Effect of the segregation of alloying elements on the grain growth in nanocrystalline alloys: coupling Monte Carlo and Molecular Dynamics simulations

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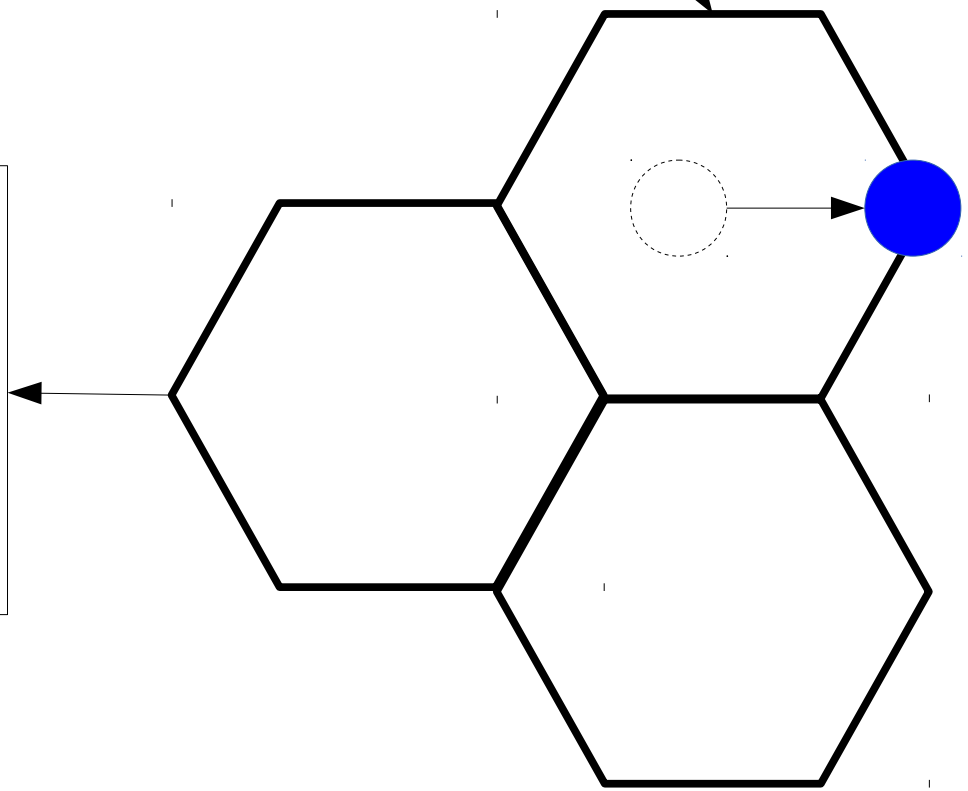
This work: Motivation

Nanocrystalline materials → Too many atoms at grain boundaries (high energy sites) → Driving force for rapid grain growth even at low temperatures

Nanocrystalline structure stabilization by alloying



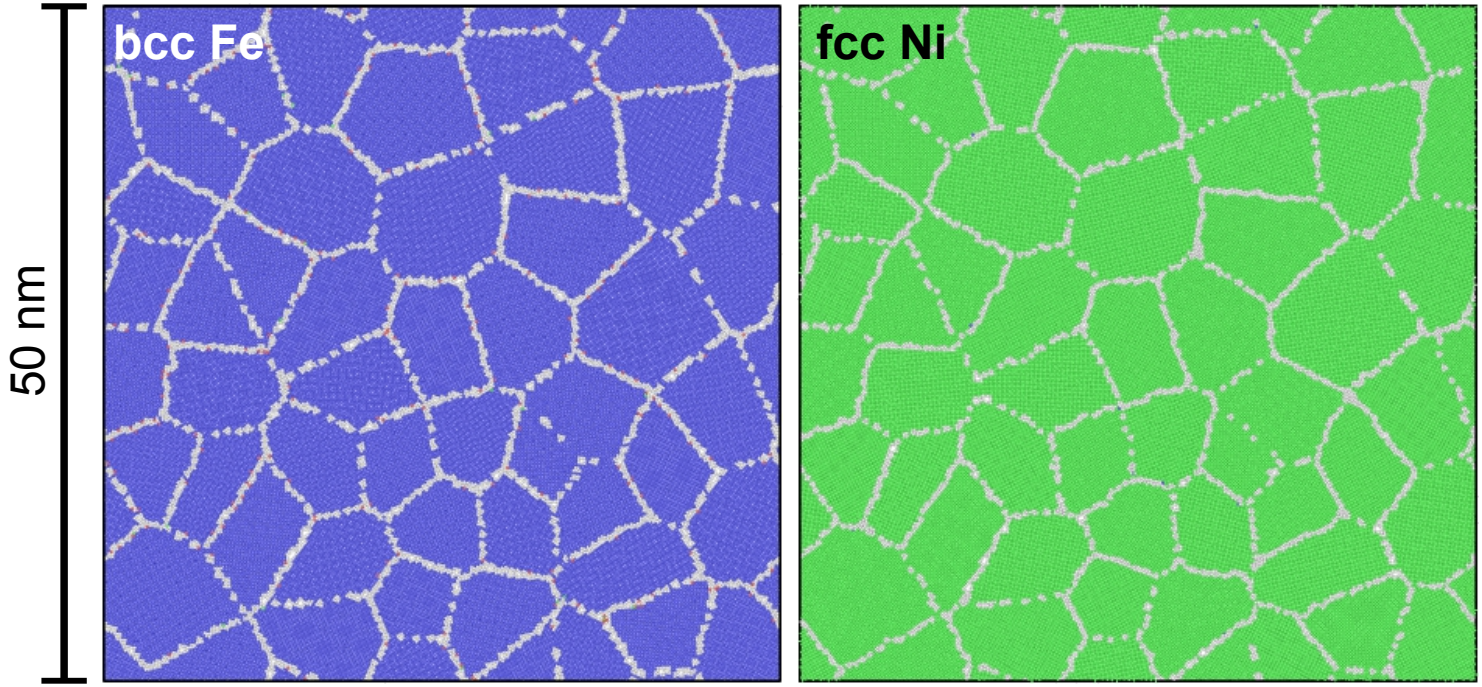
Example:
Experimental evidence of stable nc-Ni with W as alloying element
[*Acta Materialia* **55**, 371 (2007)]

Also studied by atomistic simulations → W segregation at grain boundaries
[*Acta Materialia* **55**, 4221 (2007)]

This work: Objective

To implement a simulation protocol coupling two distinct computational techniques – Monte Carlo and Molecular Dynamics – to investigate the segregation of alloying elements at grain boundaries in nanocrystalline materials and its effect (if any) on grain growth.

The model: Columnar nanostructures



Same initial structure in both cases → 50 grains (random orientation)

Average grain size → 7 nm

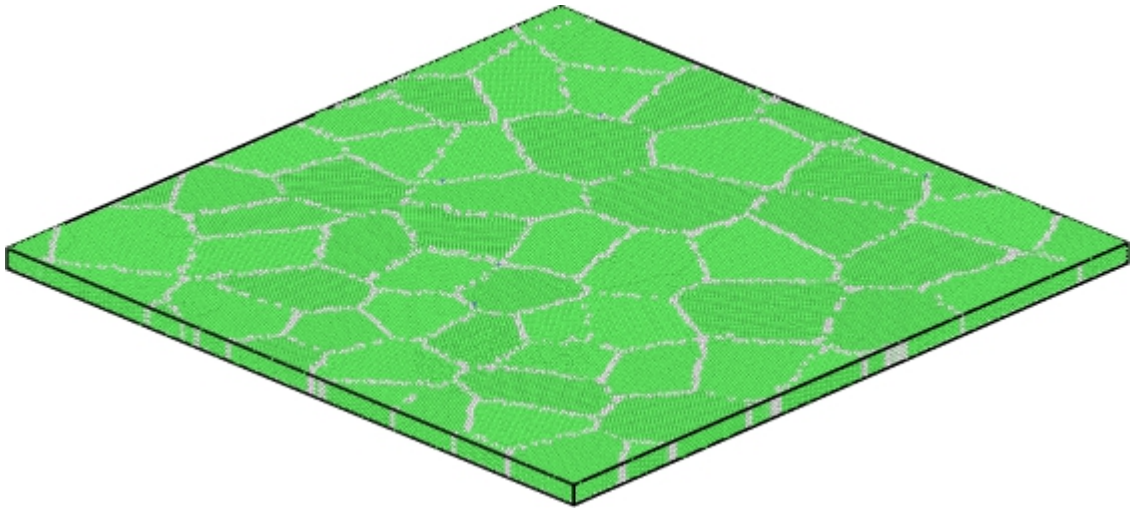
Only [100] tilt boundaries

Average disorientation → ~26°

Minimum disorientation → ~8°

Length along *z* → ~1.5 nm

The model: Columnar nanostructures



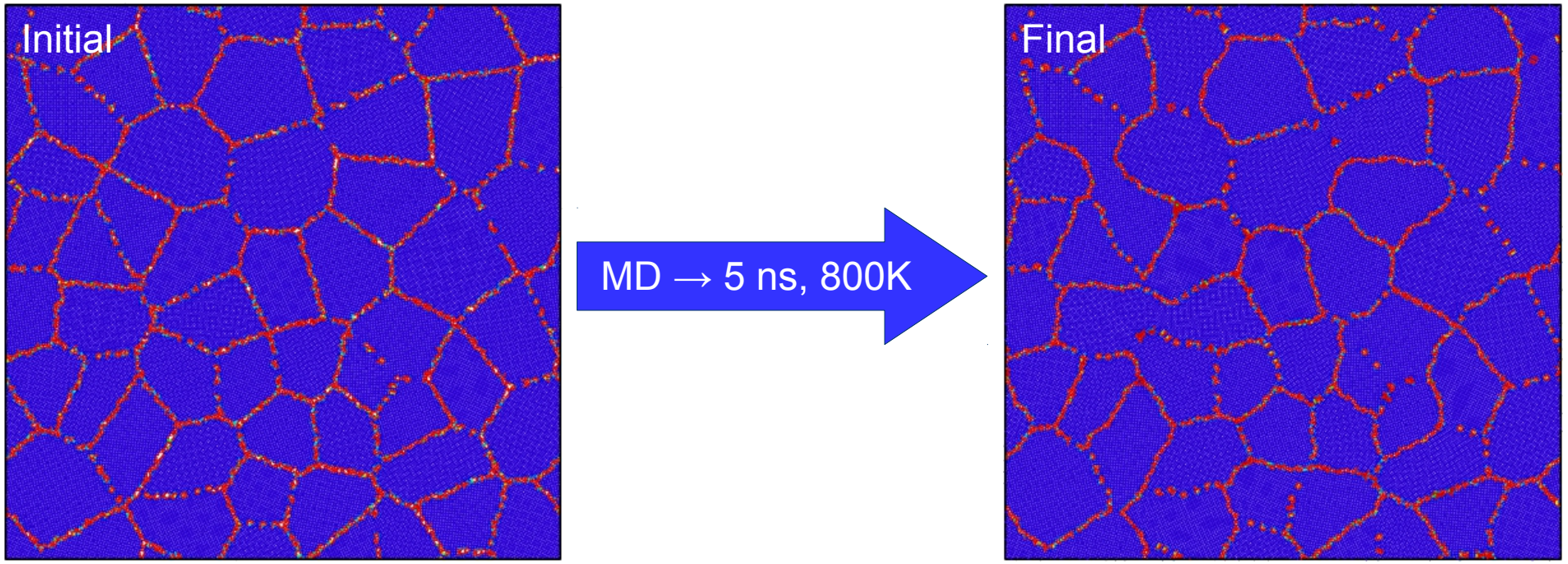
Advantages:
Easy to visualize the microstructure and its evolution in simulations

