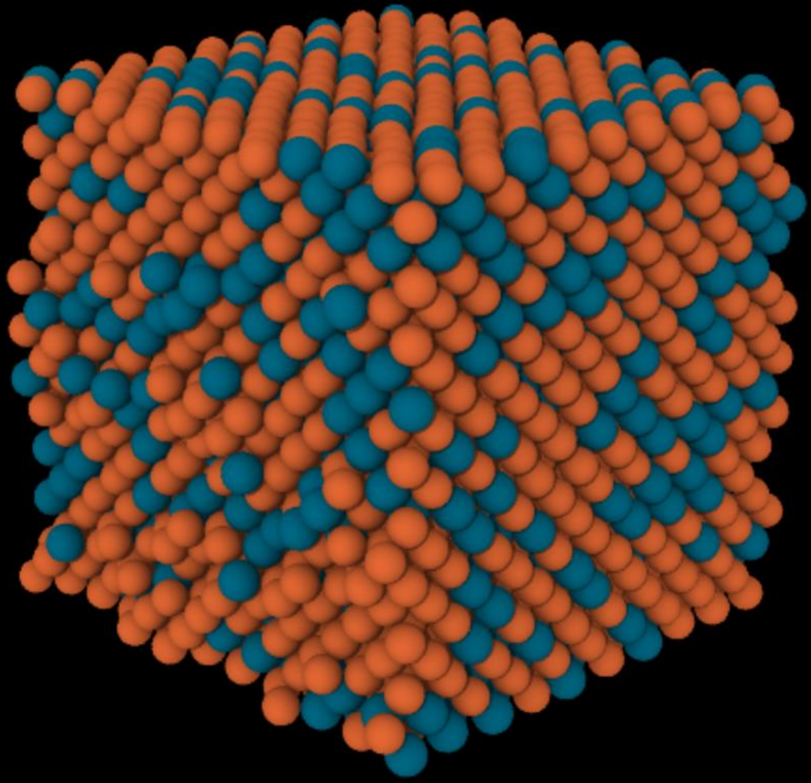
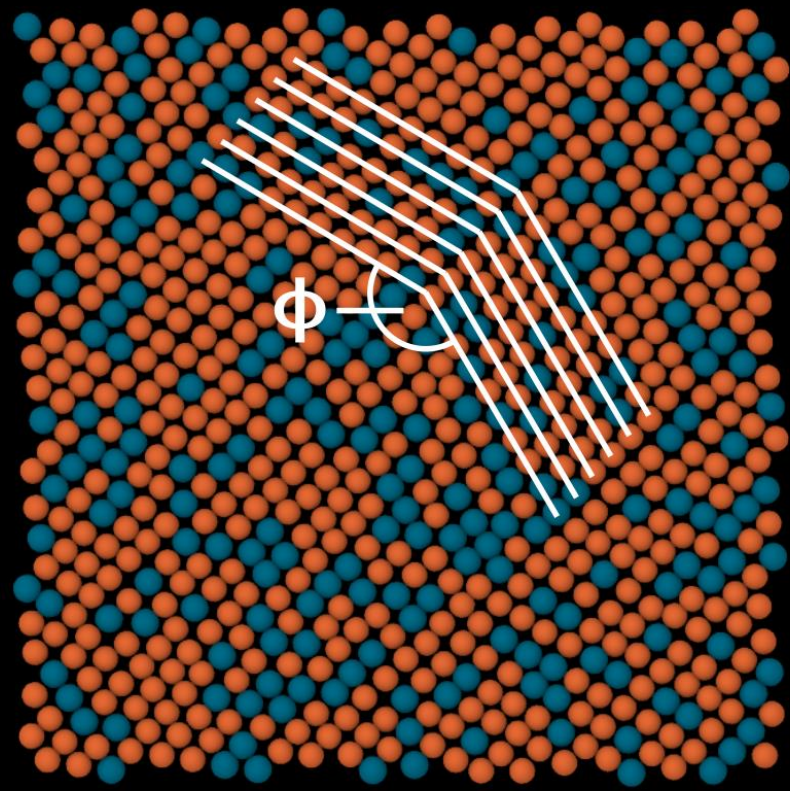




Molecular Dynamics Simulations on the Austenite-Martensite Phase Transition in Fe_7Pd_3

CompPhys17, November 30 – December 2, 2017

Alexander Holm

IOM
Leibniz Institute of Surface Modification

Motivational Introduction

Shape Changing Effects

- Thermal Shape Memory Effect
- Invar Effect
- Ferromagnetic Shape Memory Effect

Mechanical Properties

- High and low temperature solid state phases
- Martensitic transformations
- Highly ductile
- Magnetically anisotropic
- High Currie temperature (*720 K*)

Biocompatibility

- No foreign body reactions
- Good adhesion properties

Fe_7Pd_3

Functional Surfaces

Applications

- Mechanically active coatings for prosthesis
- Vascular Grafts
- Magnetically controllable actuators for medical applications [*]

[*] K. Ullakko, L. Wendell, A. Smith, P. Müllner, and G. Hampikian, Smart Mater. and Struct. 21, 115020 (2012).

Outline

Martensitic Transformations

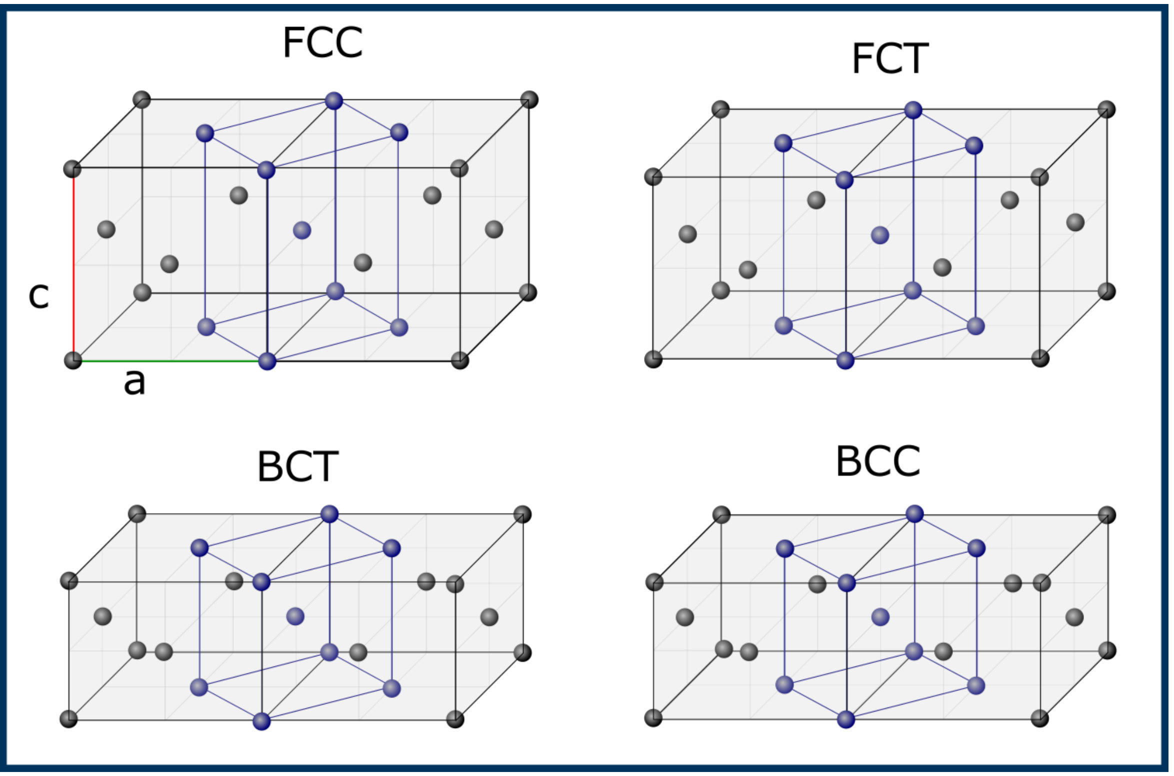
- Transformations between high temperature, high symmetric austenite and low temperature, lower symmetric martensite phase

Martensitic Transformations

- Transformations between high temperature, high symmetric austenite and low temperature, lower symmetric martensite phase
- Changes of the lattice structure and shape

Martensitic Transformations

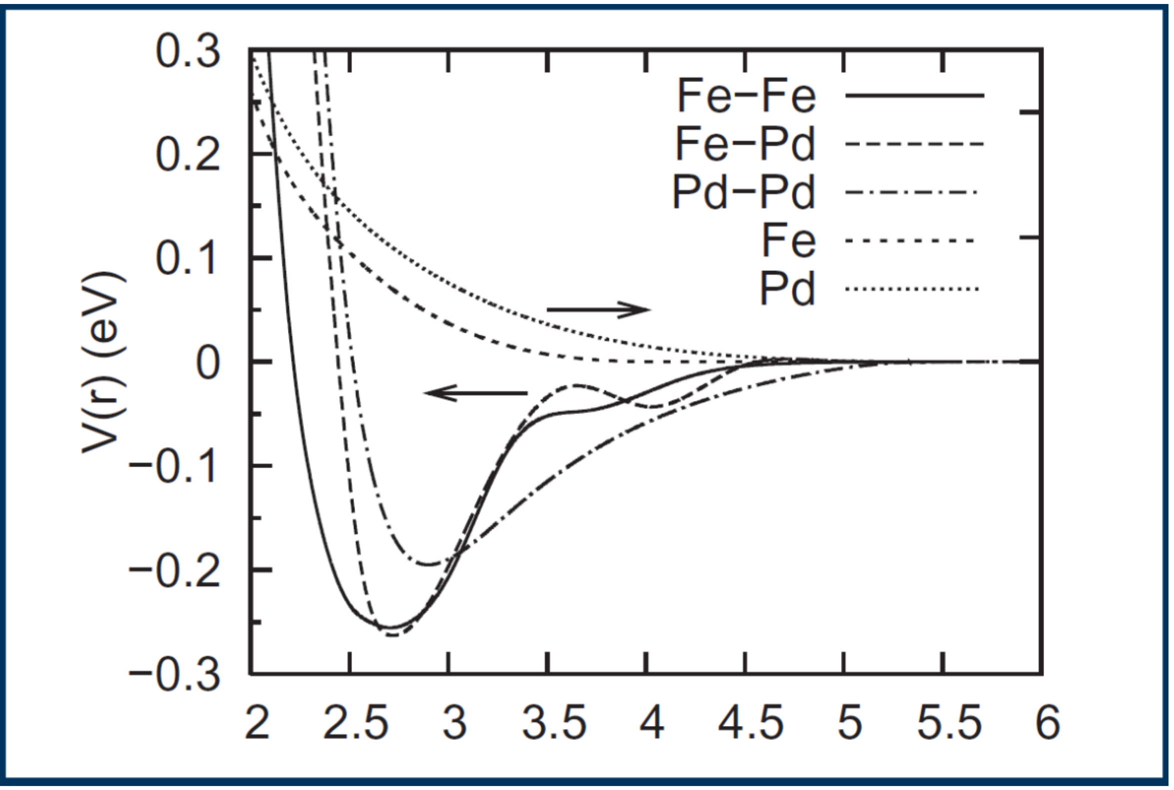
- Transformations between high temperature, high symmetric austenite and low temperature, lower symmetric martensite phase
- Changes of the lattice structure and shape
- Different transformation mechanisms proposed
  → Small ranges of atomic movement
  → Conservation of nearest neighbour relations



Bain Path

- Uniaxial Deformation parallel to the c-direction of the unit cell
- four stable structures corresponding to axis ratios:

Crystal Structure	Axis Ratio (c/a)
FCC	1
FCT	0.940
BCT	0.717
BCC	0.707



Potential for Molecular Dynamics Simulations

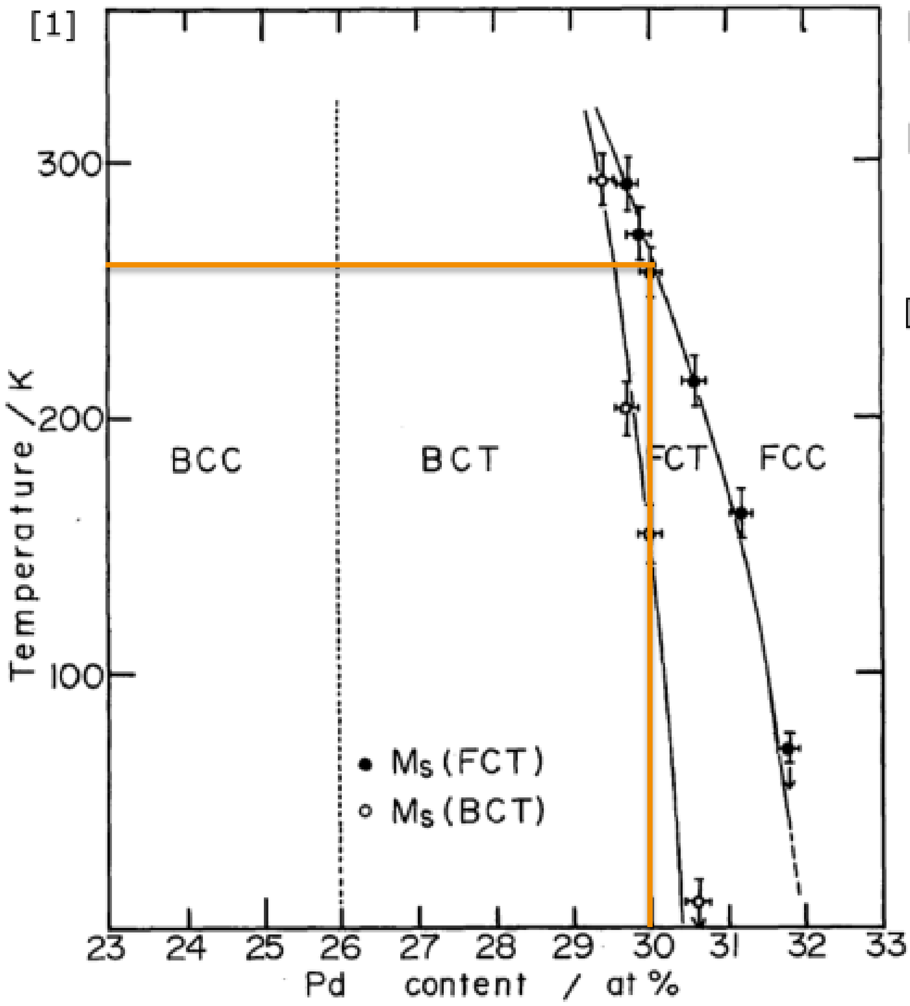
- Embedded Atom Method

$$E_{tot} = \sum_i F_i\big(\rho_i(R_i)\big) + \frac{1}{2}\sum_{i,j;j\neq i} \phi(R_{ij})$$

- Fit of the potential in order to adept Bain path properties observed in DFT simulations

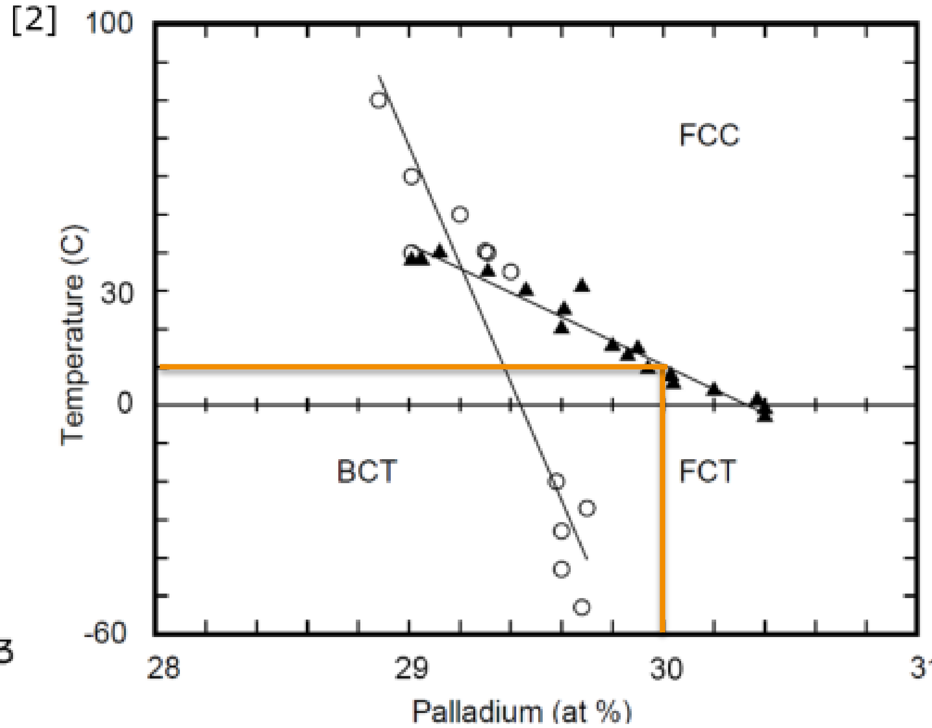
[S G Mayr and A Arabi-Hashemi 2012 *New J. Phys.* **14** 103006]

