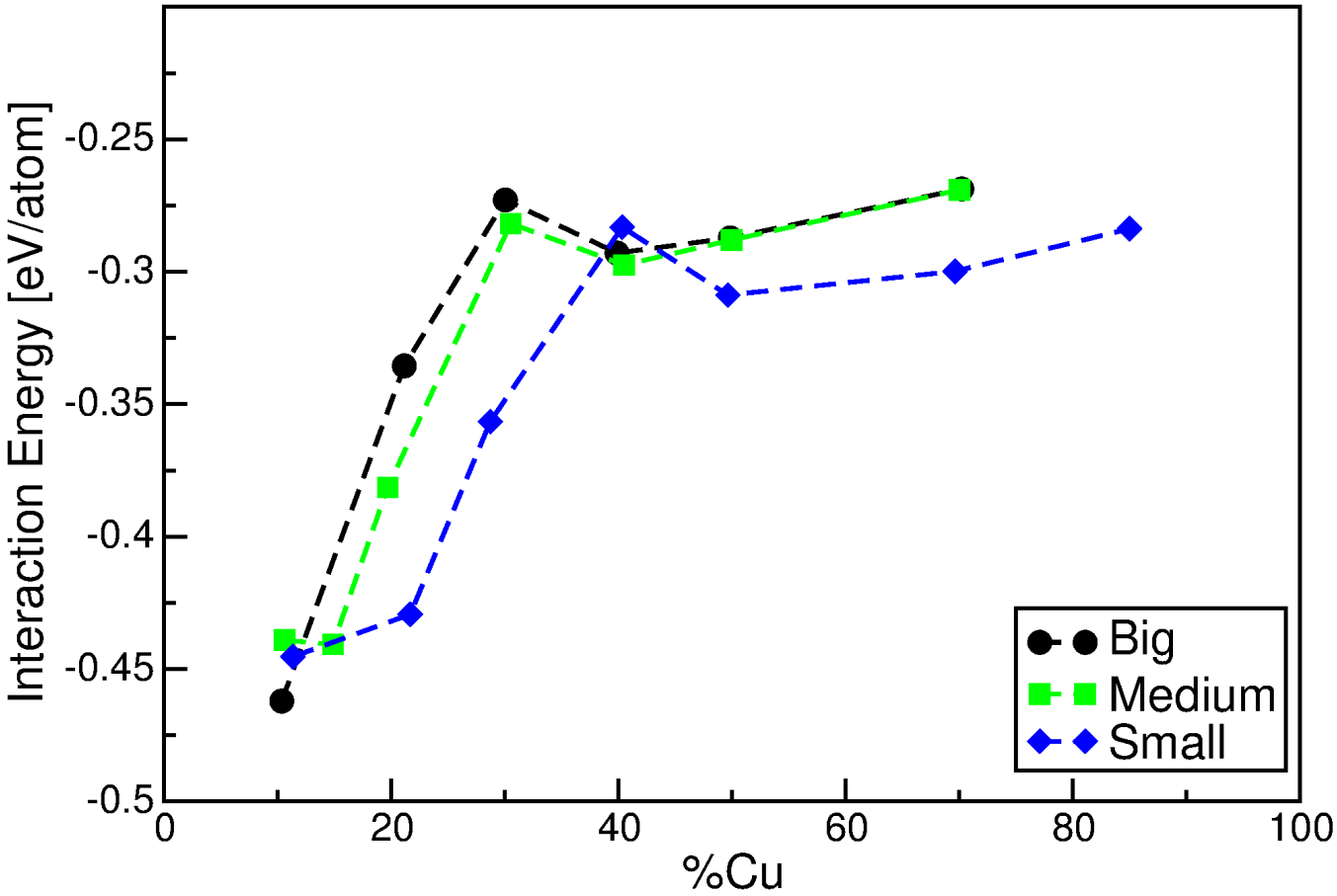


J. Rojas-Nunez et al., to be submitted

Results

Energy and configuration at different sizes and cooper concentrations

Interaction energies (Fe-Cu) show variations through the different concentrations



UdeSantiago de Chile

J. Rojas-Nunez et al., to be submitted

Summary & Perspectives

- Annealing and minimizations were applied to FeCu nanoparticles using classical molecular dynamics
- Different atomic structures have been found at different sizes and Cu concentrations
- Defects for Cu had been found at higher Cu concentrations
- Further work: Study oxidation effects over these structures

UdeSantiago de Chile

Acknowledgements

CEDENNA

UdeSantiago
de Chile

UdeSantiago
de Chile

Thank You