Thin slab → Systems much larger than 3D microstructures

Disadvantages:
Only tilt boundaries → Not a general model of a polycrystal

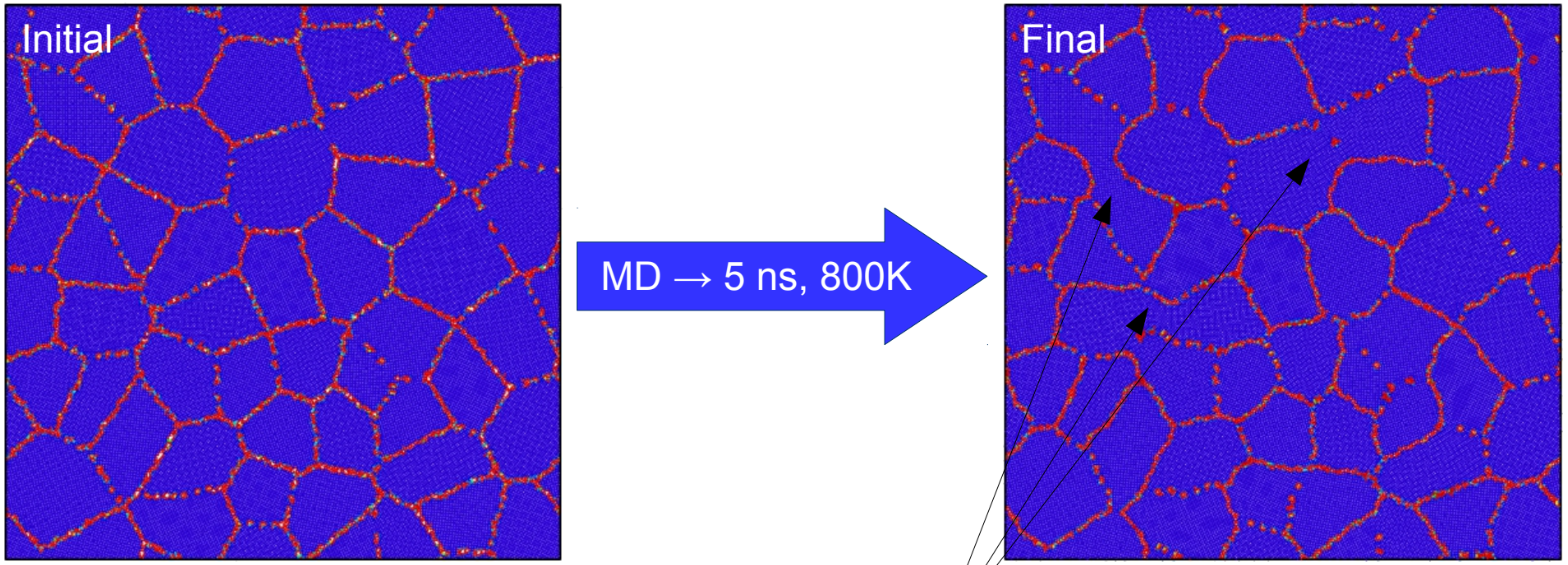
Some results: Pure metals

Iron



Some results: Pure metals

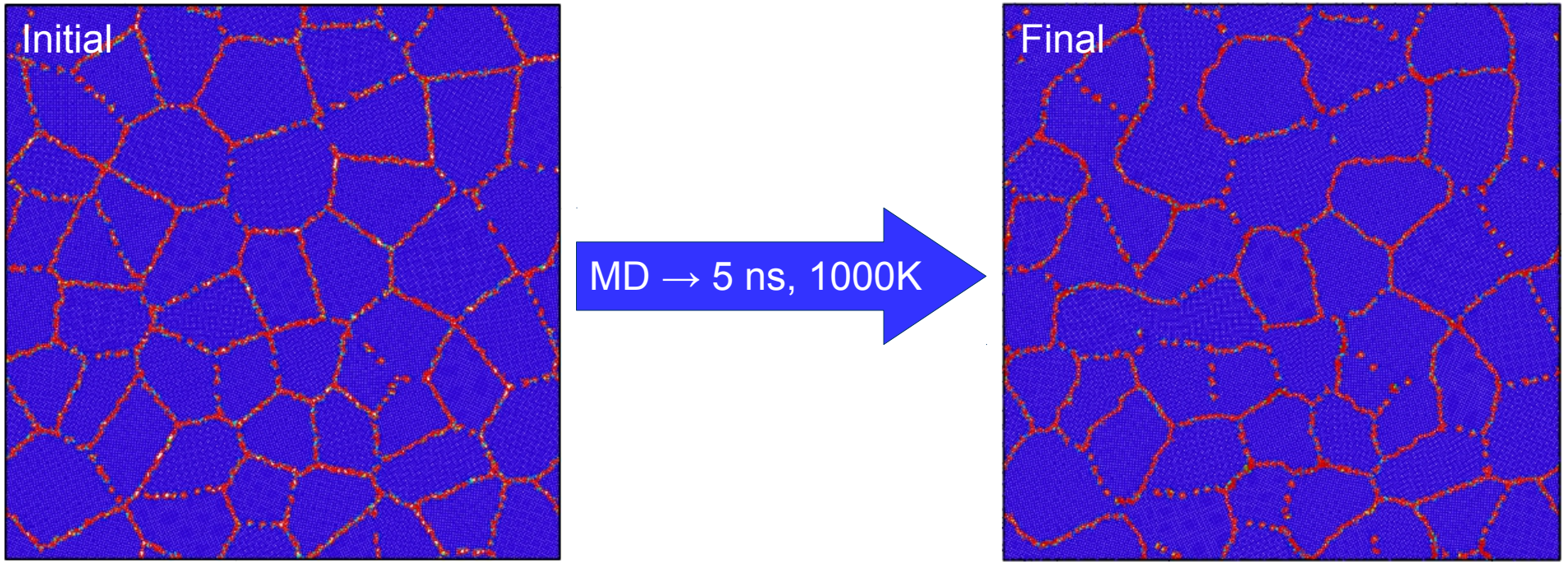
Iron



Something is happening here... but very slowly!

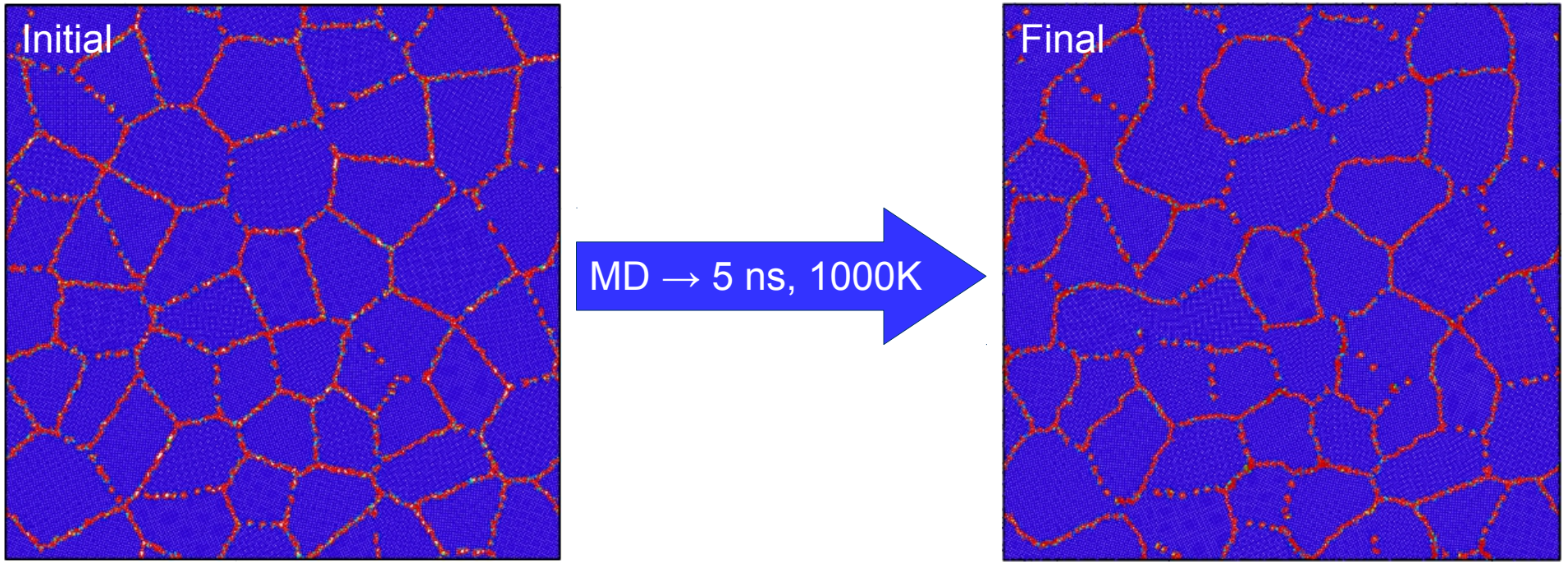
Some results: Pure metals

Iron



Some results: Pure metals

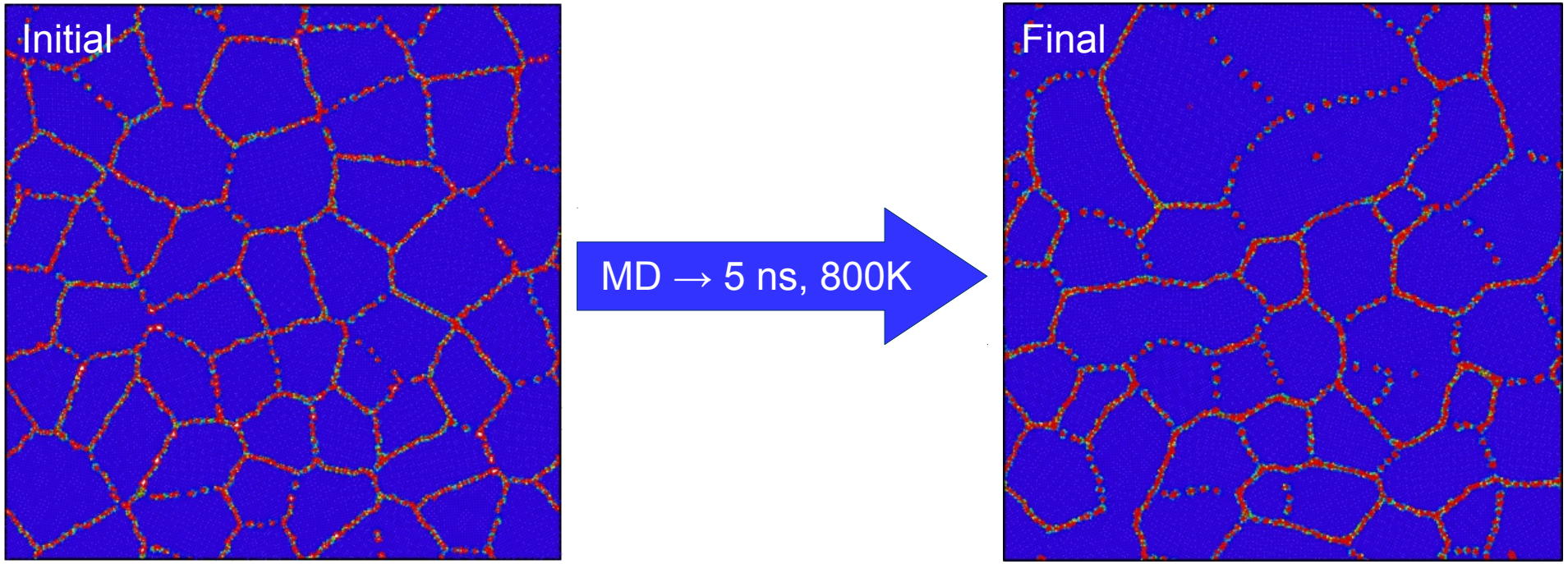
Iron



The microstructure still evolves very slowly.