Thermally Induced Phase Transition

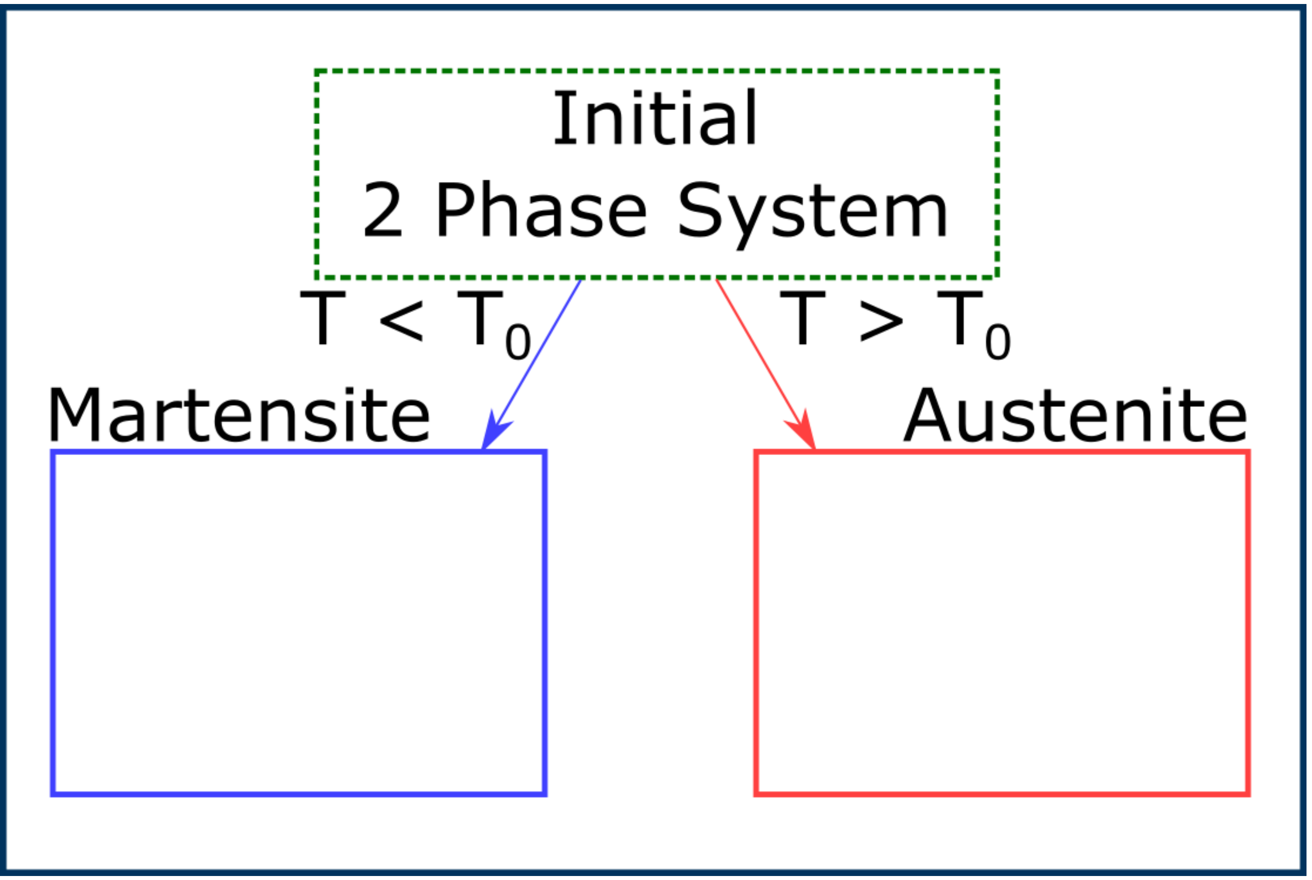


[1] M. Sugiyama, R. Oshima, and F. E. Fujita, Transactions of the Japan Institute of Metals 25, 585 (1984).

[2] J. Cui, T. Shield, and R. James, Acta Materialia 52, 35 (2004).



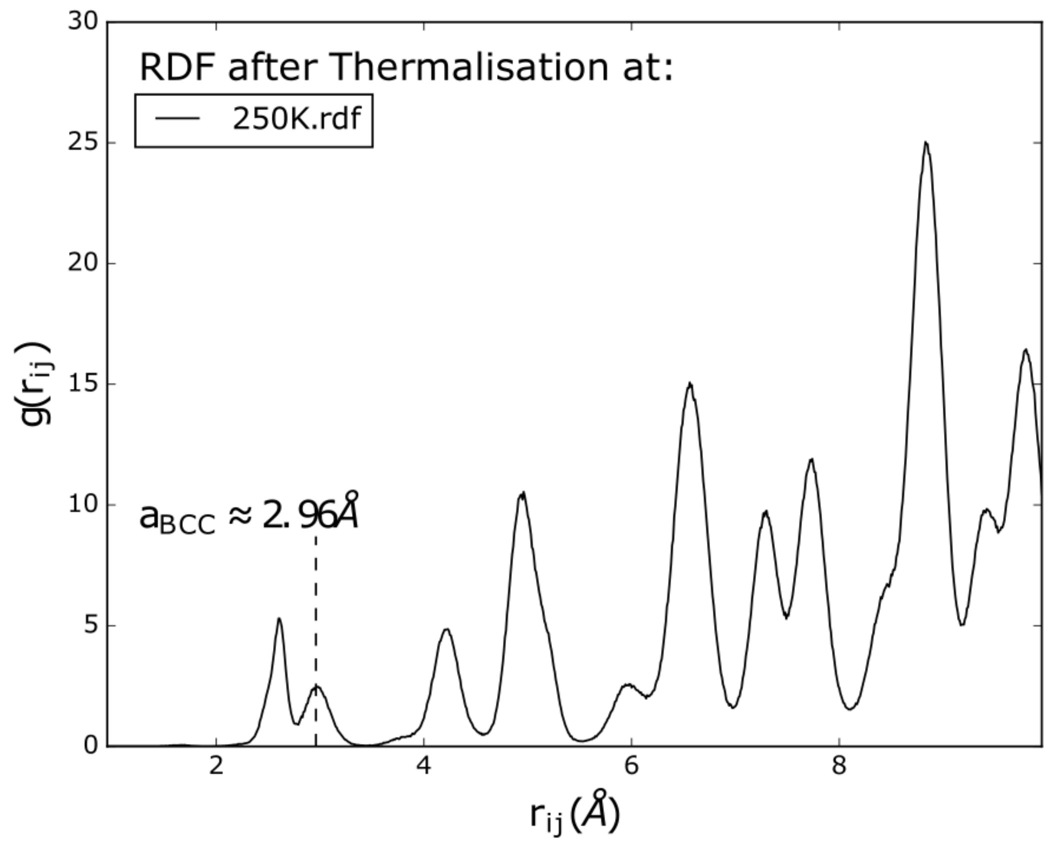
Thermally Induced Phase Transition

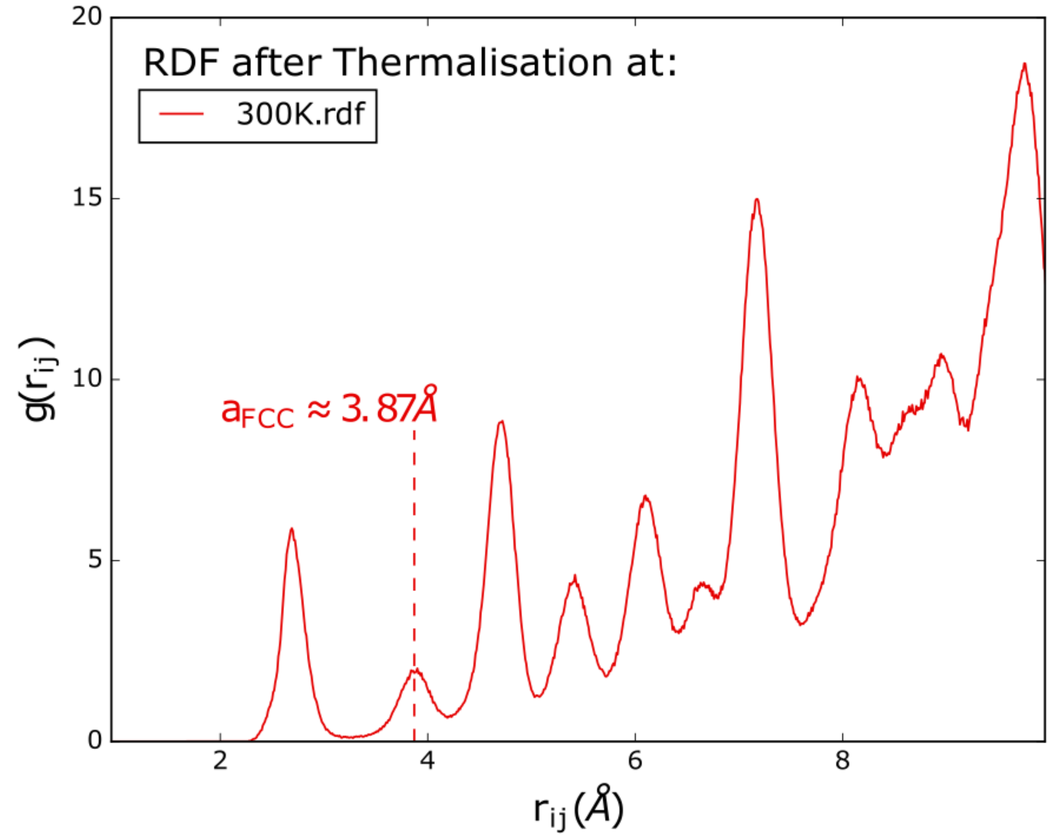


Resulting Phases

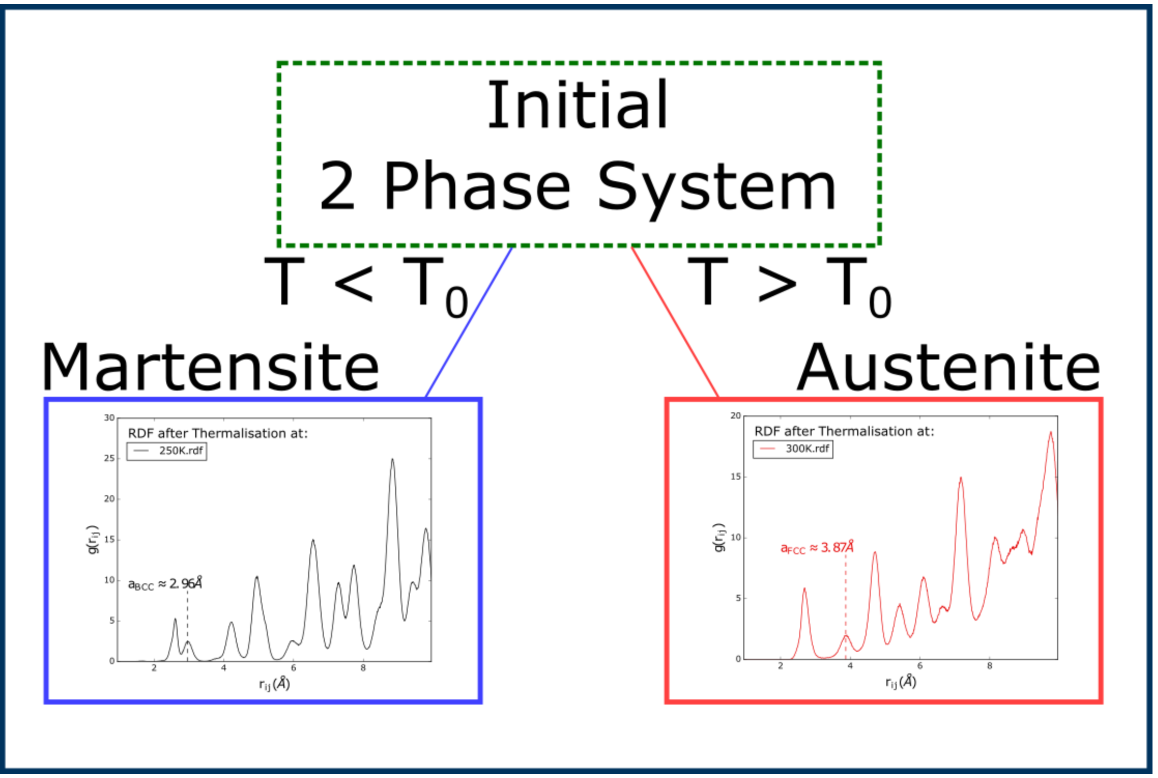
- Preparing a two phase system
- Depending on Temperature: two different equilibrium phases
- Compute the Radial Distribution Function (RDF)

Thermally Induced Phase Transition





Thermally Induced Phase Transition



Resulting Phases

- Providing 50 Temperature Sets for each Temperature to the two phase system
- Measure the relative frequentness of the *FCC* (austenite) phase compared to the *BCC* (martensite) phase

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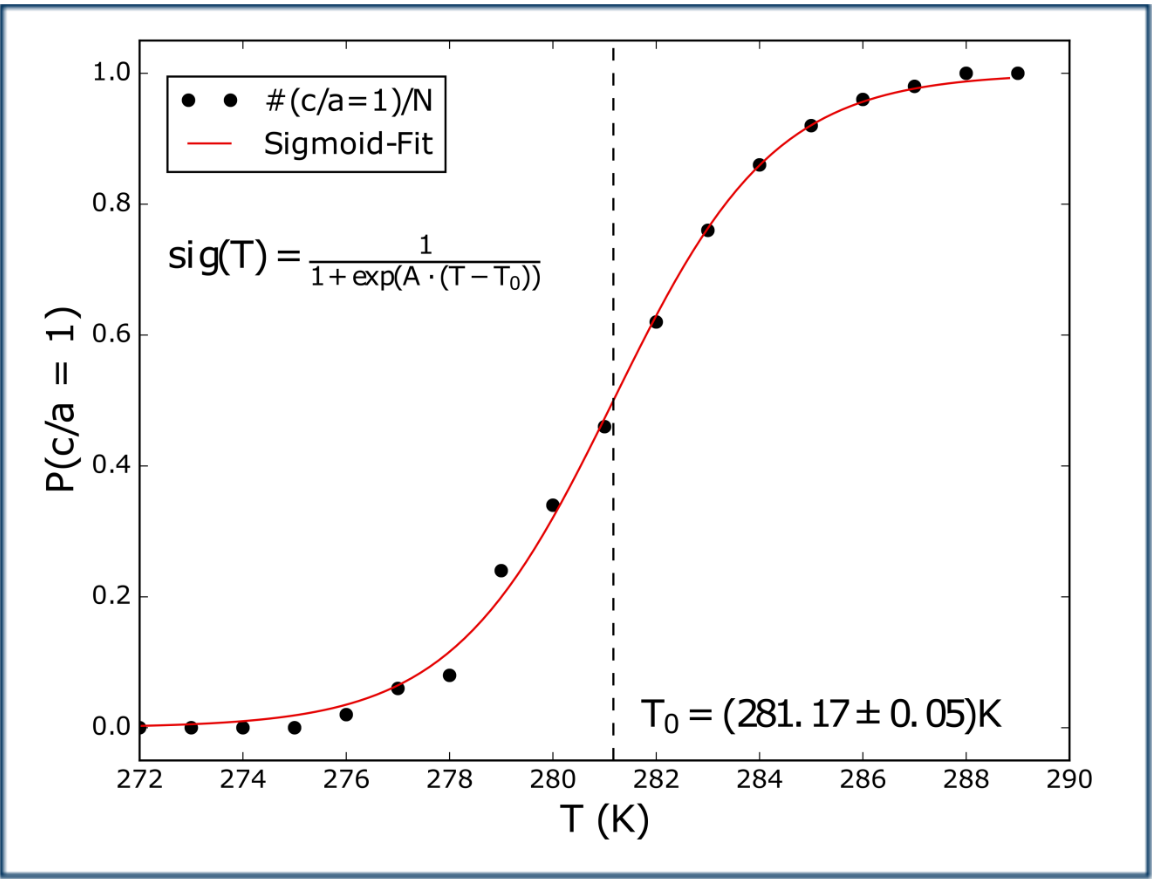
Thermally Induced Phase Transition



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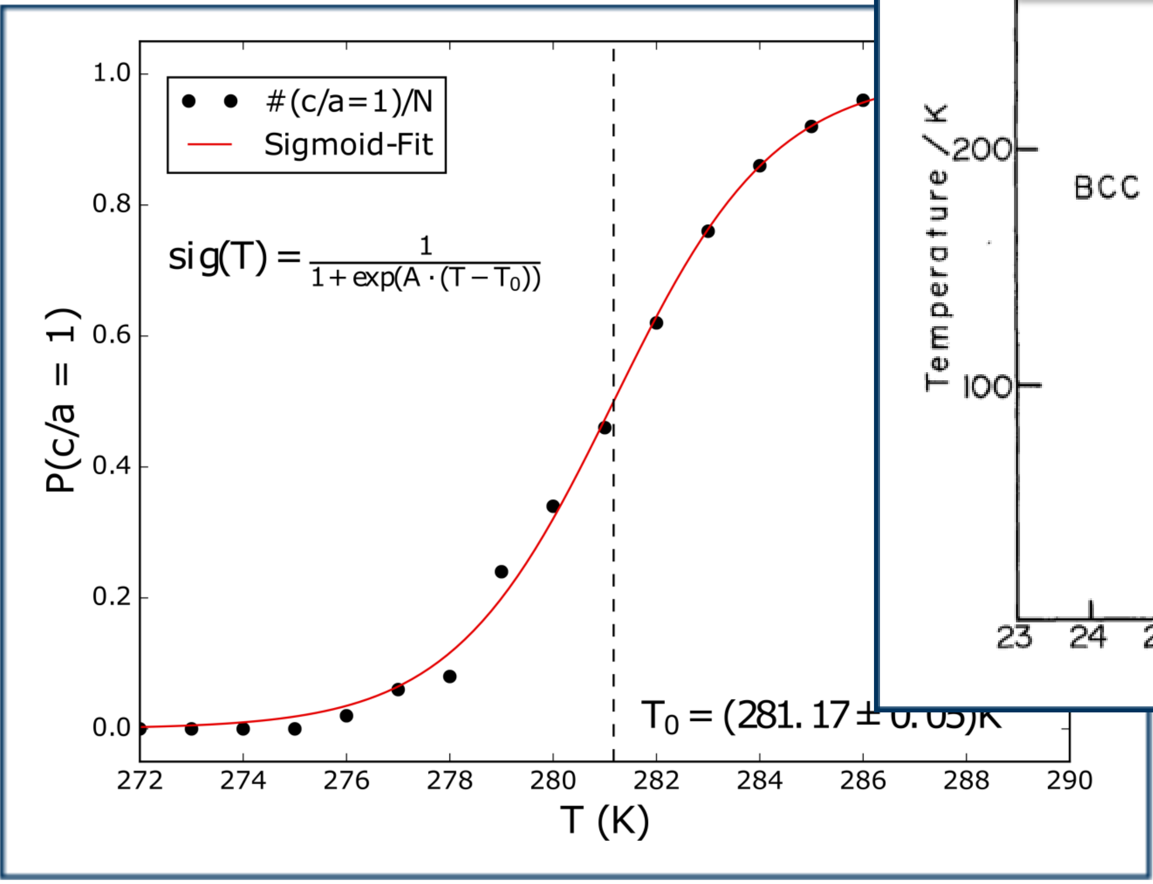

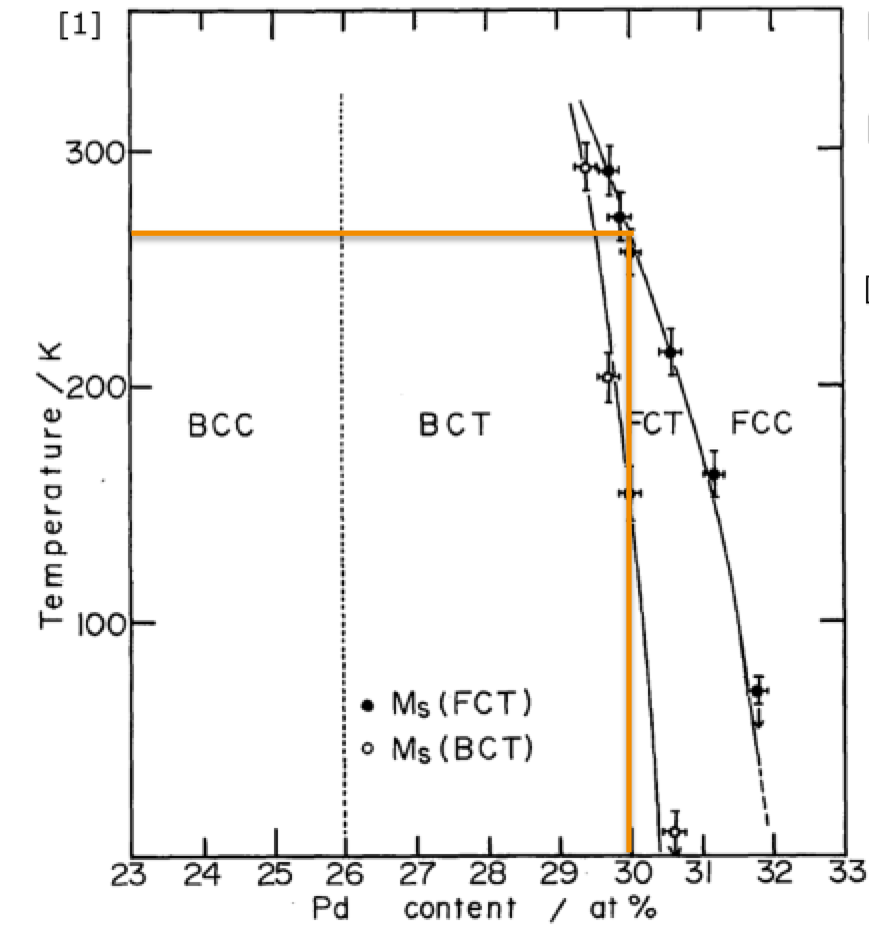

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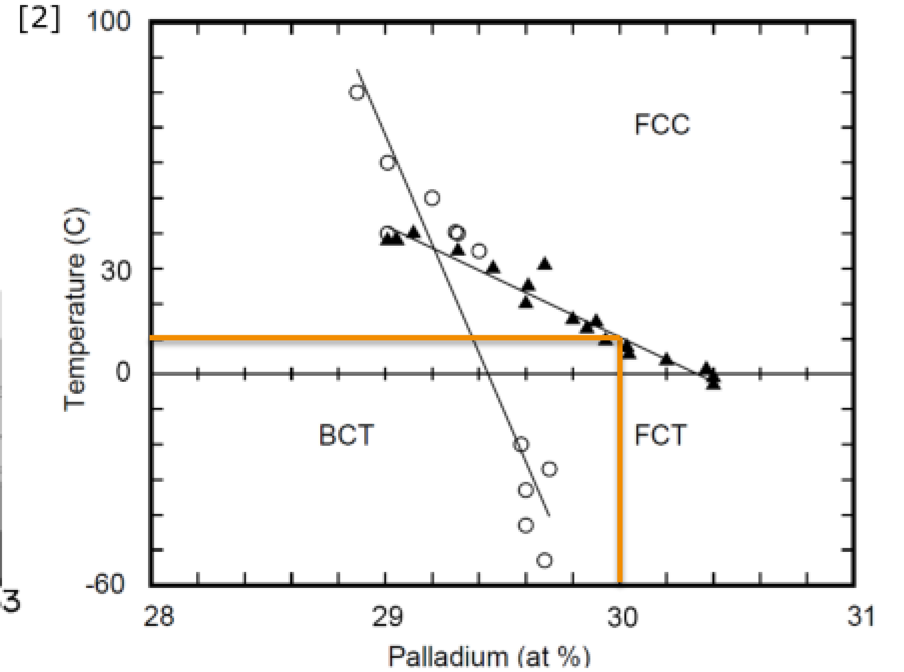
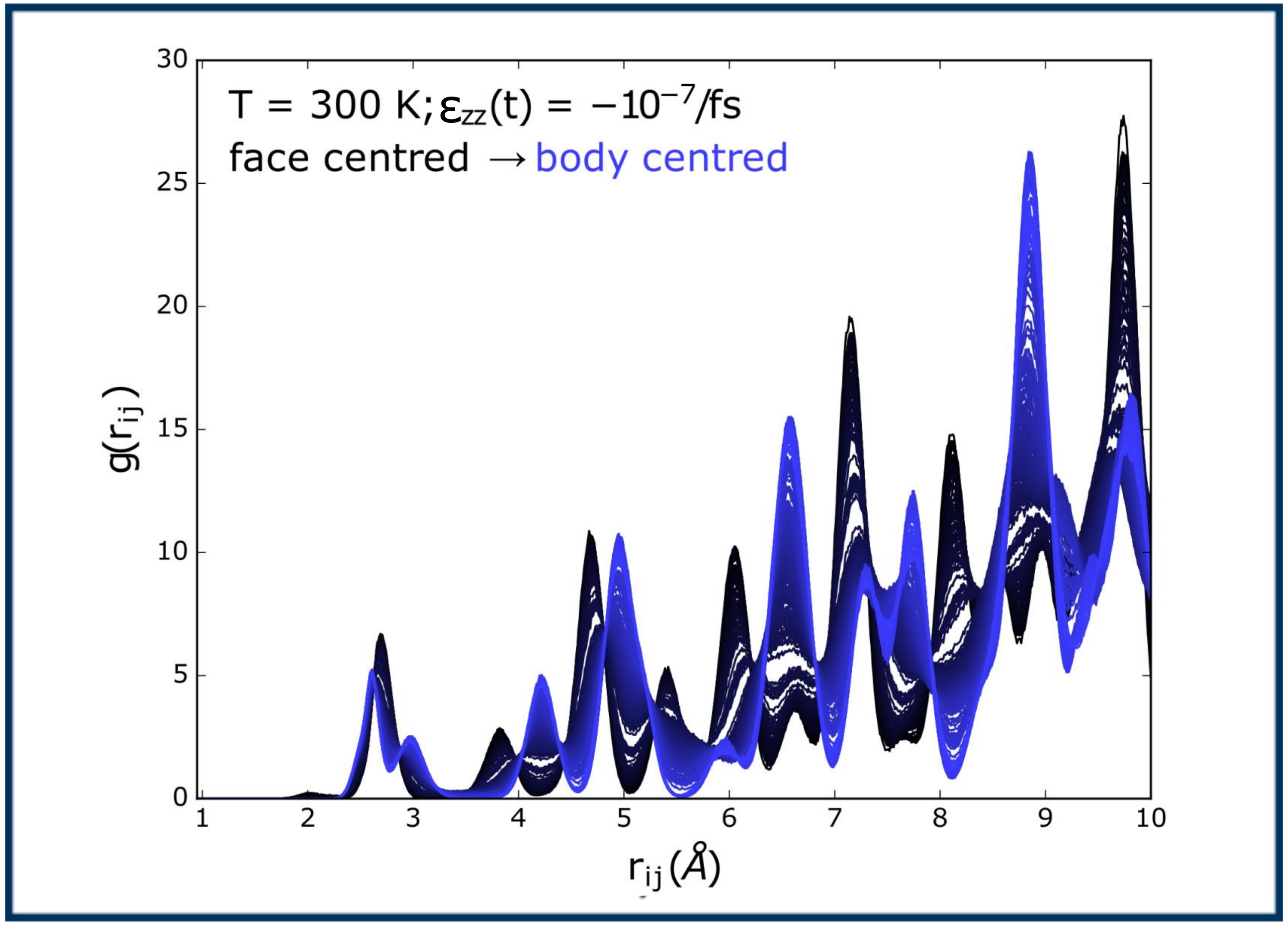


- Good accordance of the determined phase transition temperature ($(281.17 \pm 0.05)\ K$) to literature values

Strain Induced Phase Transition



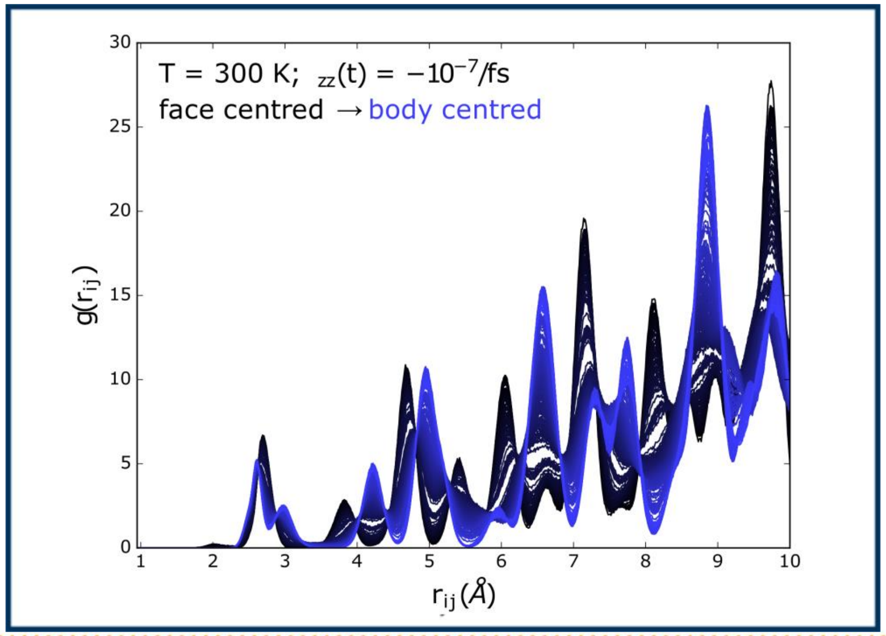
Setup according to the Bain path:

- Uniaxial deformation along the [001] direction with a constant strainrate of $\varepsilon_{zz}(t) = -0.1\ z_0/\mathrm{ns}$
- 2 ns of simulated time
- Calculated RDF every 10 ps