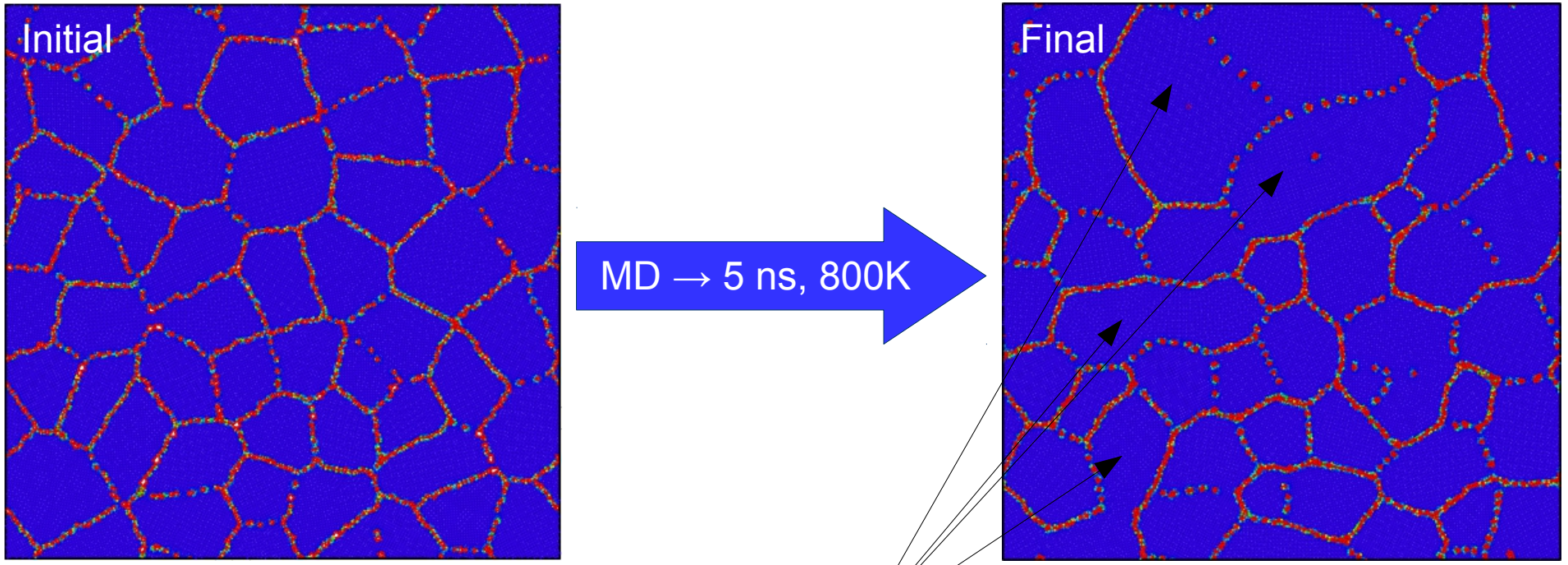
Some results: Pure metals

Nickel



Some results: Pure metals

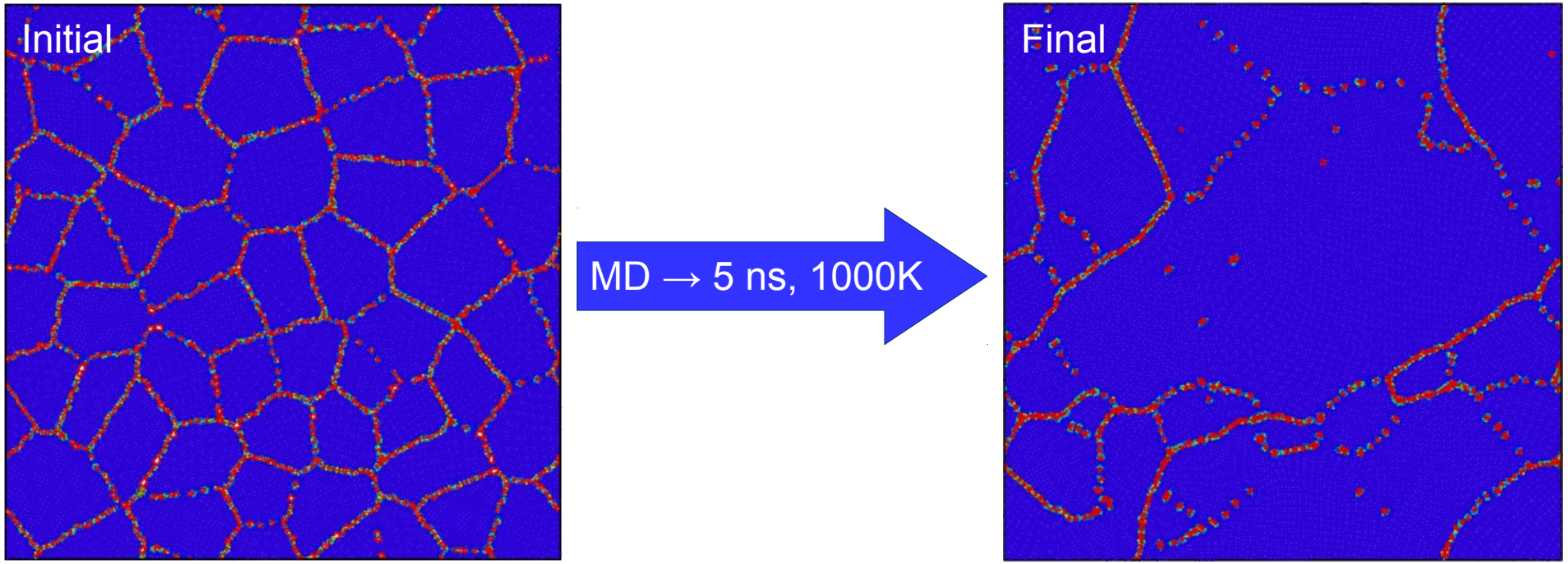
Nickel



Grain boundaries moved much faster!

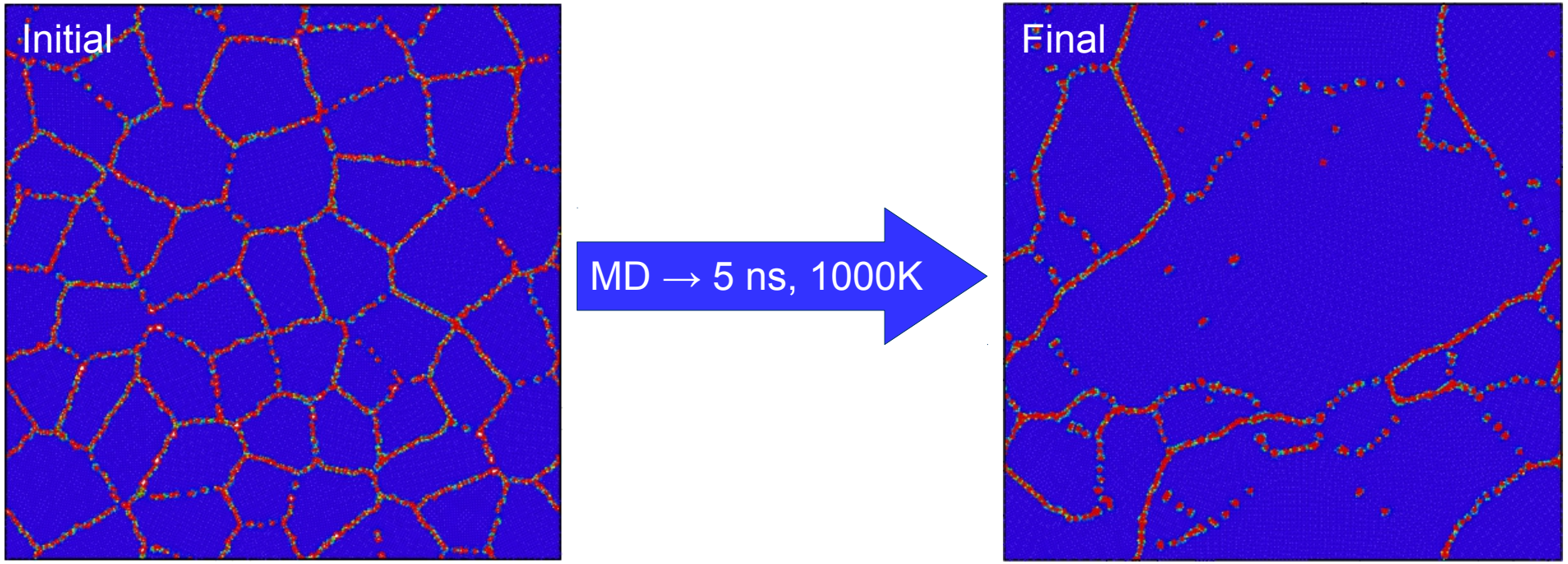
Some results: Pure metals

Nickel



Some results: Pure metals

Nickel



Let's start with Ni!

Segregation at grain boundaries
Monte Carlo simulations

Two different sites defined → GB and bulk

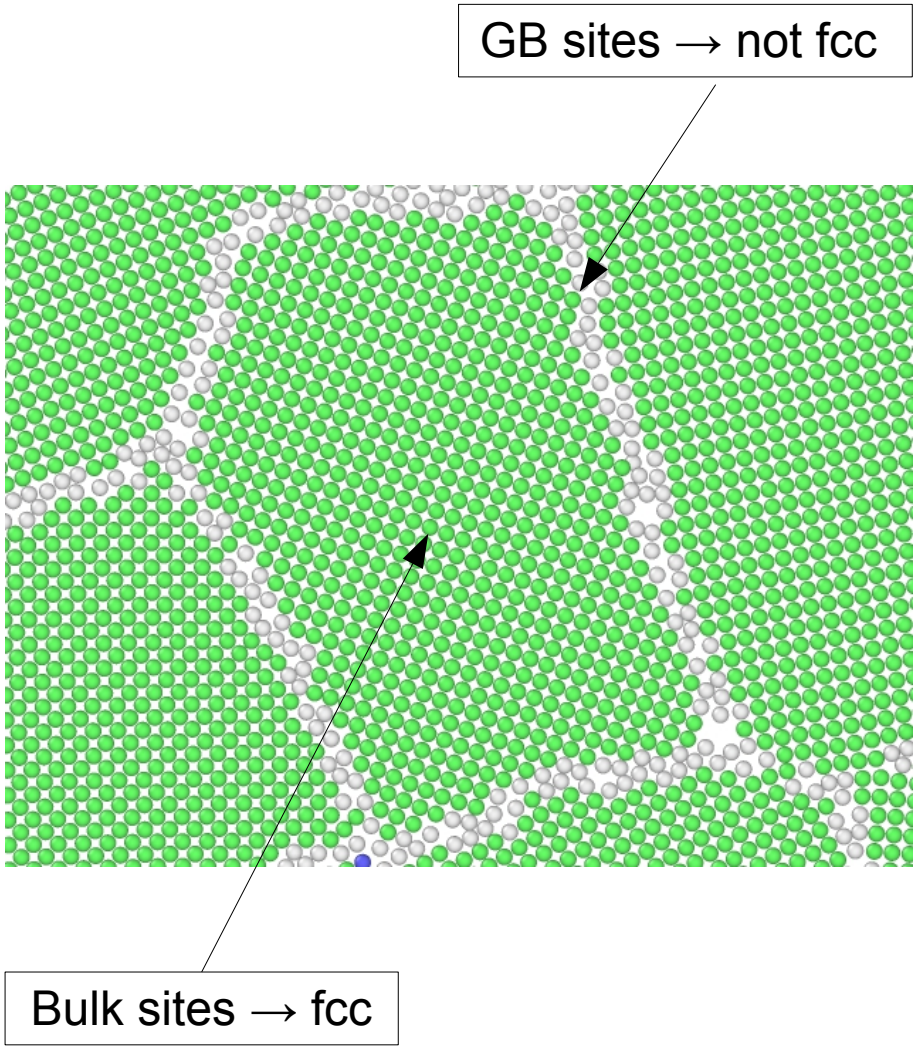
Allowed MC moves → bulk↔GB and GB↔GB → **Speeds up the simulations!**