RDF Structure Analysis

Radial Distribution Function

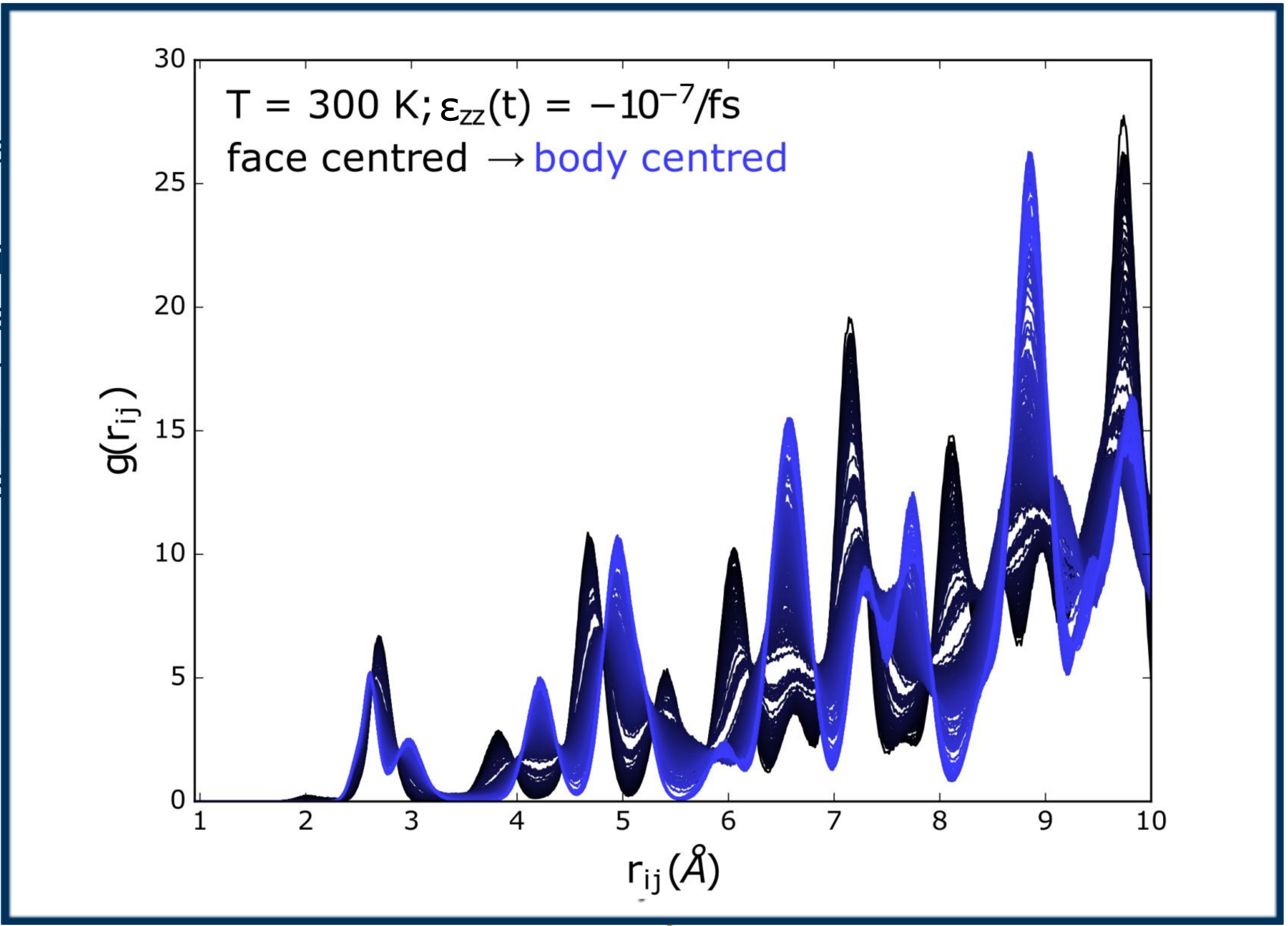
- Rather continuous transformation from *FC* zu *BC* structure
- Limited to resolve internal structures or events



Strain Induced Phase Transition

Radia

- Limi
  tetra
- Rath
  tran
  BC s



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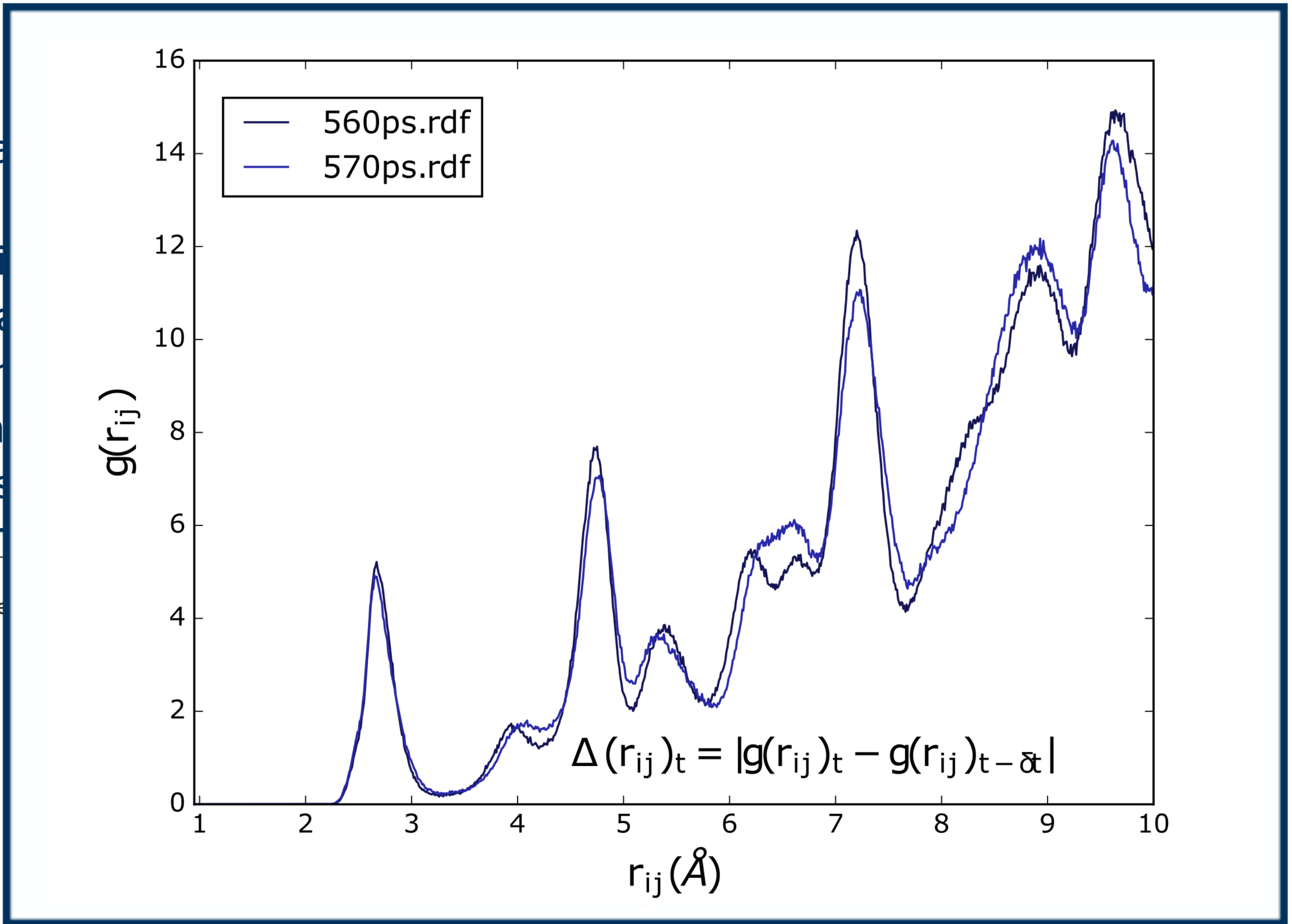

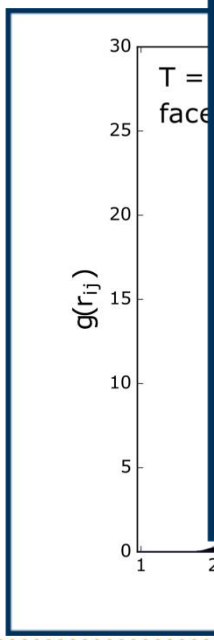

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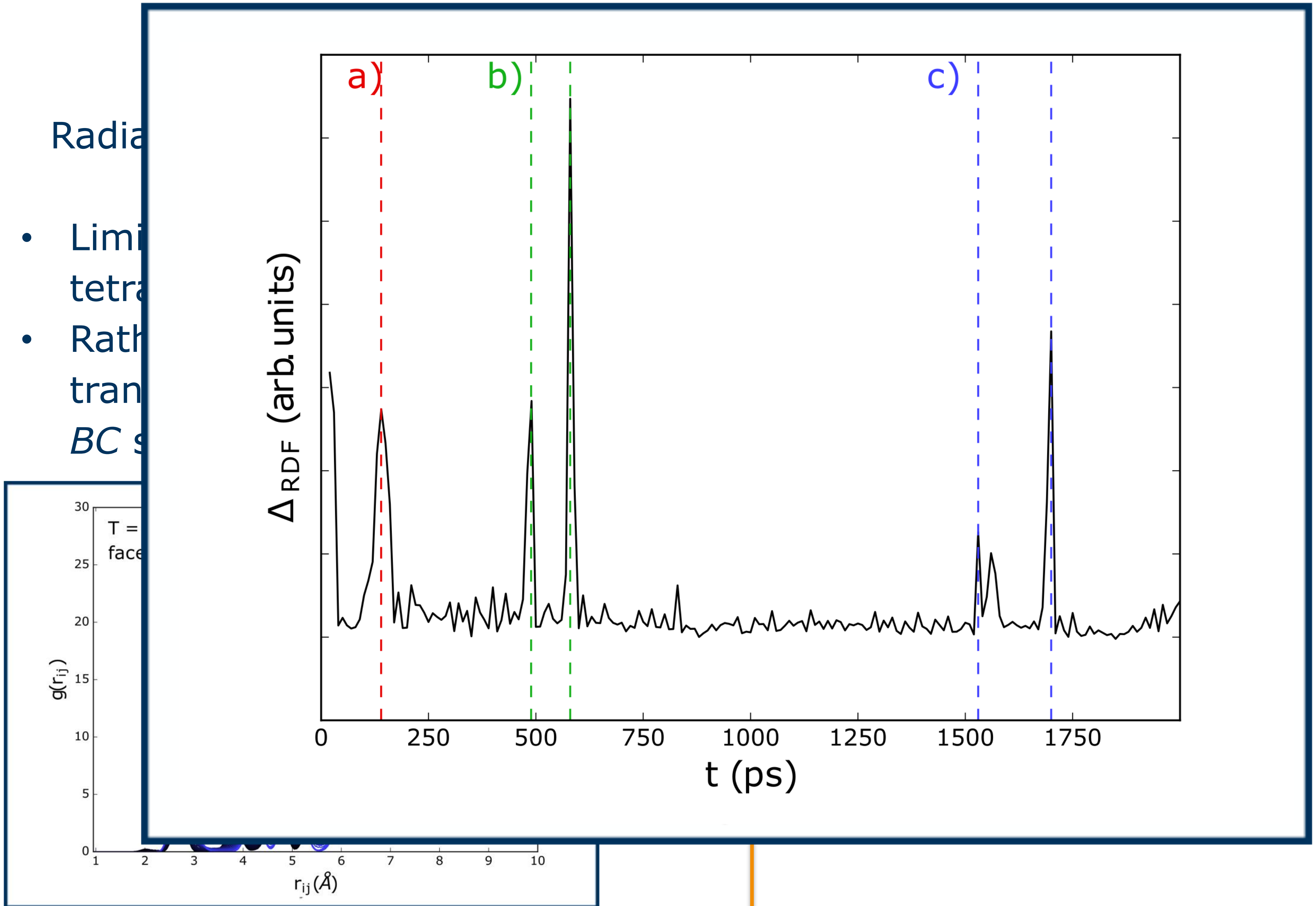

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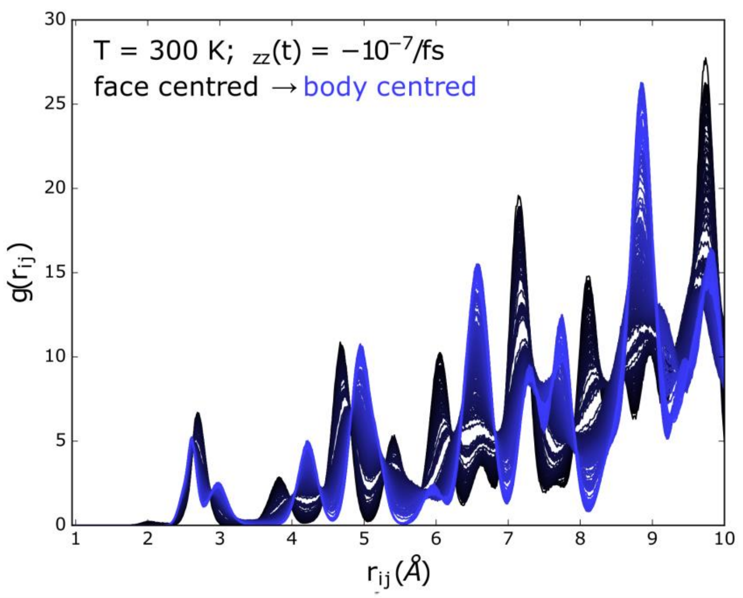
Structure Analysis

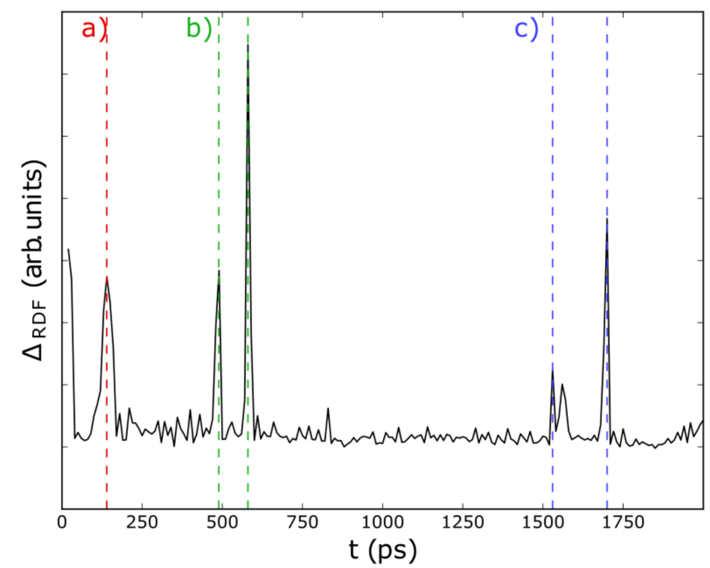
Radial Distribution Function

- Limited to resolve tetragonal phases
- Rather continuous transformation from *FC* zu *BC* structure



RDF Separation Function

- $\Delta_{RDF} = \int_{r_{ij}} |g(r_{ij})_{t0} - g(r_{ij})_{t0\_}| dr_{ij}$
- Indication of "avalanche" events



Common Neighbour Analysis

- Evaluation of lattice enviornment of atomic positions
- Output of the associated lattice type per atom