Metropolis algorithm → **No dynamics!**

10% of the atoms of the main constituent (in our case, Ni) randomly replaced by atoms of the alloying element (Al, Co, Mo, Pd, Ta, Ti, W)

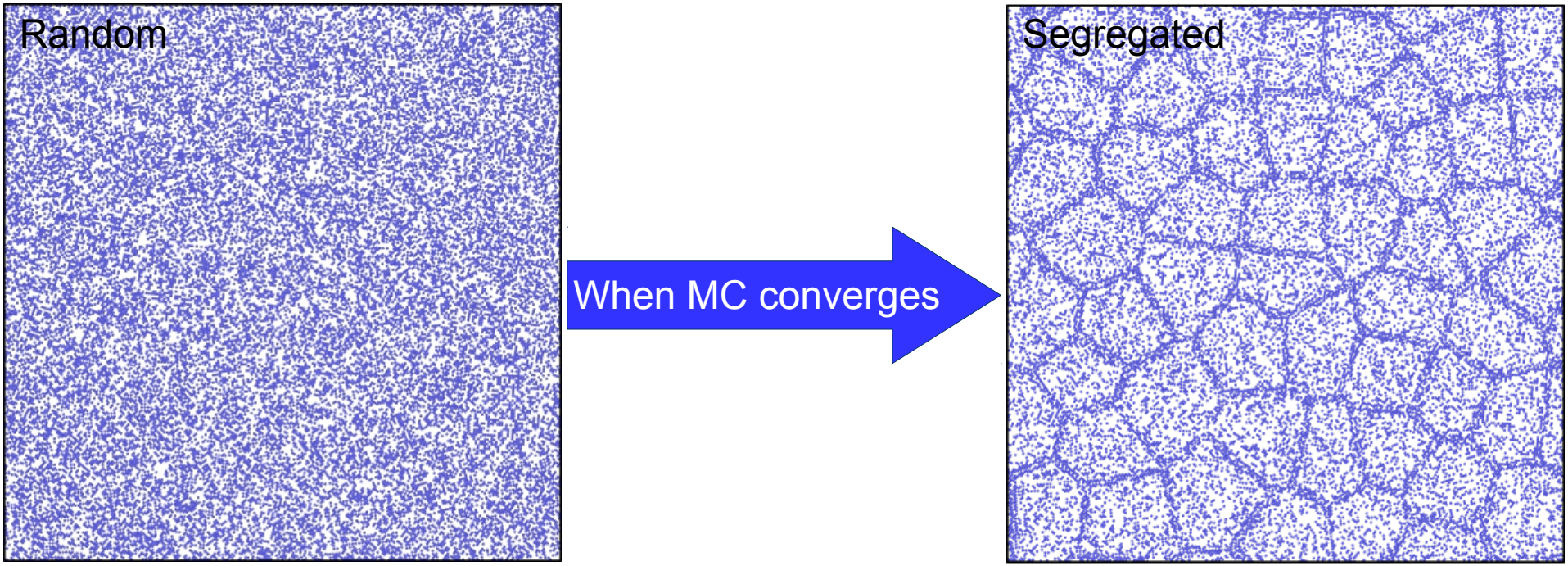
Total energy of each tested configuration → LAMMPS

T=350 K



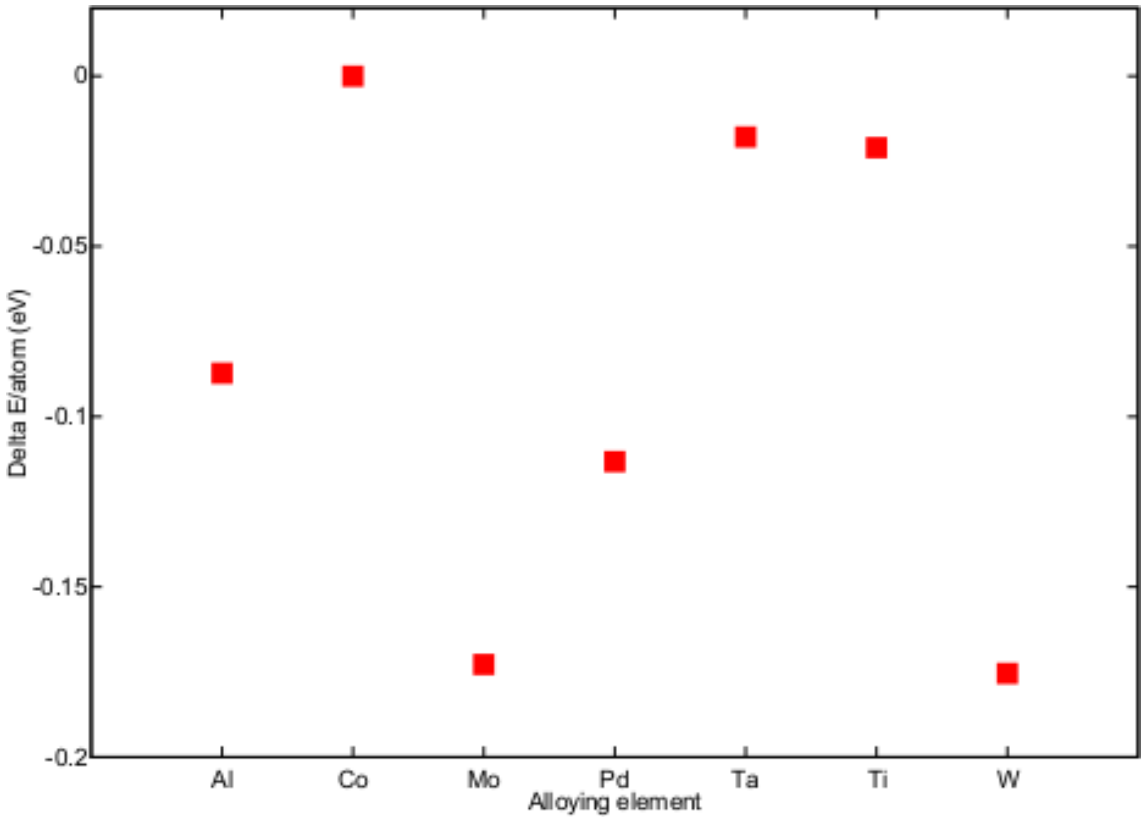
Segregation at grain boundaries
Monte Carlo simulations

Example → Ni-W



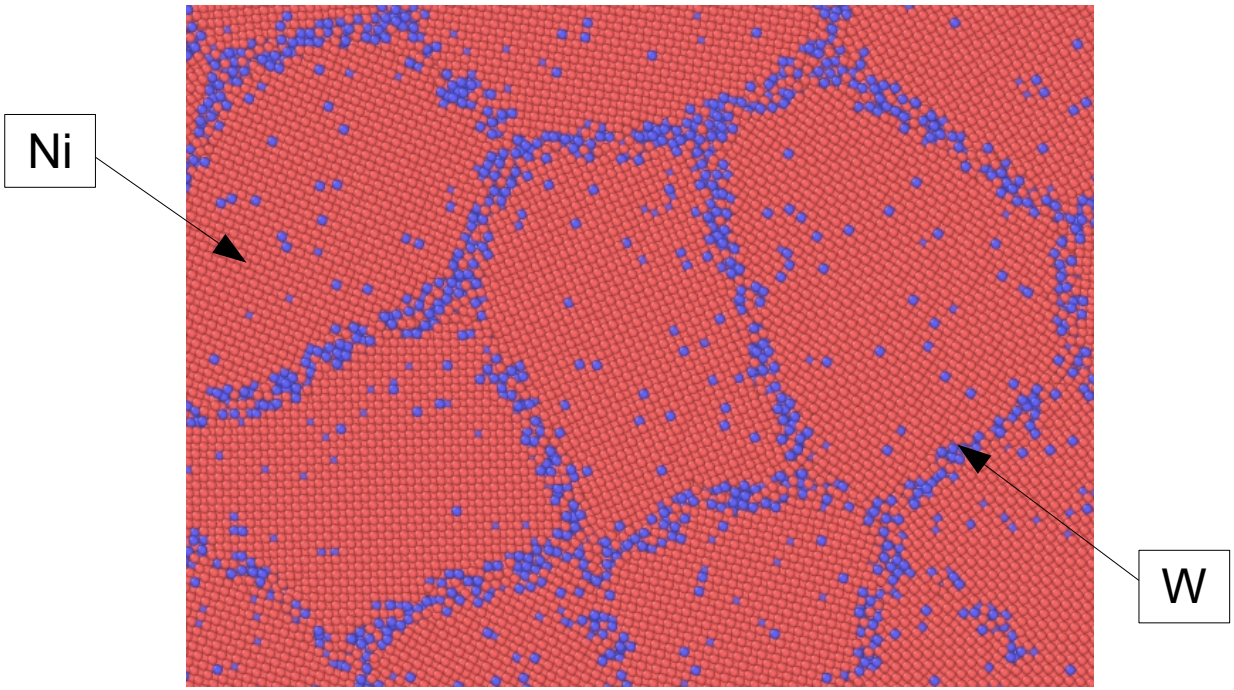
Segregation at grain boundaries
Monte Carlo simulations