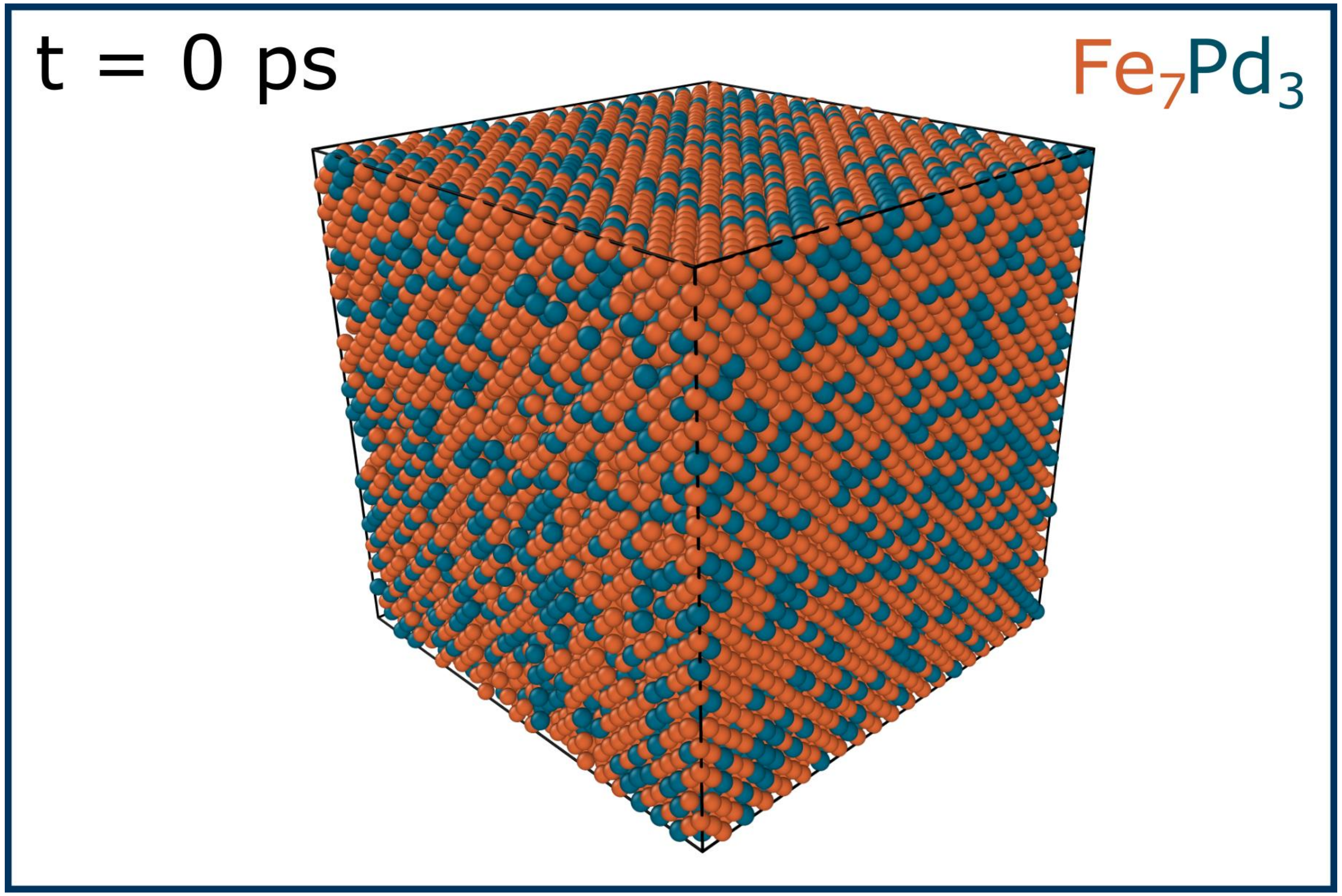
[Honeycutt and Andersen, J. Phys. Chem. 91, 4950]

Dislocation Analysis

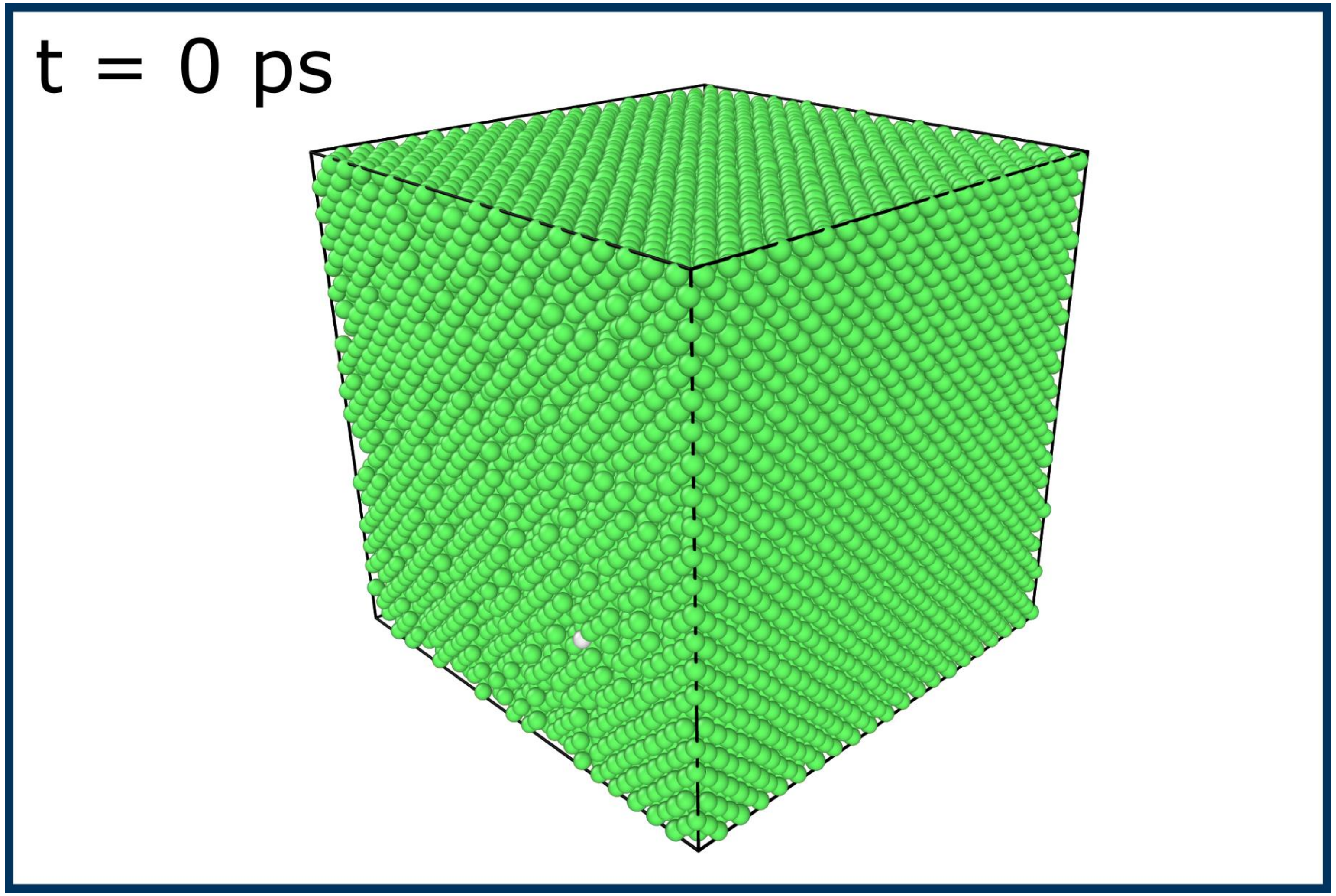
- Identyfication of all defects in a crystal of **given** lattice structure
- Output of defect mesh: triangulated surface deviding the "good" and the "bad" crystal region

[A. Stukowski, V.V. Bulatov and A. Arsenlis. Modelling Simul. Mater. Sci. Eng. 2 0, 085007 (2012)]

Strain Induced Phase Transition



Strain Induced Phase Transition



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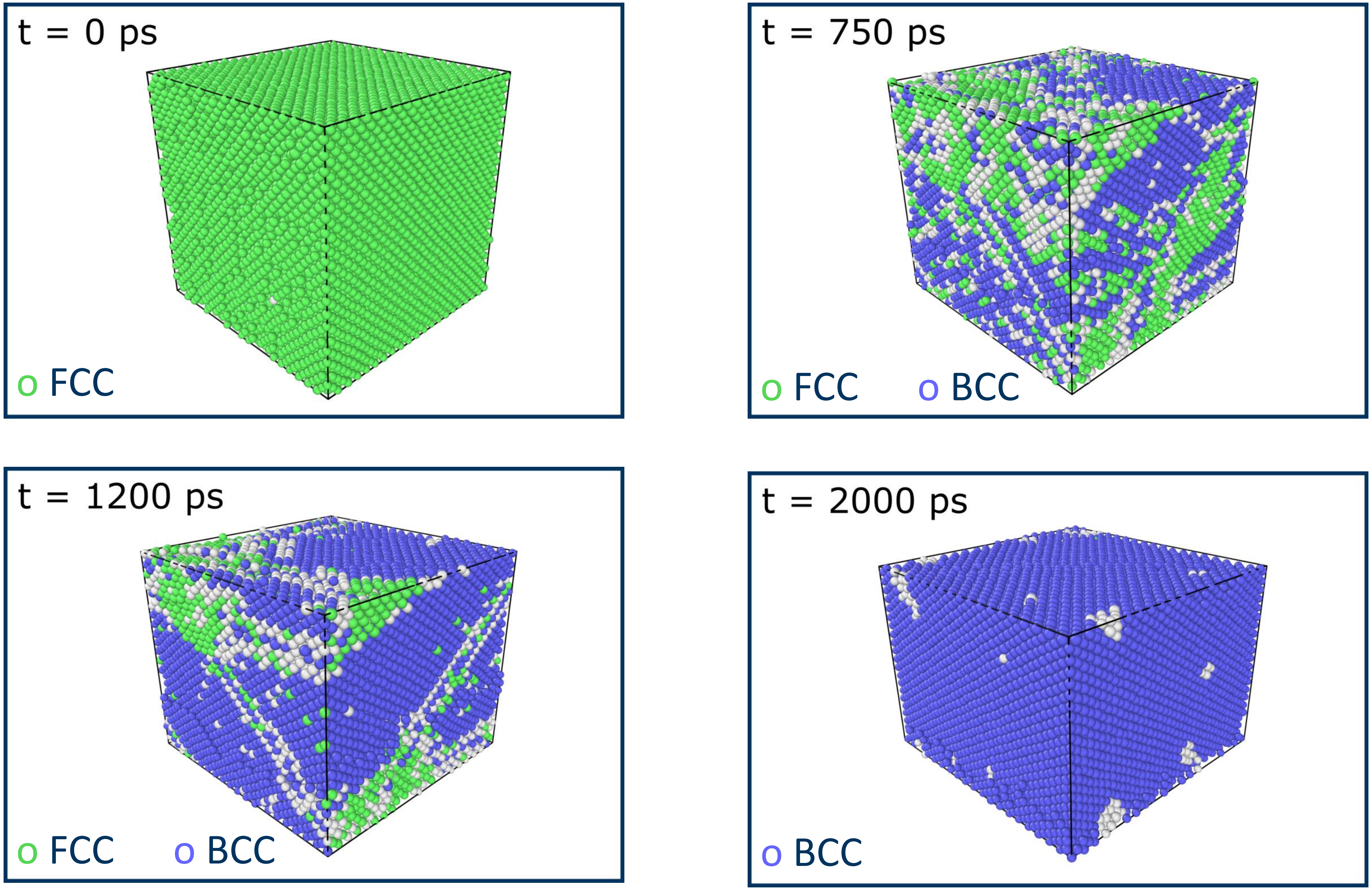

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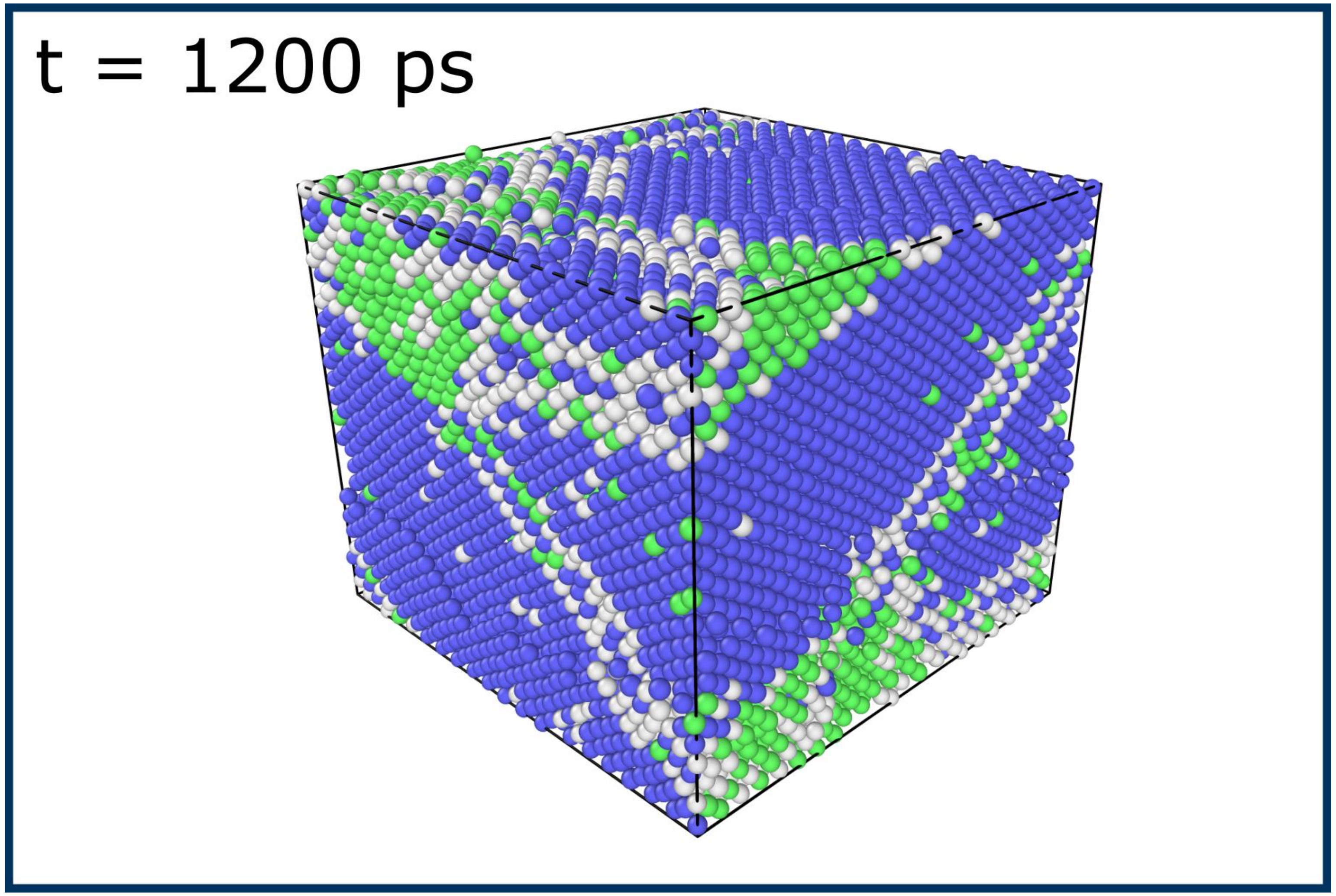

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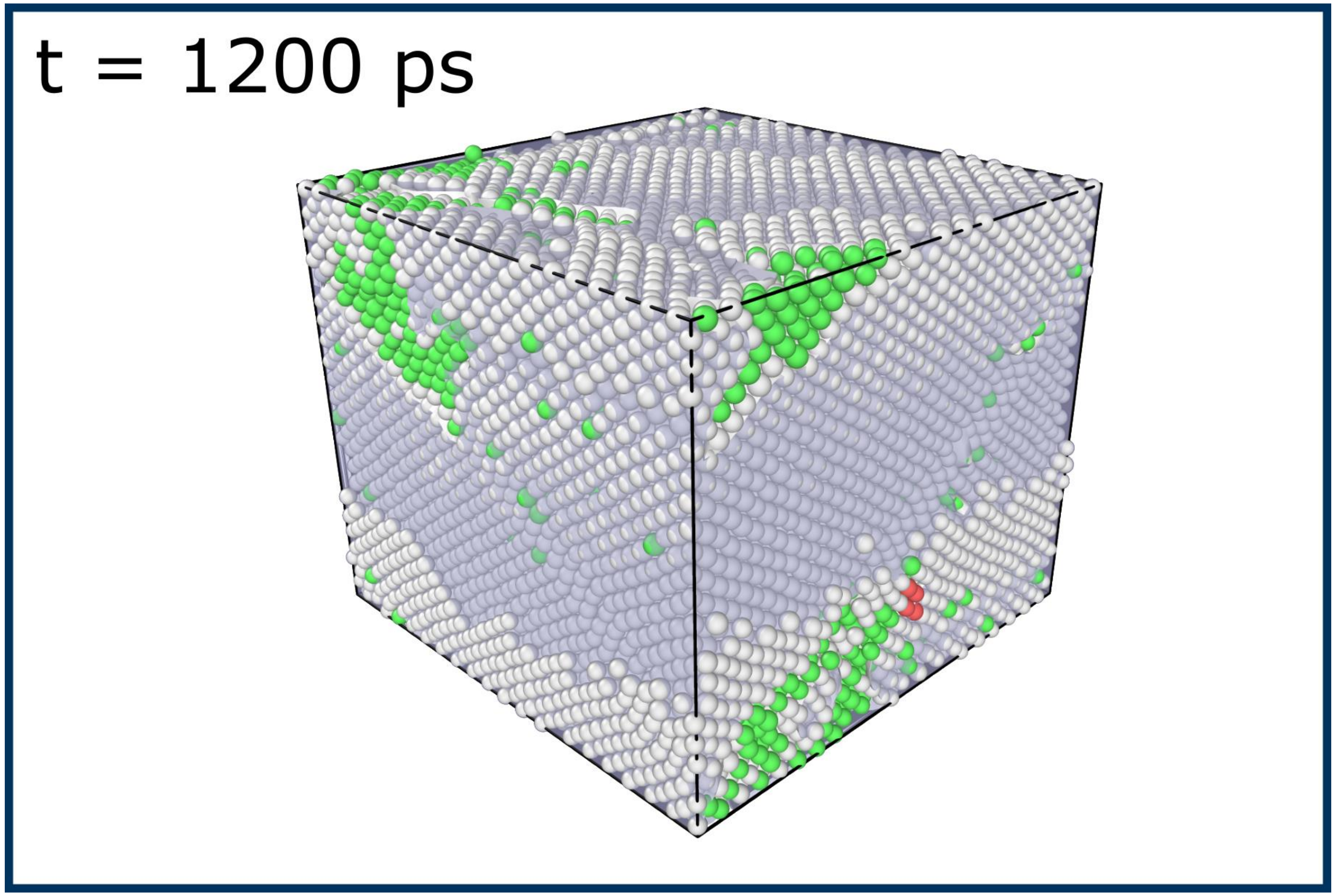