Enery variation (per atom) from random to segregated condition



Segregation at grain boundaries
Monte Carlo simulations

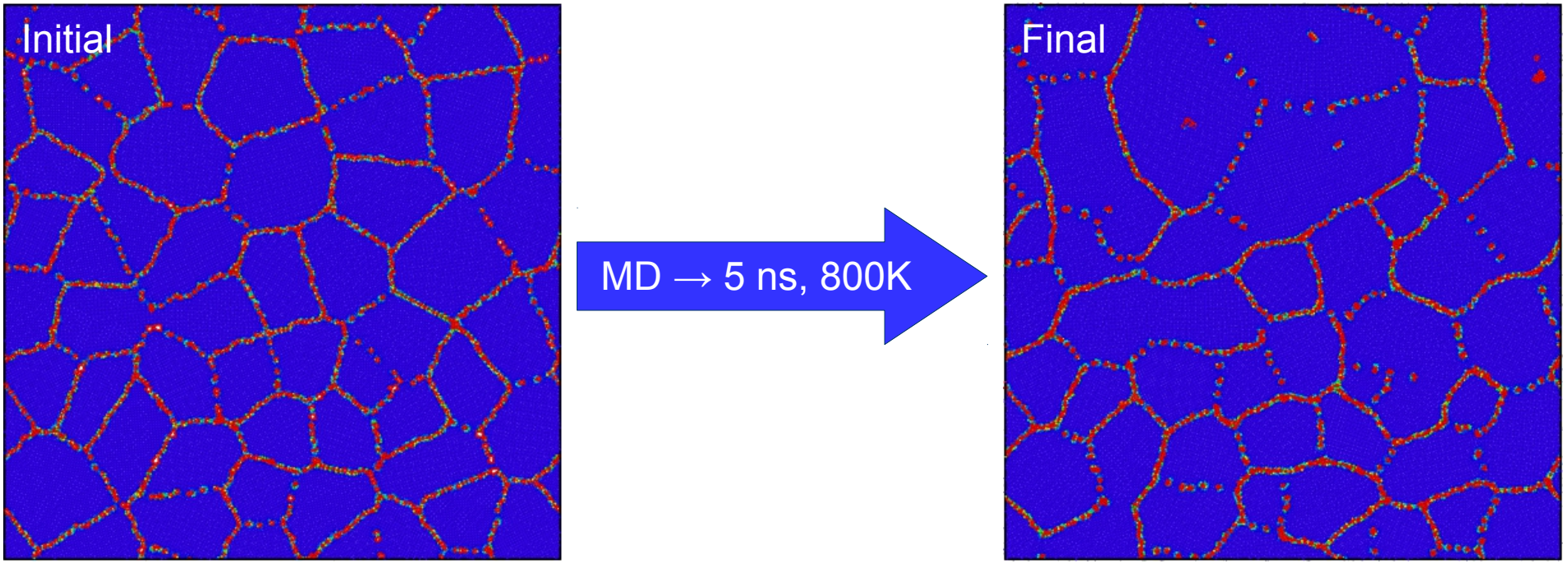
Example → Ni-W



From converged MC simulations → initial structure to be simulated with MD

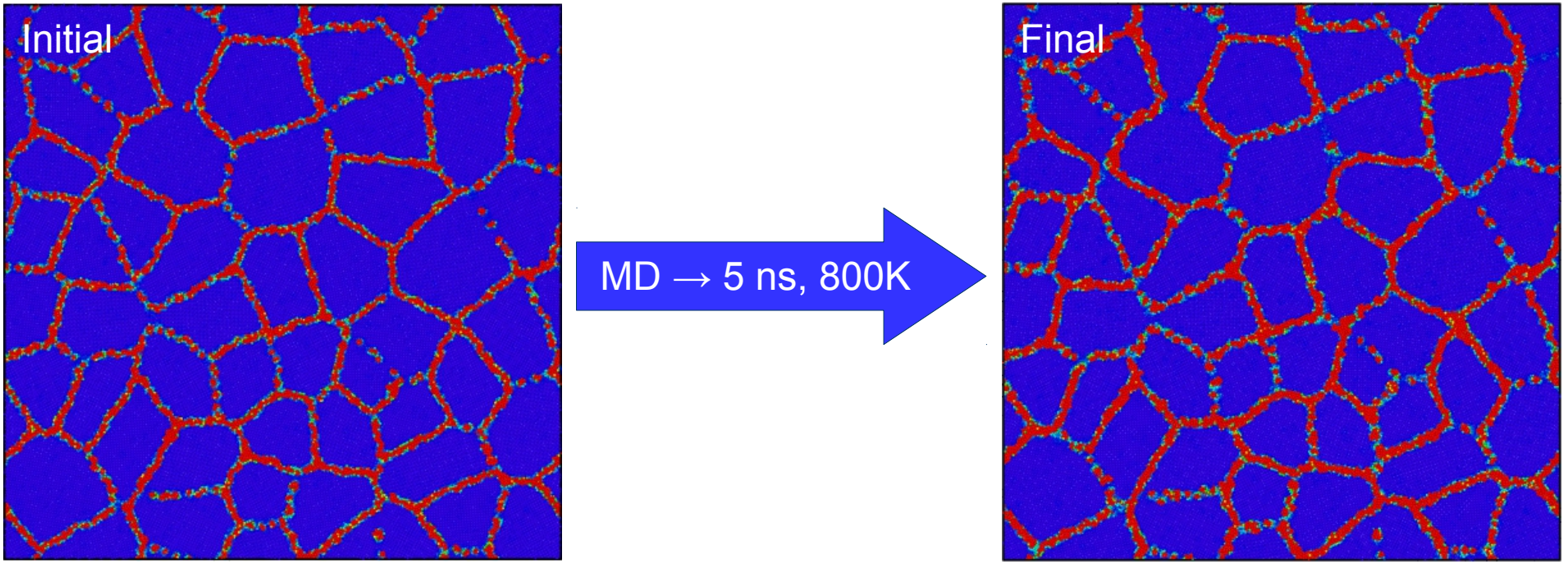
More results: Nickel alloys

Nickel-Cobalt



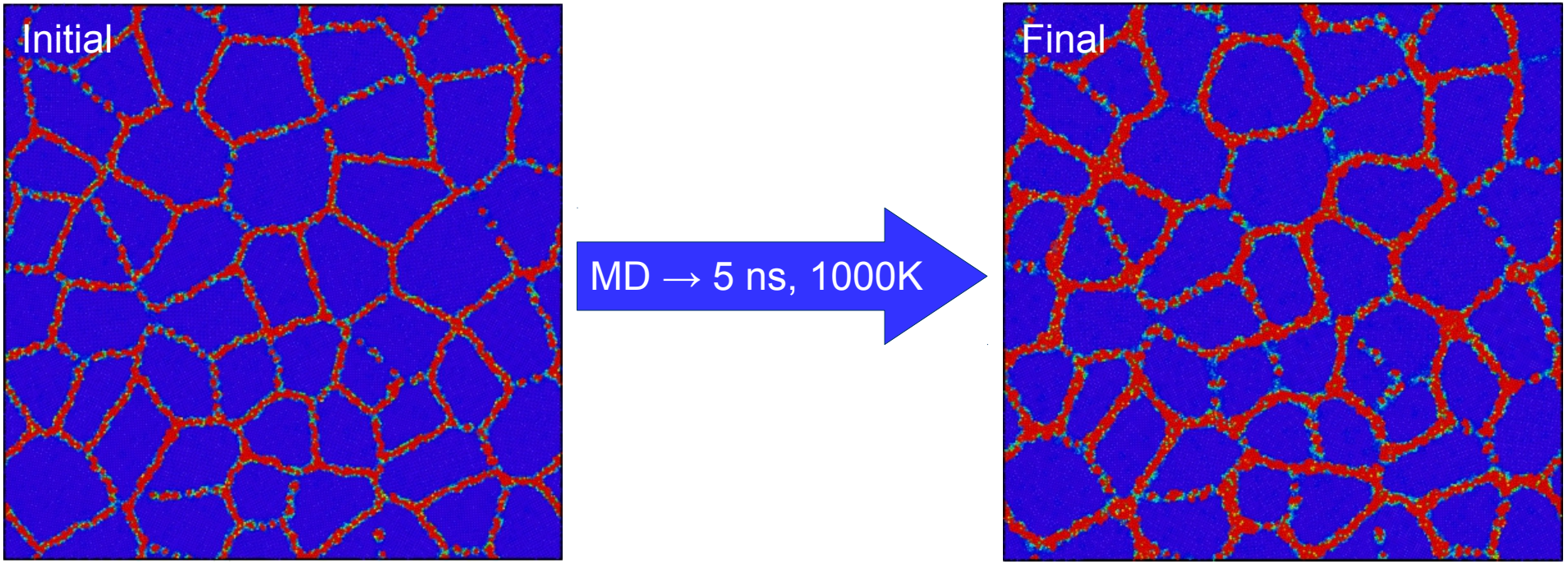
More results: Nickel alloys

Nickel-Aluminium



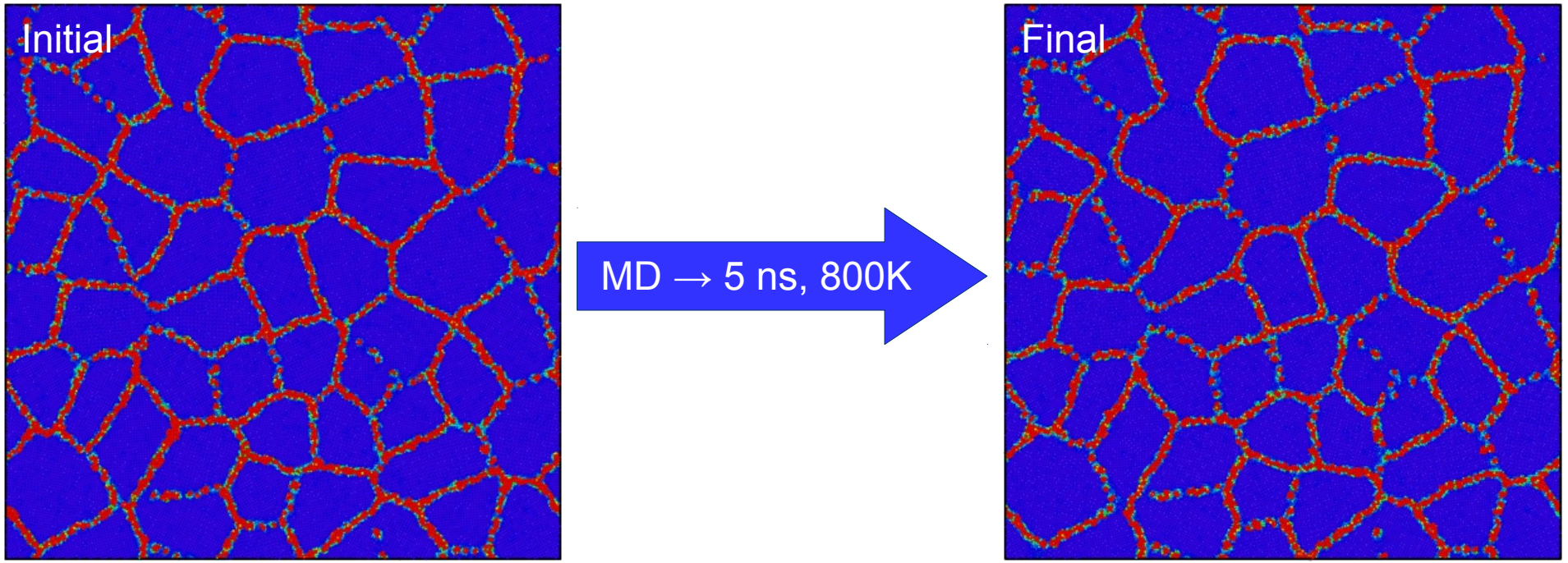
More results: Nickel alloys

Nickel-Aluminium



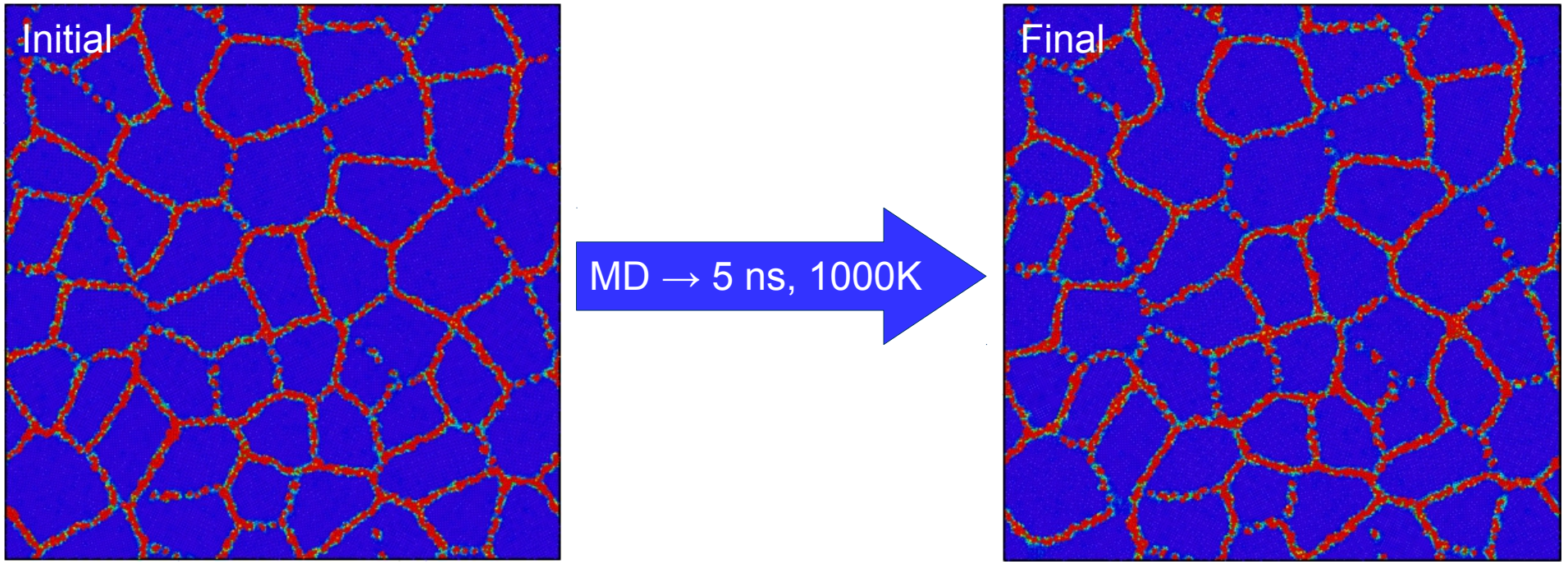
More results: Nickel alloys

Nickel-Palladium



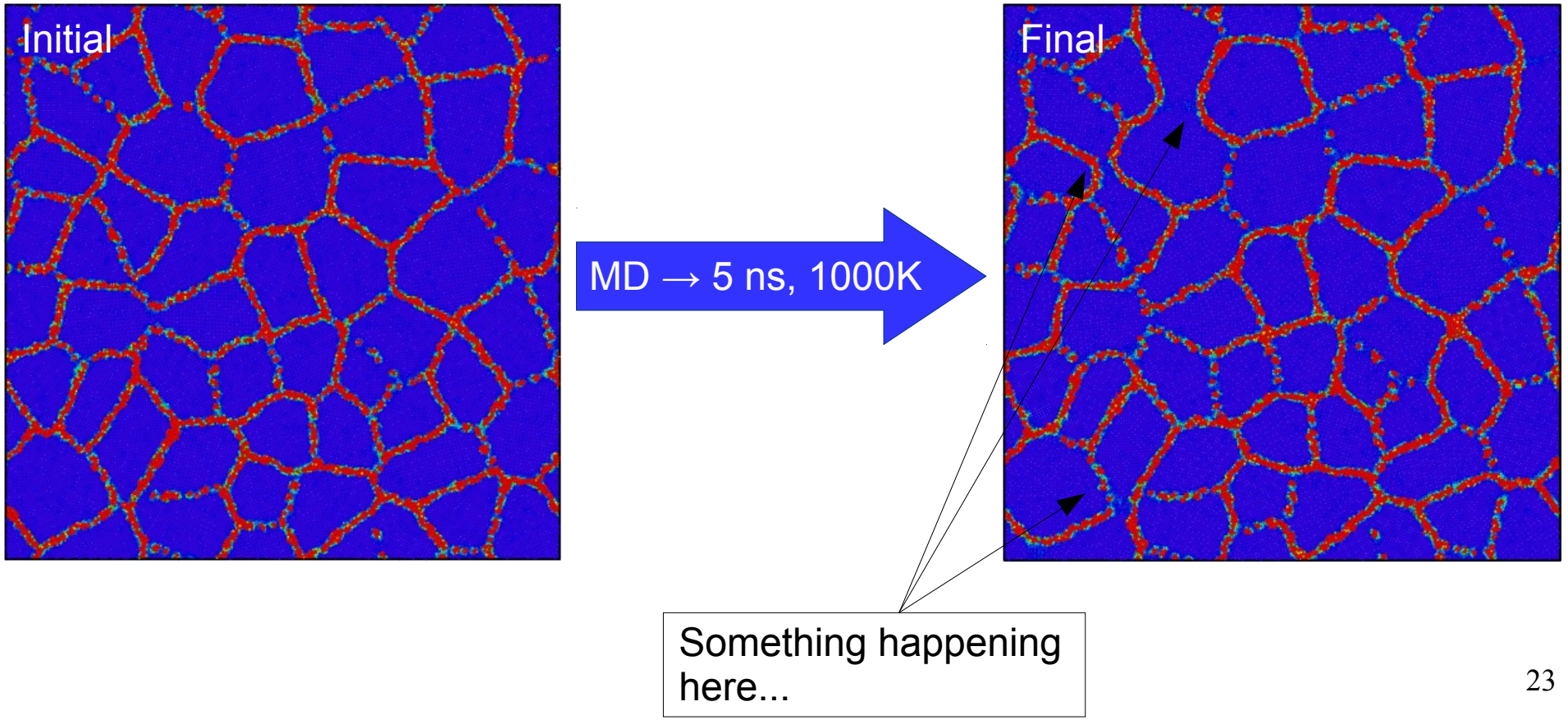
More results: Nickel alloys

Nickel-Palladium



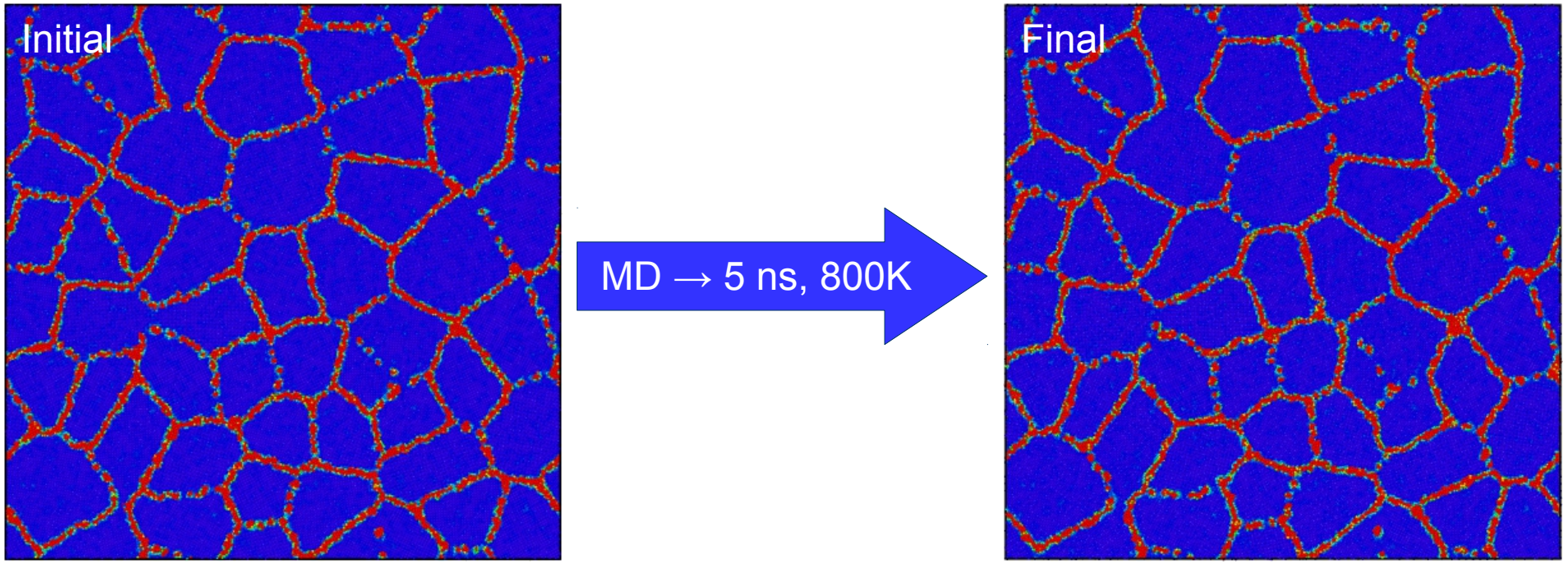
More results: Nickel alloys

Nickel-Palladium



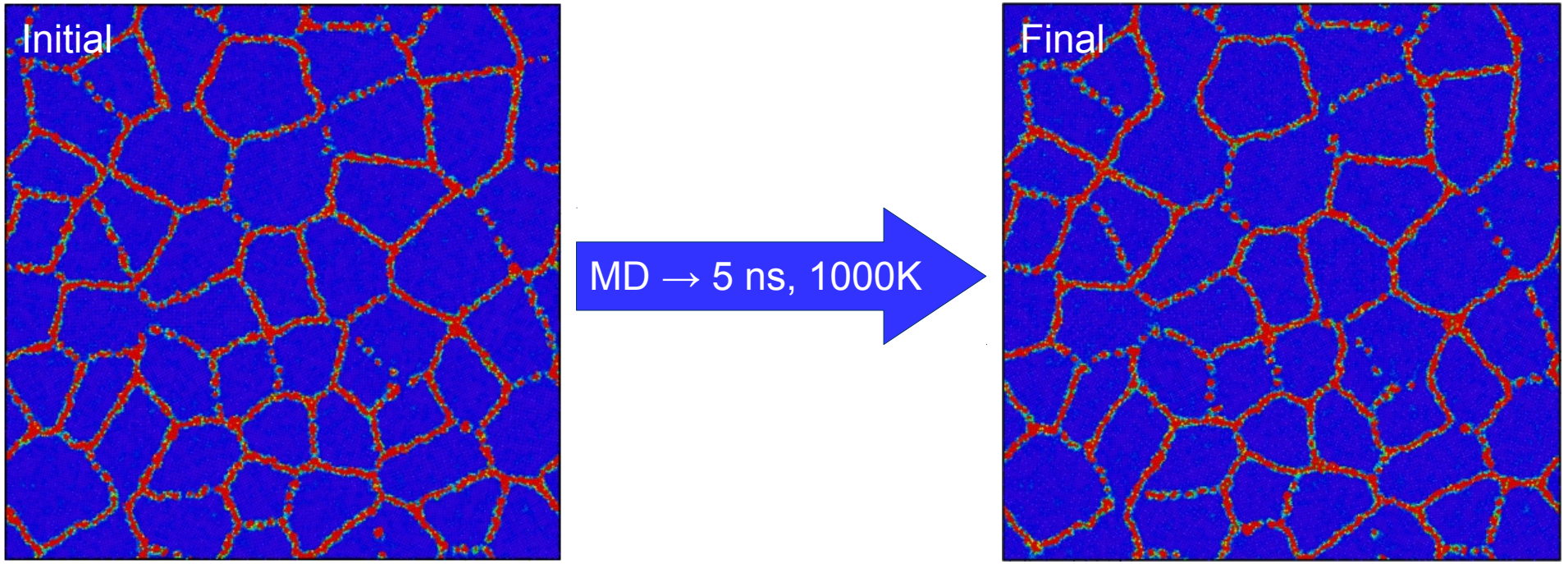
More results: Nickel alloys

Nickel-Tantalum



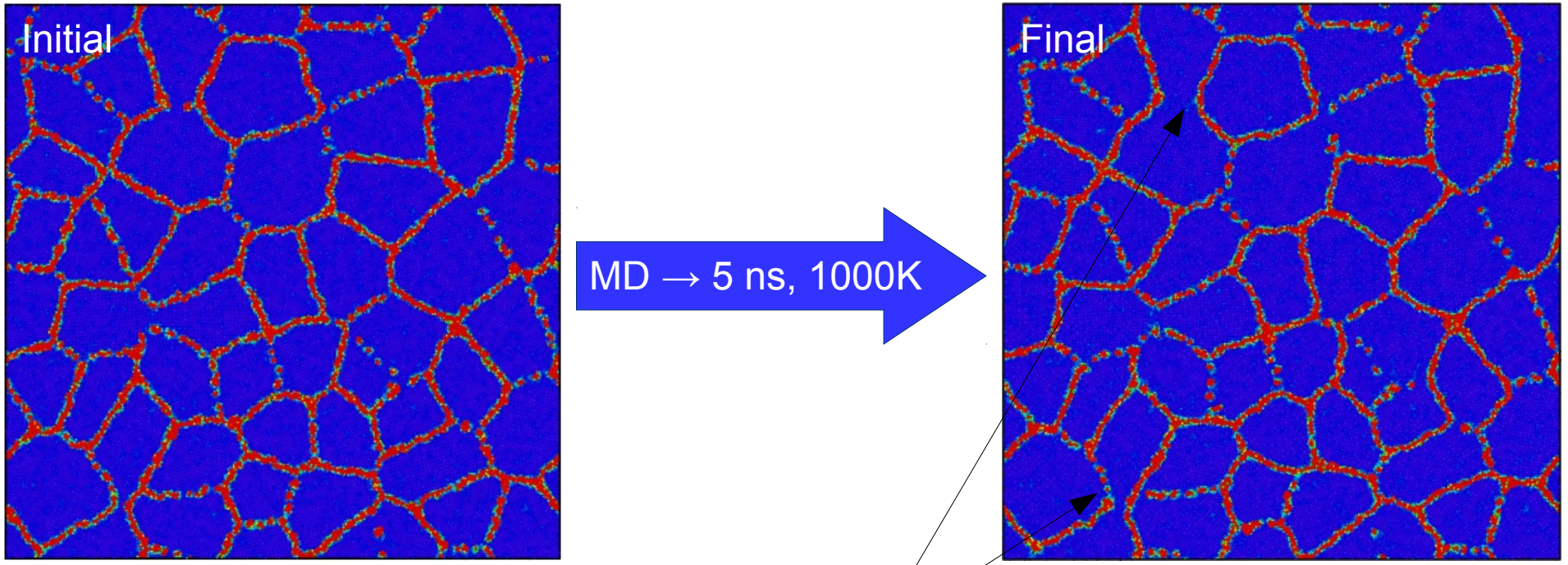
More results: Nickel alloys

Nickel-Tantalum



More results: Nickel alloys

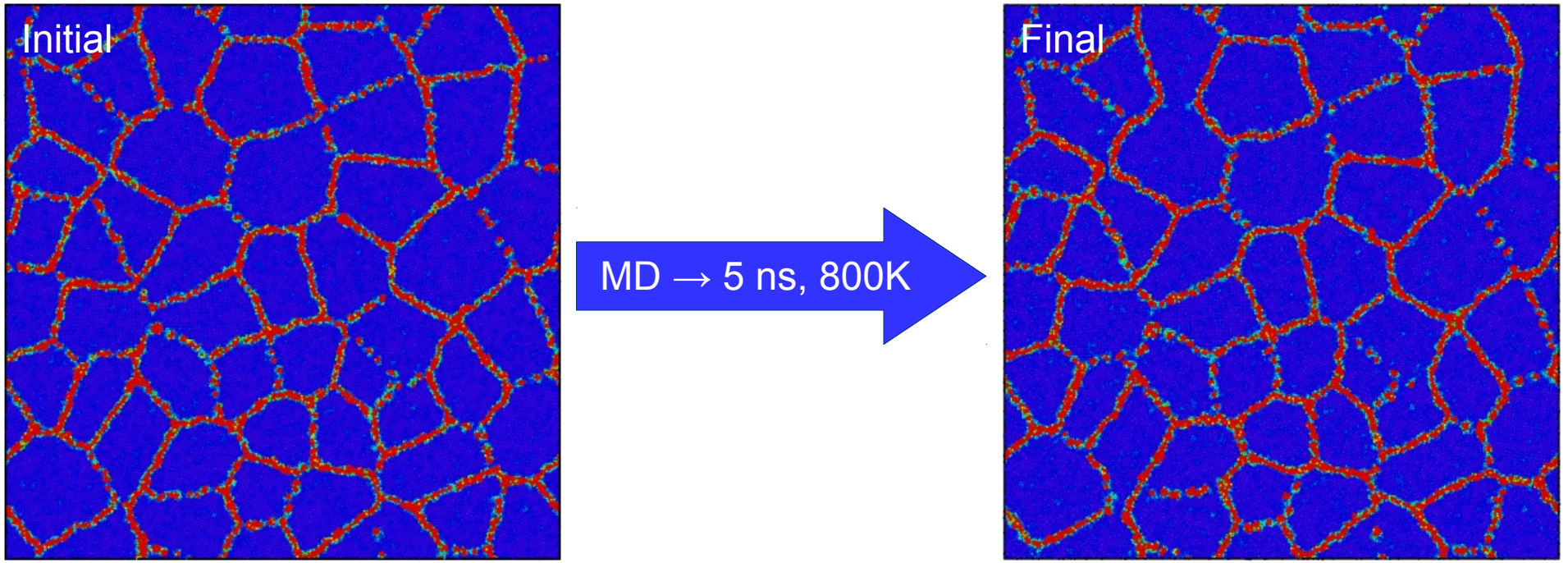
Nickel-Tantalum



Grain boundaries moving slower... but visibly moving.