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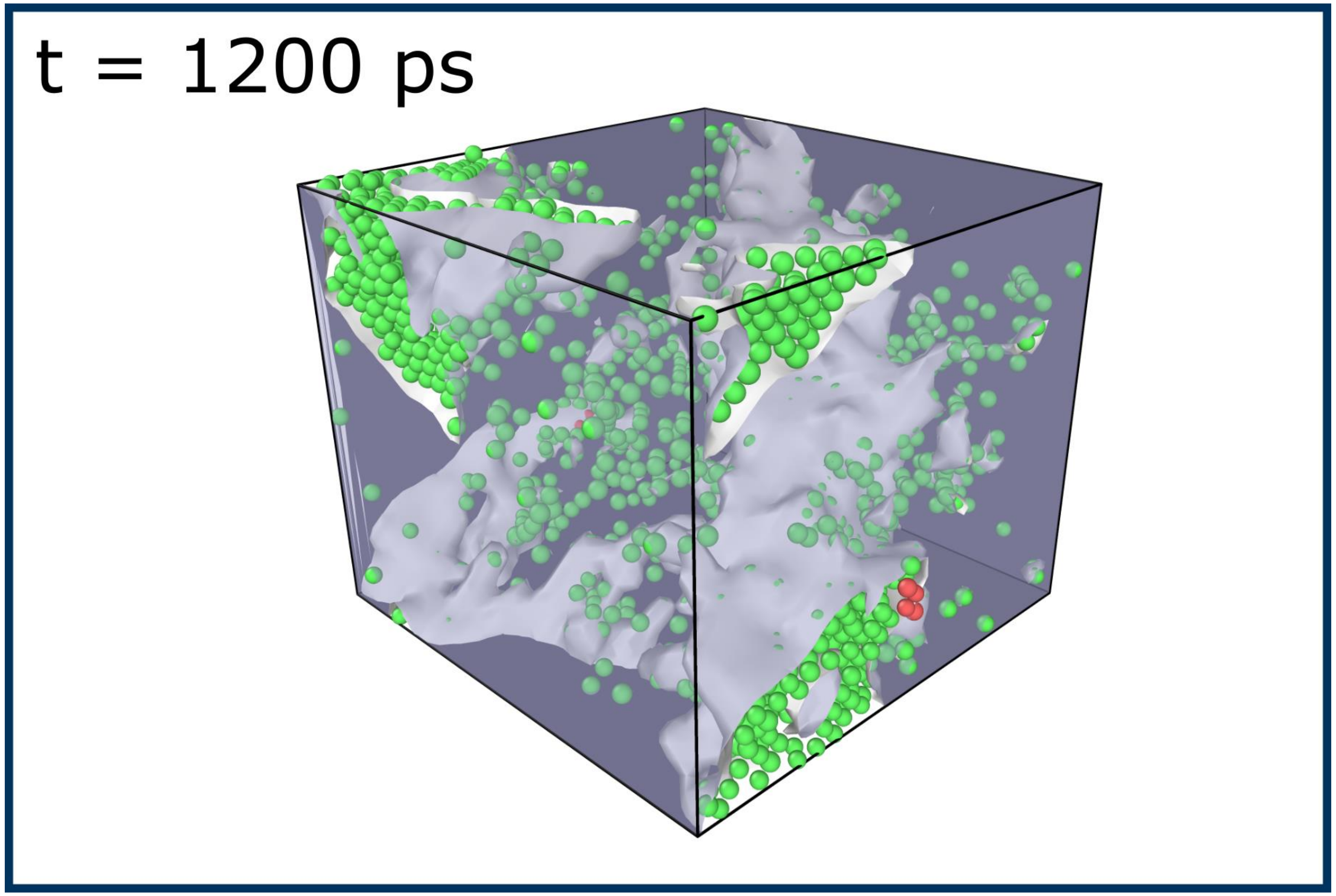

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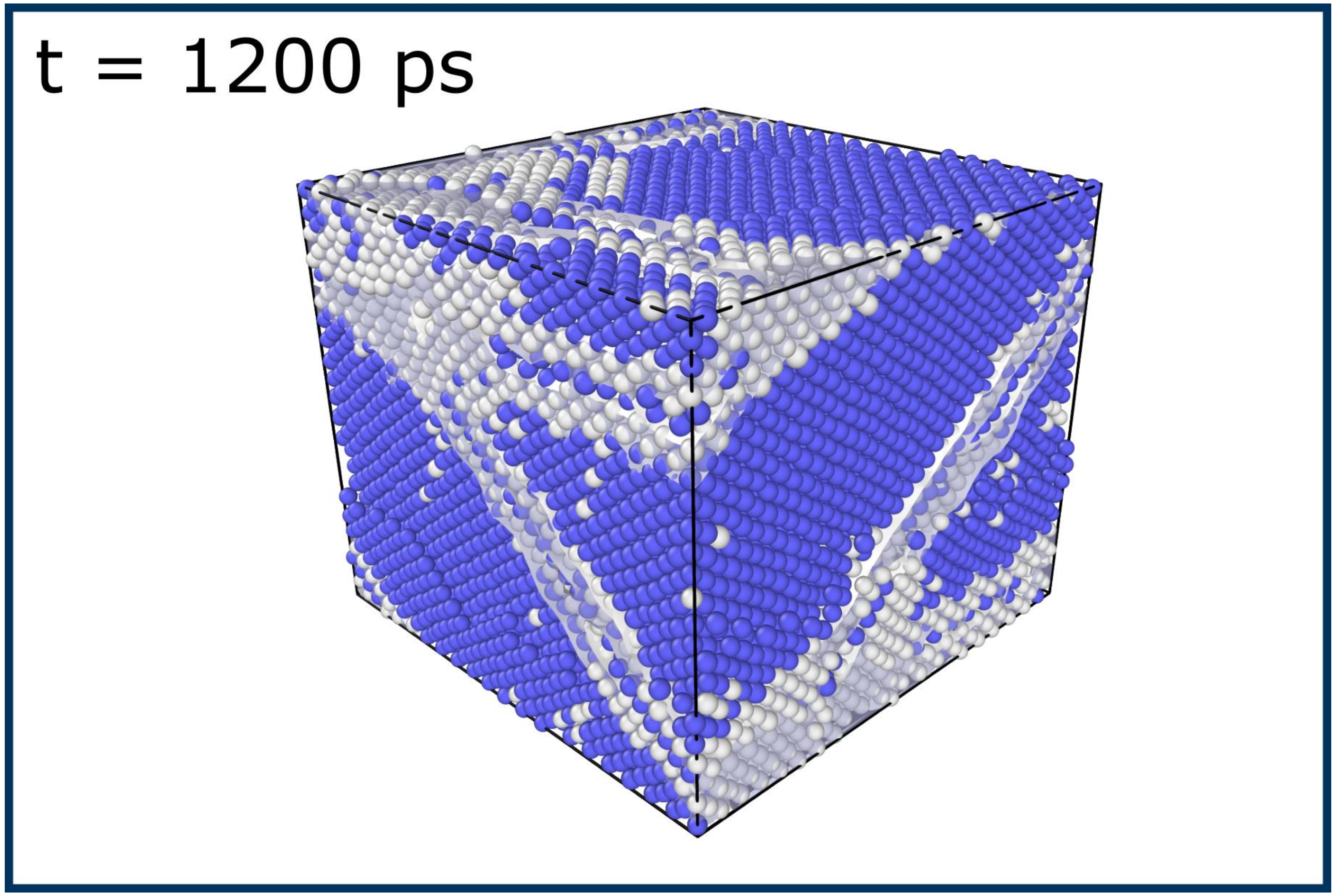

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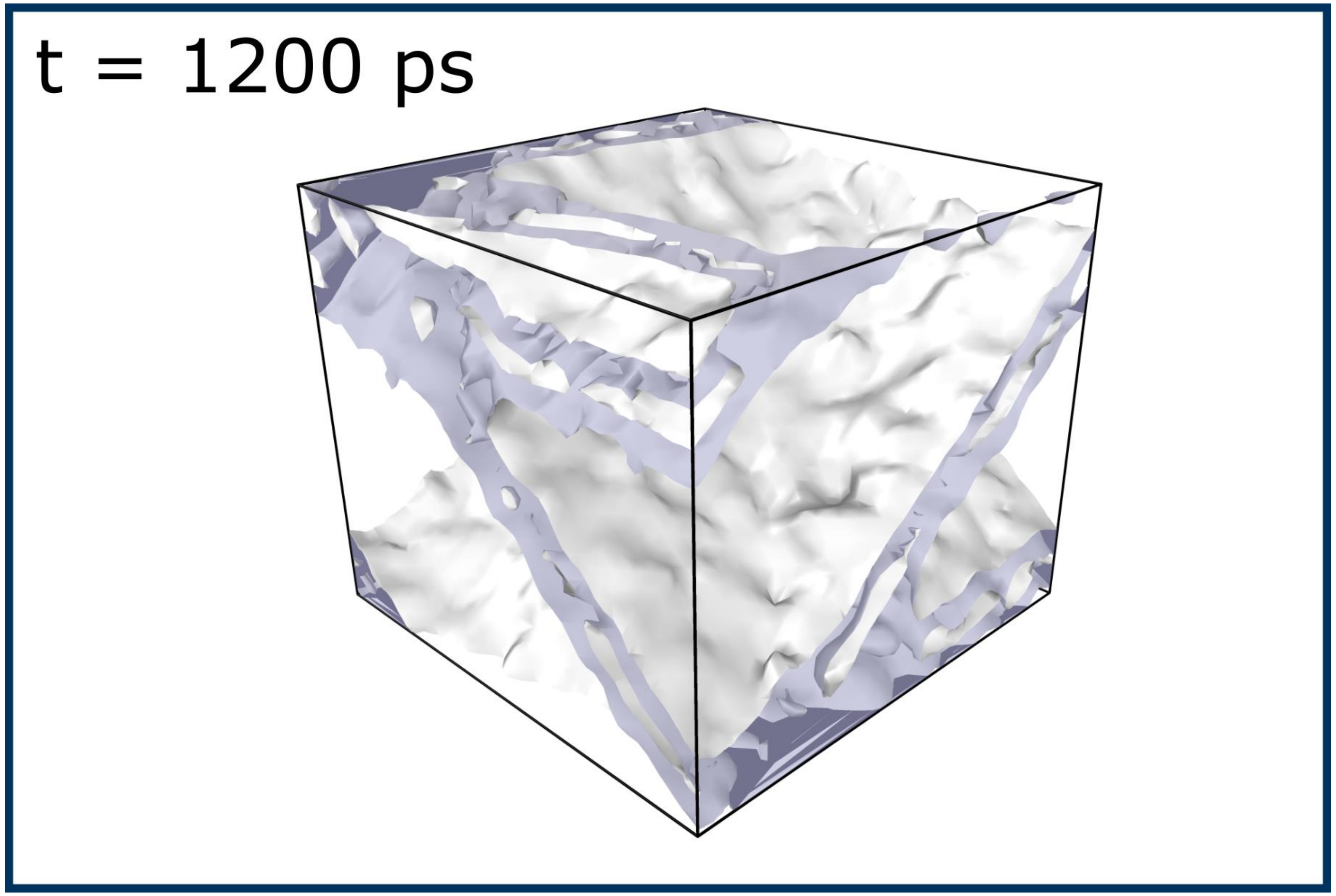