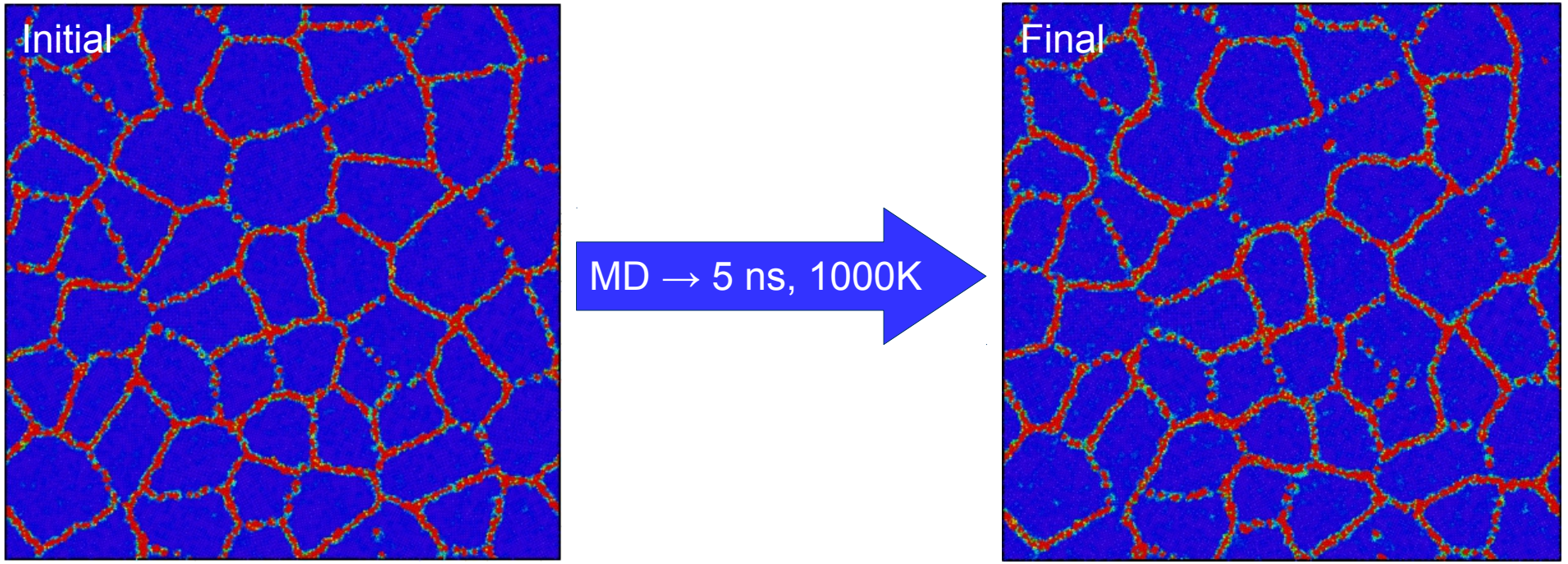
More results: Nickel alloys

Nickel-Titanium



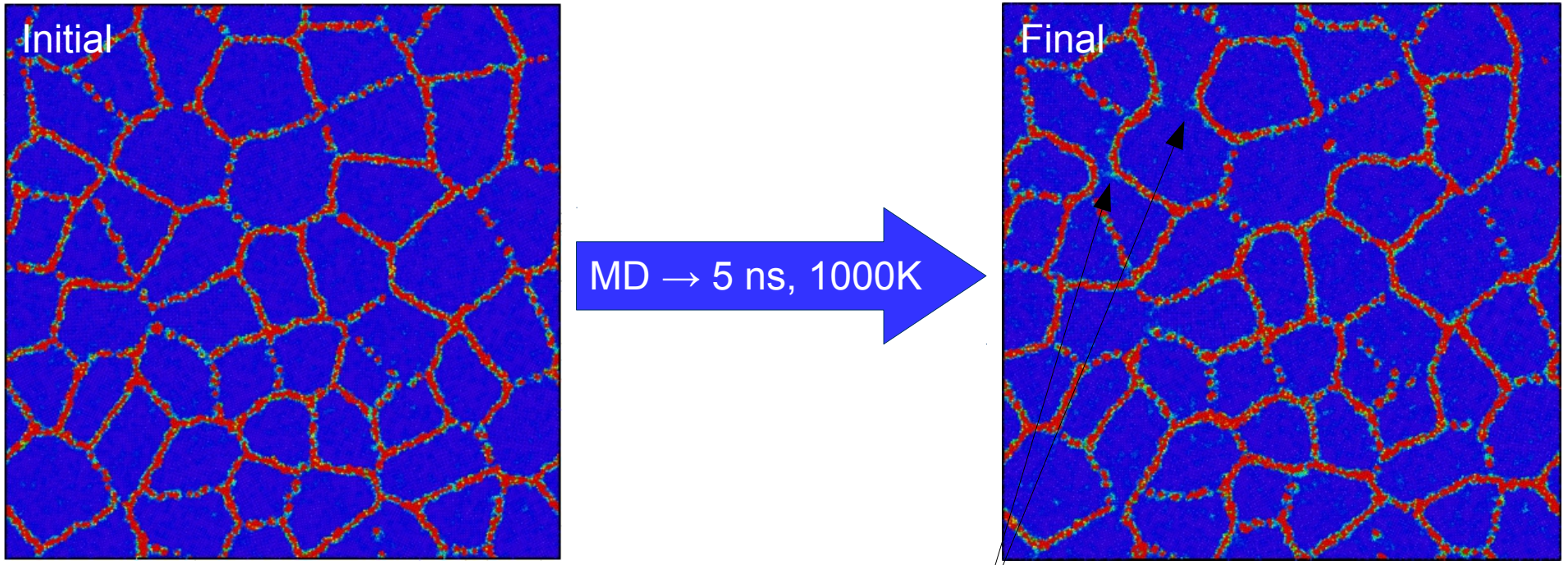
More results: Nickel alloys

Nickel-Titanium



More results: Nickel alloys

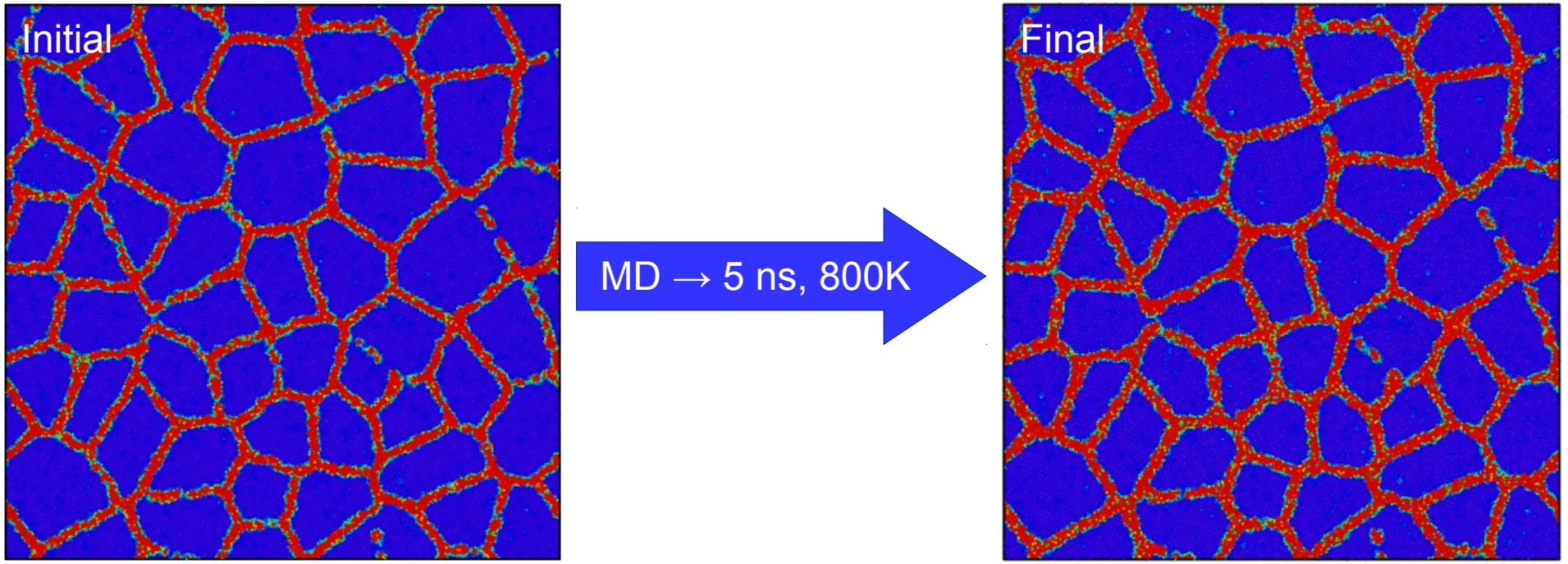
Nickel-Titanium



Grain boundaries moving slower... but moving.

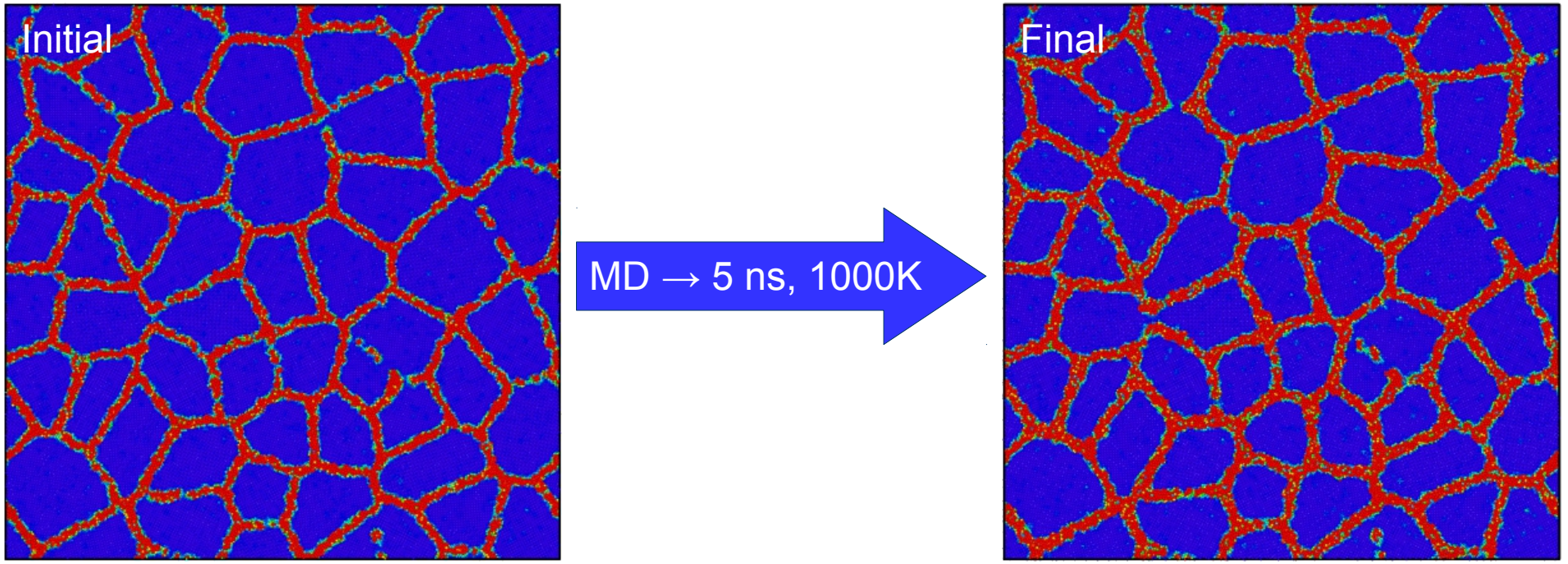
More results: Nickel alloys

Nickel-Molybdenum



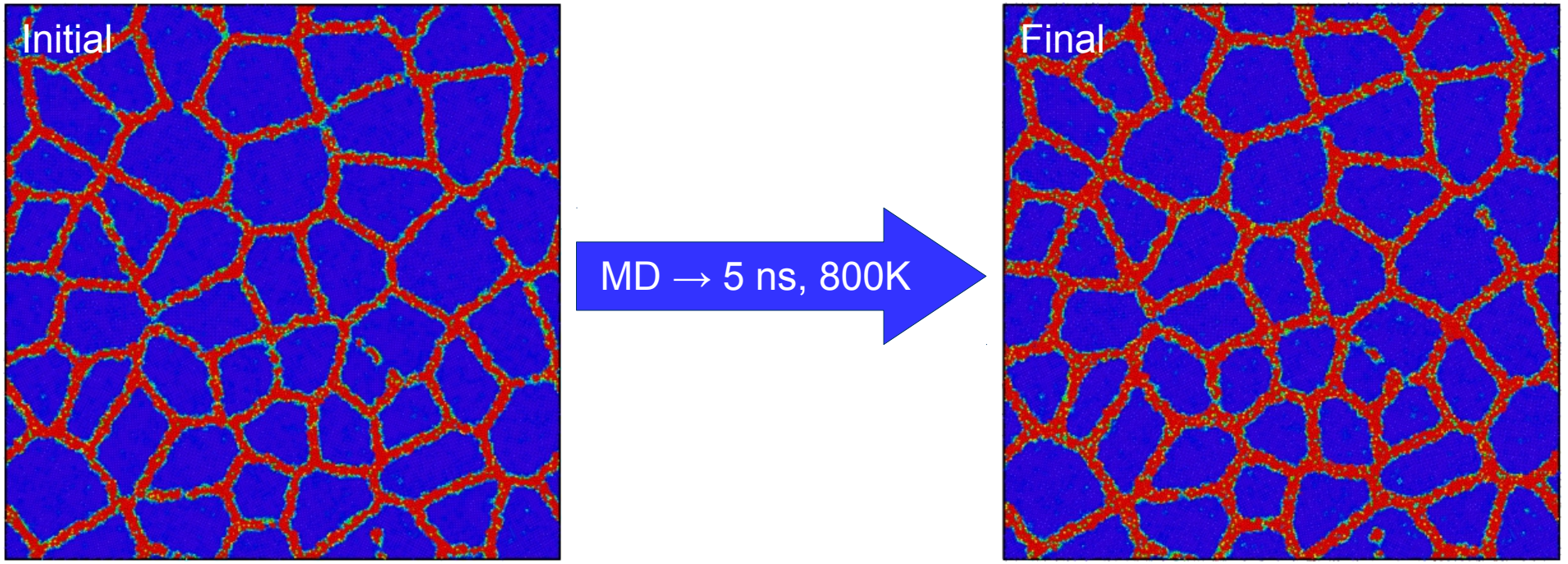
More results: Nickel alloys

Nickel-Molybdenum



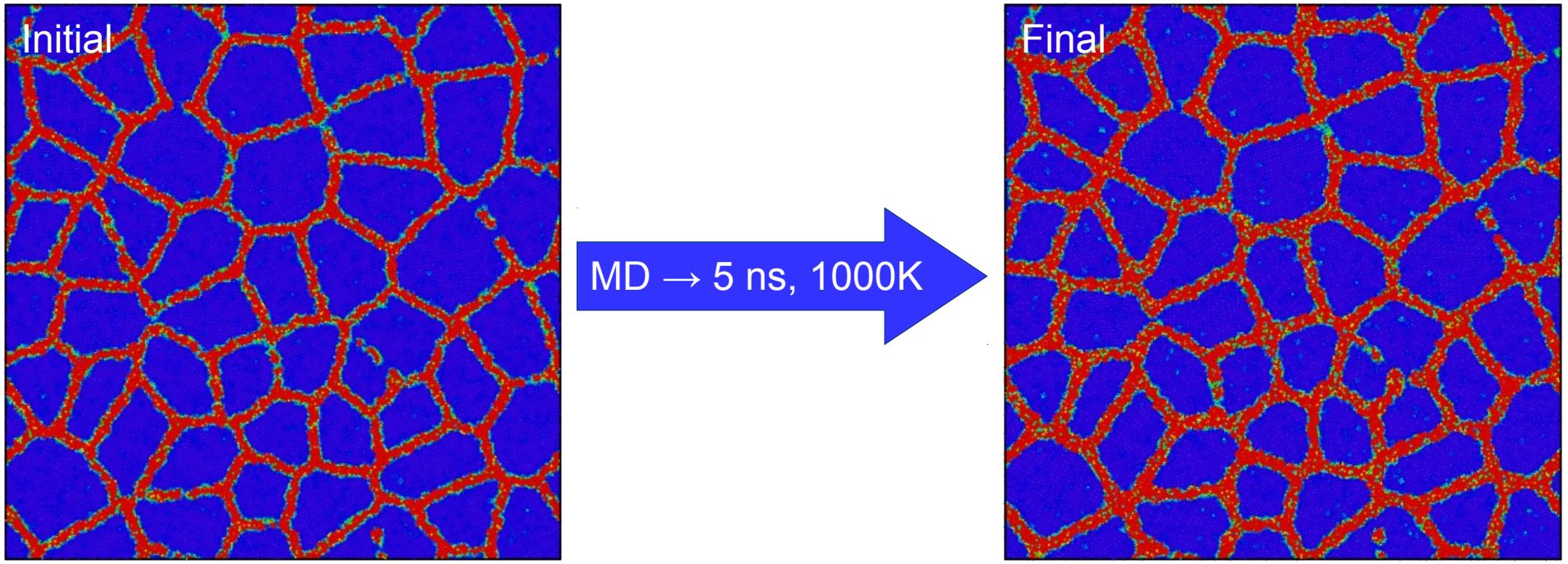
More results: Nickel alloys

Nickel-Tungsten



Some results: Nickel alloys

Nickel-Tungsten



Just to summarize

With Monte Carlo → From random to segregated stable (low energy) structures
With MD (using MC-simulated segregated structures) → Grain boundary behavior

Major conclusions:

Co has no significant effect on grain growth in the model system.

Al, Pd, Ta, and Ti apparently slow down grain growth in the model system.

W (as previously shown in experiments and simulations) and Mo appear to freeze the nanocrystalline structure of Ni.

For nc-Fe, the MD simulation time (5 ns) seem to be too short to observe significant grain growth even at 1000 K.

Next steps

Change the concentration of alloying elements → Saturation effects on segregation and grain growth

Run longer MD simulations for nc-Fe → More significant evolution of the microstructure

Run MC and MD for more than one alloying element

Test 3D structures → More general model of a nanocrystalline alloy

Consider segregation (e.g., carbon) at austenite/ferrite interface

This work used computational facilities provided by the USP/Rice University agreement (Blue Gene P supercomputer)

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Thank you for your attention