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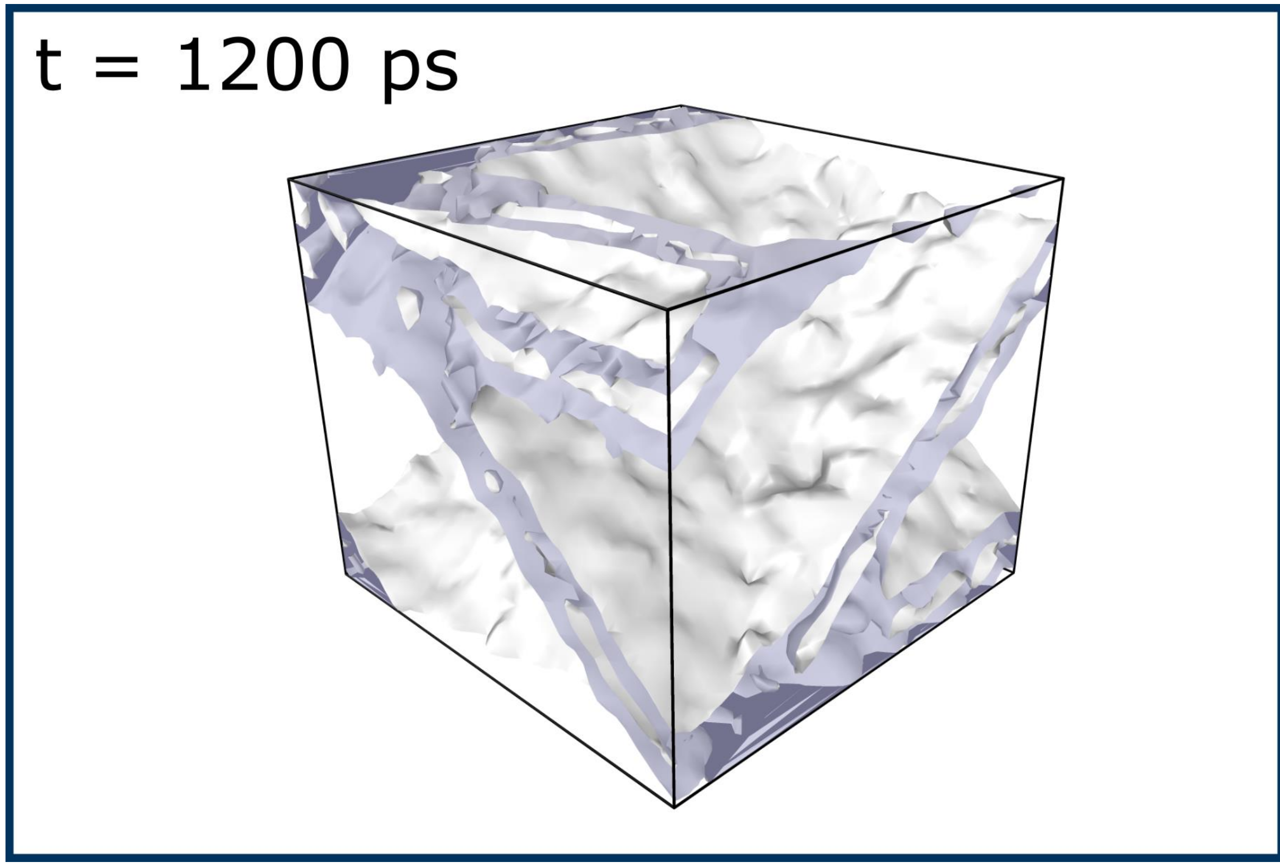
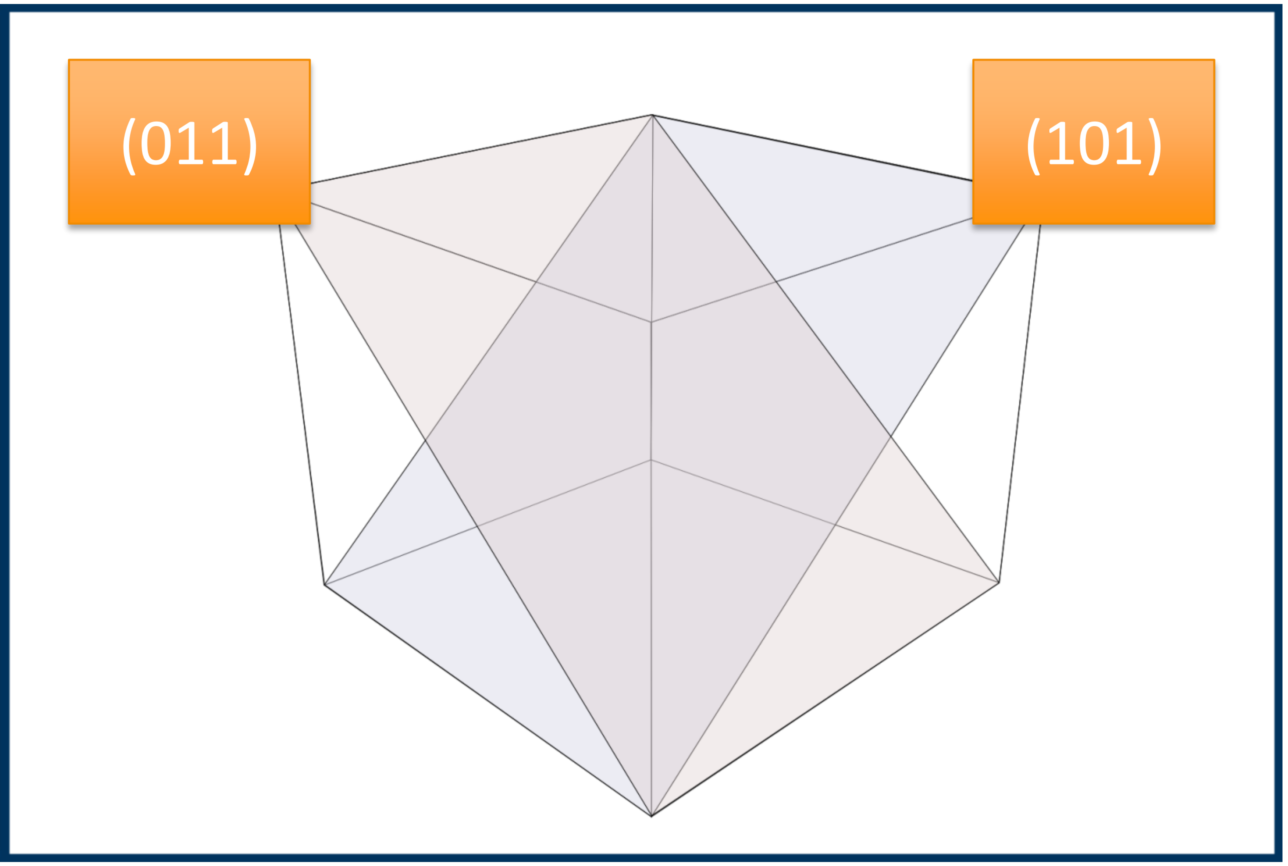
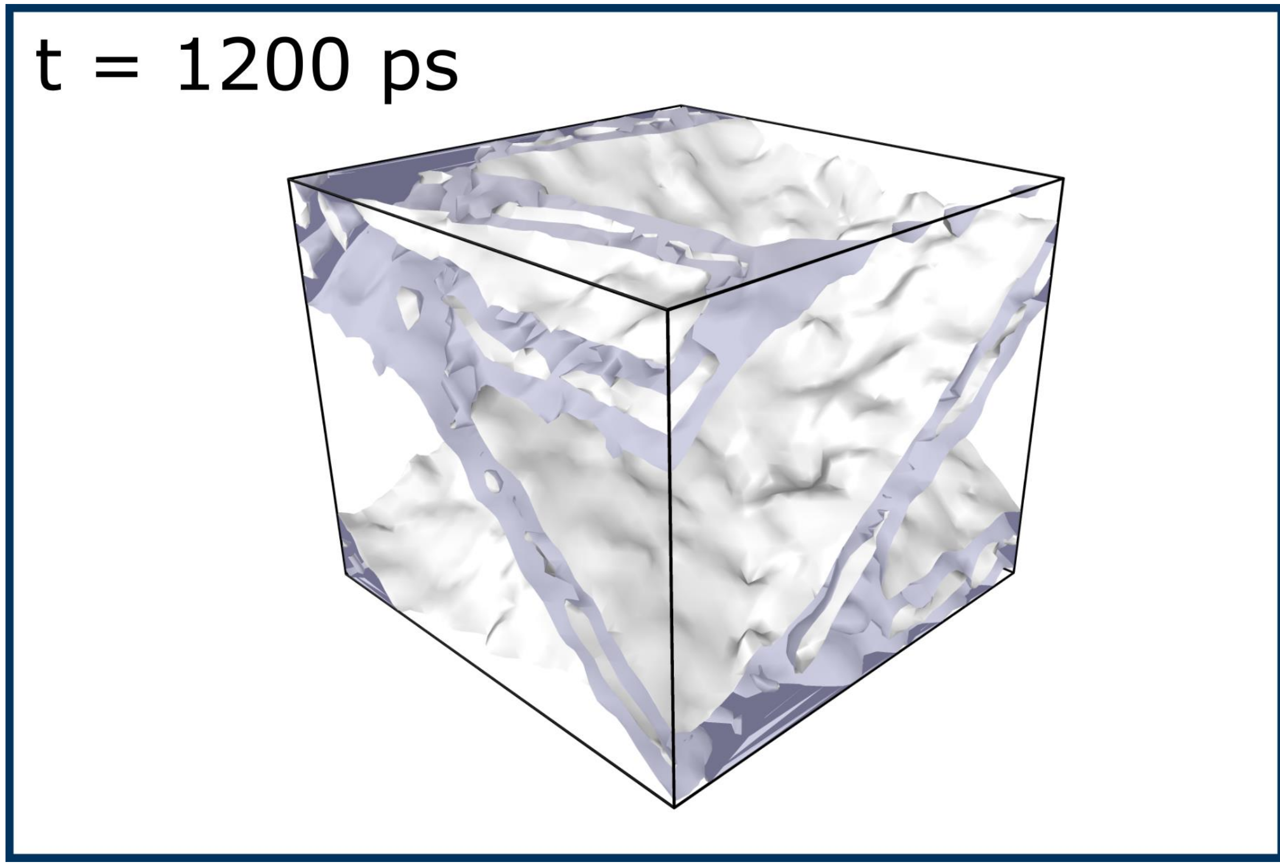
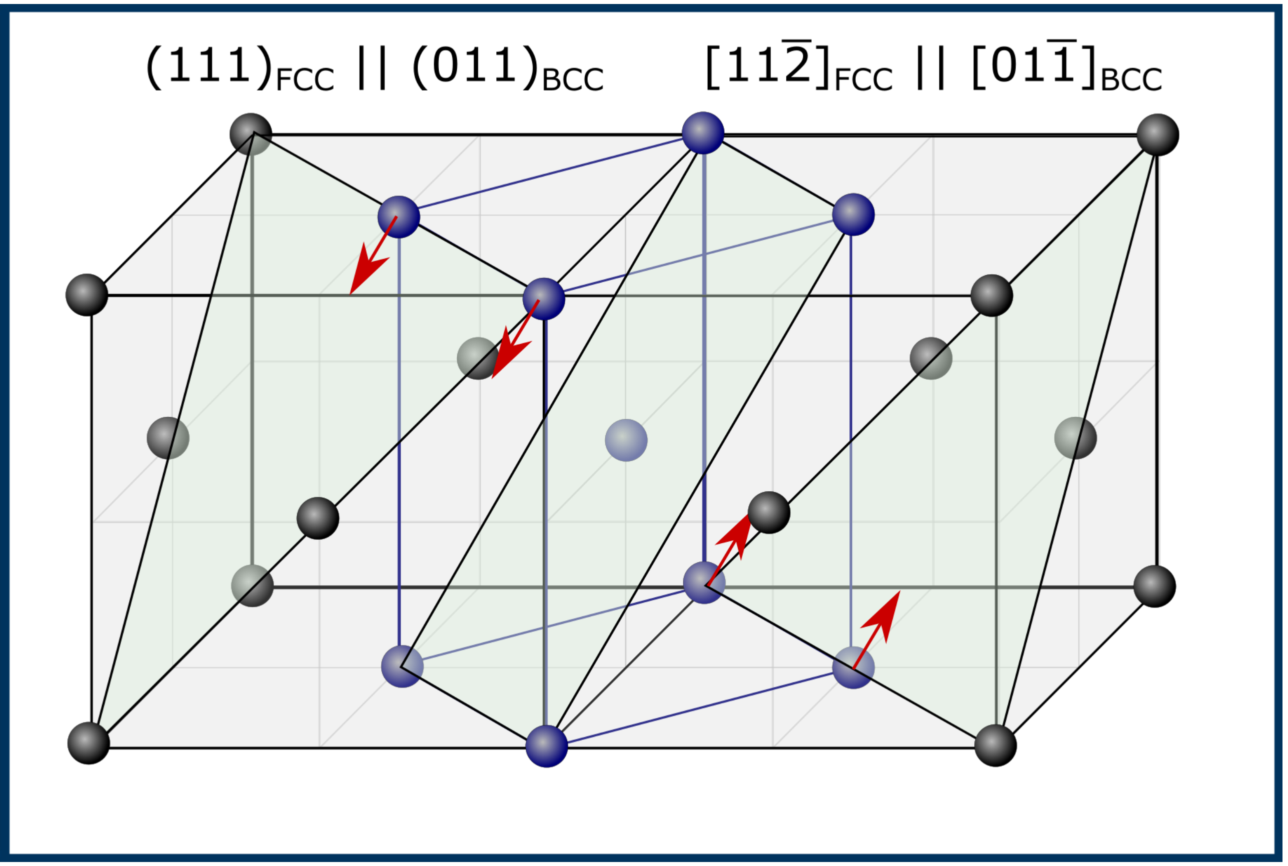


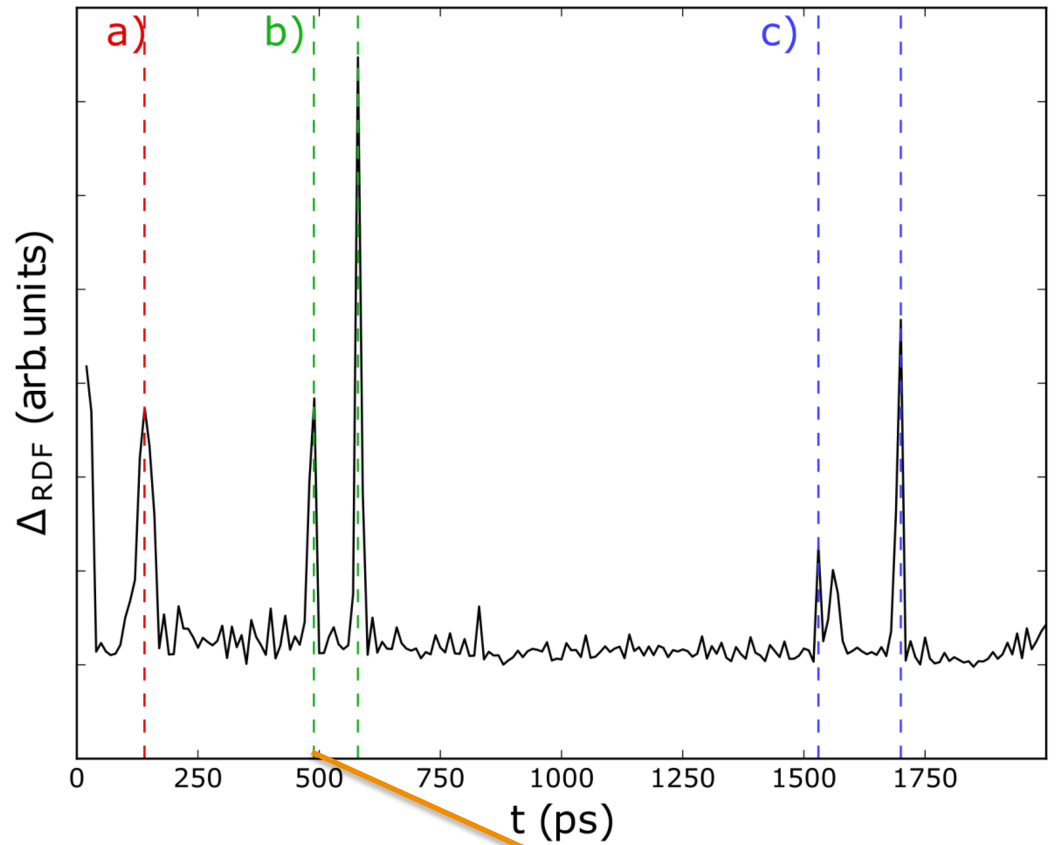


Nishiyama - Wassermann

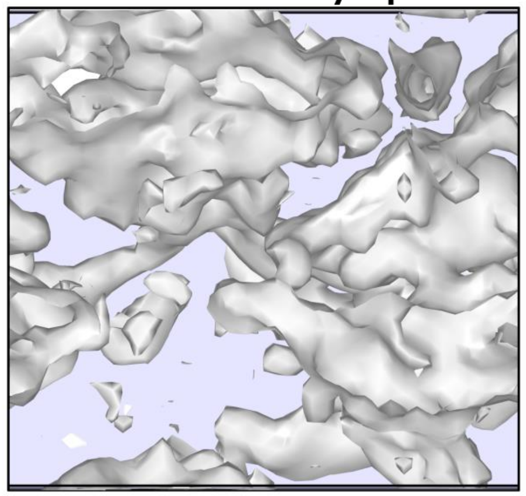




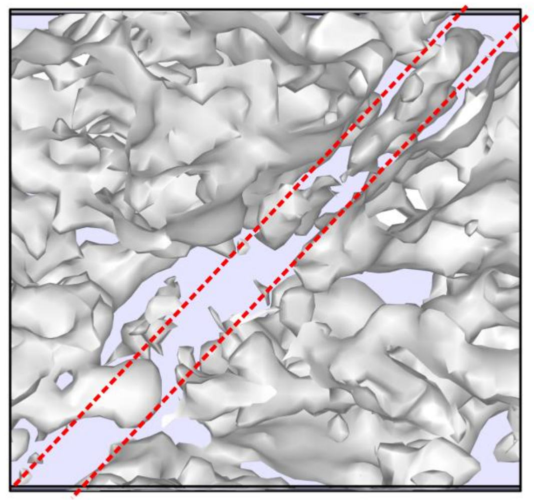
Analysing the Peaks



t = 470 ps View on y-plane



t = 480 ps



Formation of (101) habit planes

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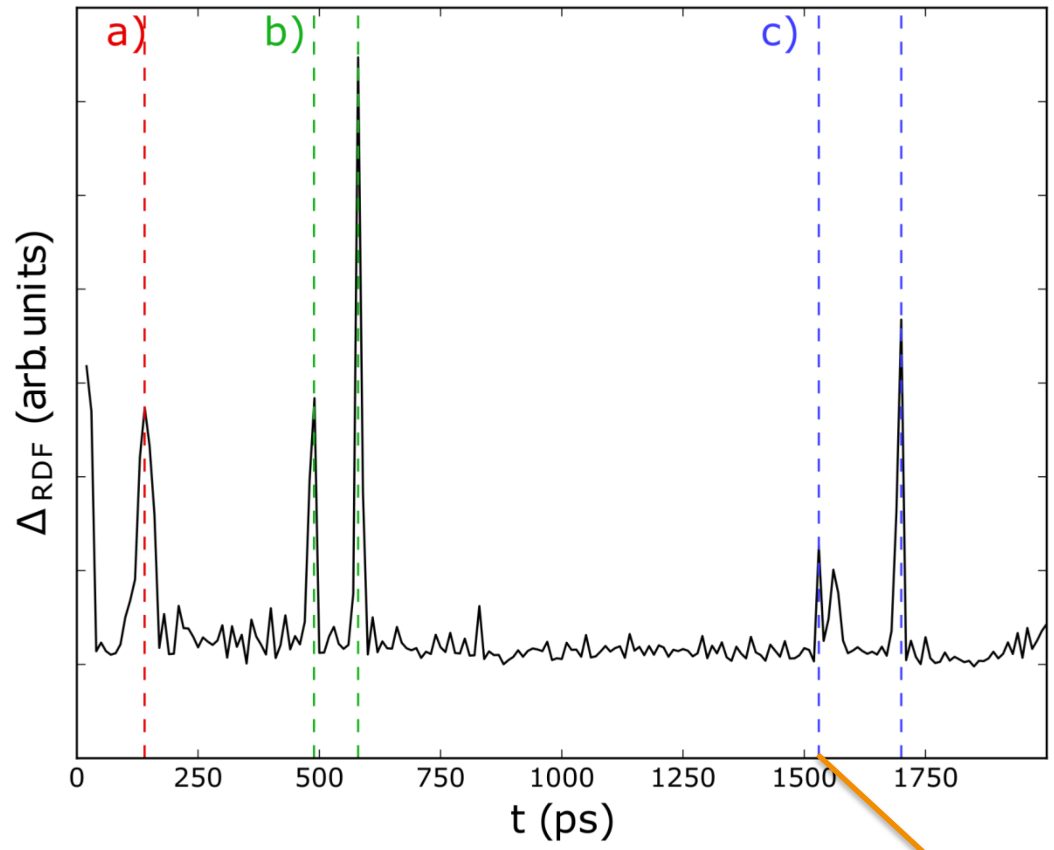
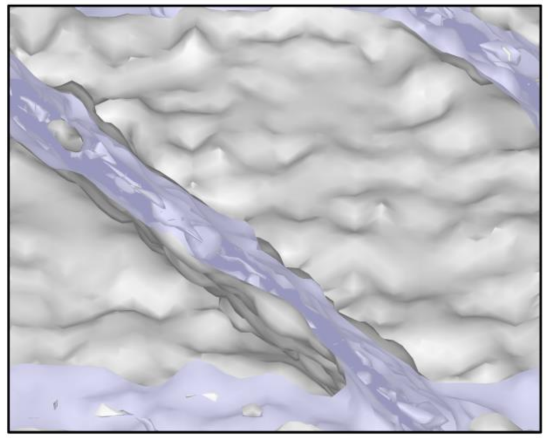
Analysing the Peaks

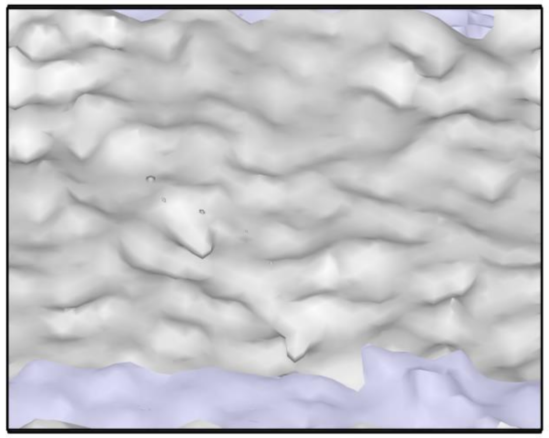


Vanishing of (011) habit planes

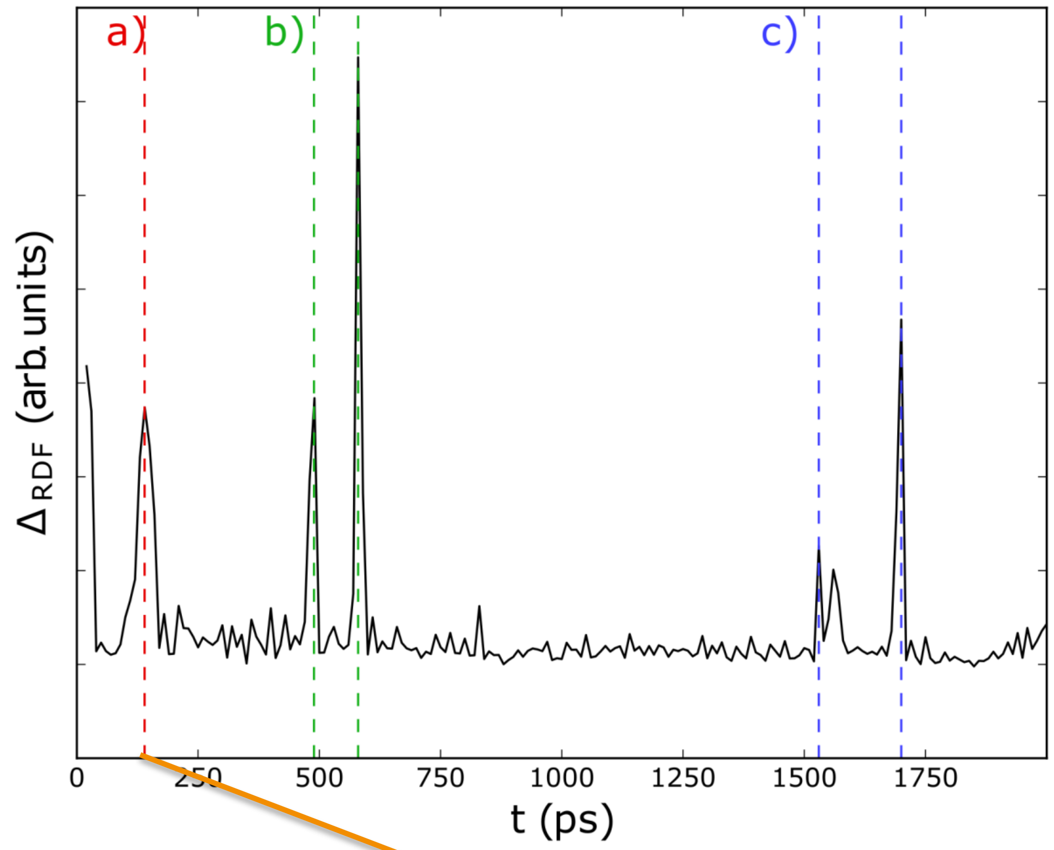
t = 1520 ps View on x-plane



t = 1540 ps



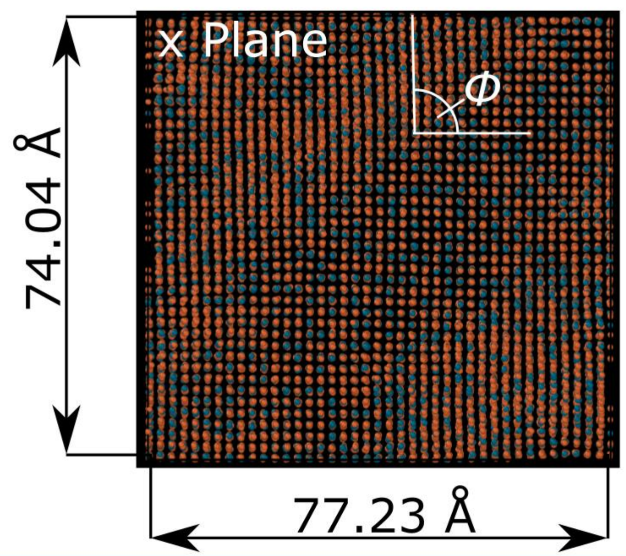
Analysing the Peaks



Angle of Tilt Dislocations

- $\varphi = 2\left(\arctan\left(\frac{c_t}{a_t}\right) - \frac{\pi}{4}\right)$ [1]

[1] A. Khachaturyan, S. Shapiro, and S. Semenovskaya, Physical Review B 43, 10832 (1991).



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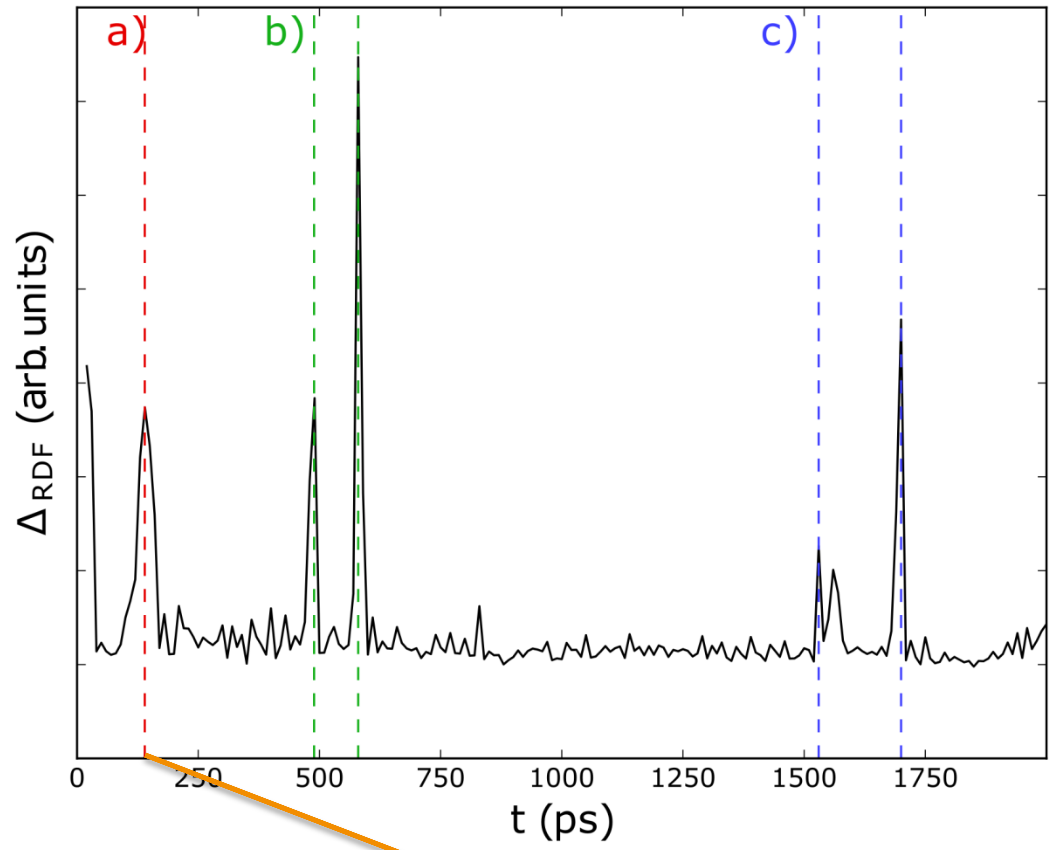
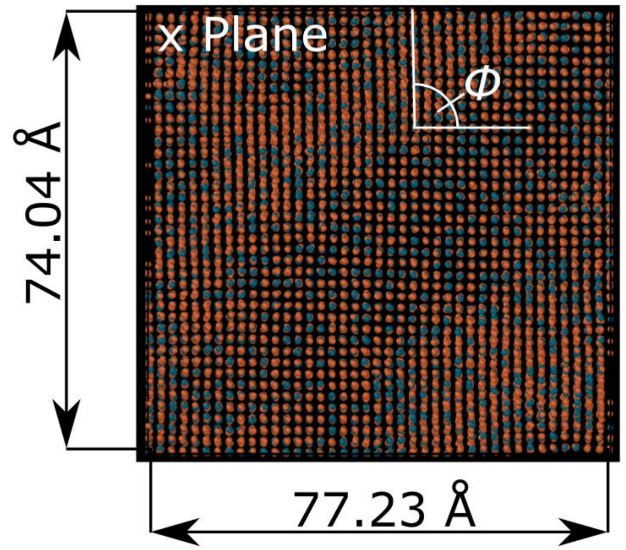
Analysing the Peaks



Angle of Tilt Dislocations

- $\varphi = 2\left(\arctan\left(\frac{c_t}{a_t}\right) - \frac{\pi}{4}\right)$
- Indication of a temporary *FCT* phase



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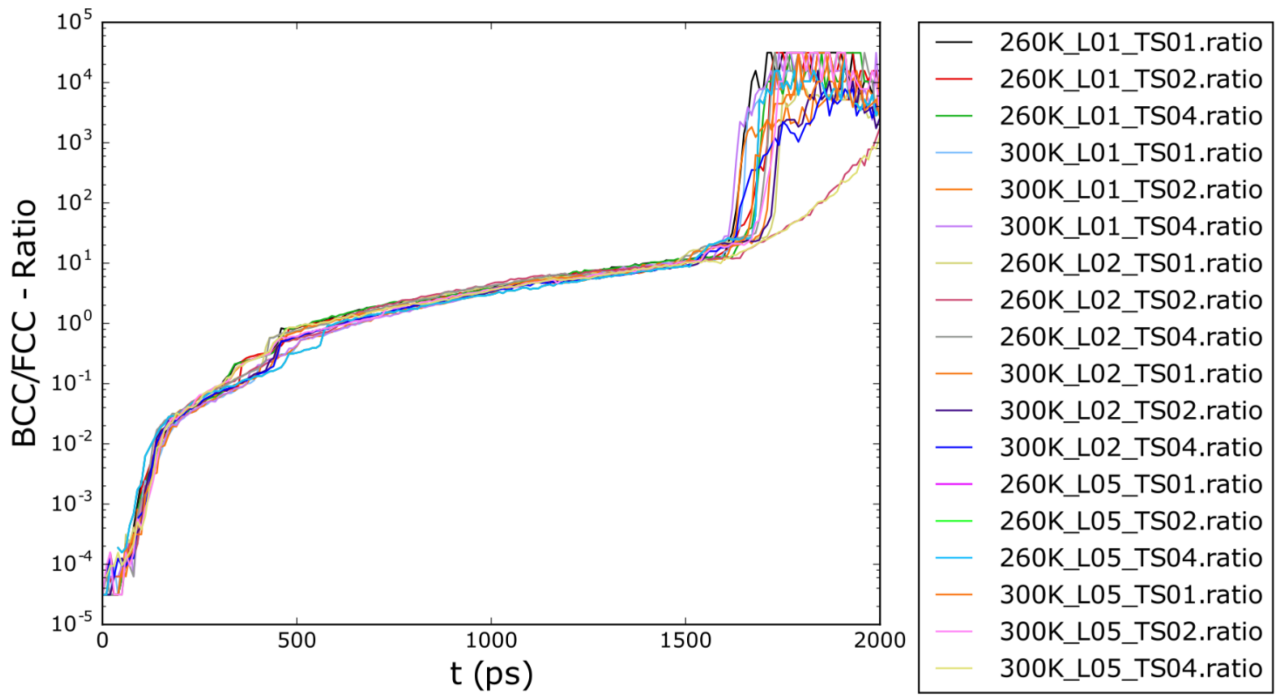

Check Bain Path for Different Temperatures, Temperature Sets and Atomic Orders

- Every simulation exhibits the same pattern of *(101)* and *(011)* habit planes
- *BCC/FCC* ratio graphs: all simulated transitions follow the same pattern (except for minor fluctuations)

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Conclusion

- Successfully determined a phase transition temperature
- Nishiyama – Wassermann Transformation vs. Bain Path
- Avalanche effects:
    - Habit plane formation due to shear deformation
- RDF-Separation-Function complementary method to investigate structural changes

Acknowledgements

- Prof. Stefan G. Mayr
- “AG Mayr” work group
- Open Visualization Tool – “Ovito”
  [www.ovito.org – Alexander Stukowski]
- Prof. Wolfhard Janke
- You!

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Strain Induced Phase Transition