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Simulation of X-ray diffraction peaks of single crystal superalloys

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Nickel based superalloy (2 phases)

- Precipitates Ni₃Al γ' : structure L1₂
- Matrix Ni γ (structure FCC)

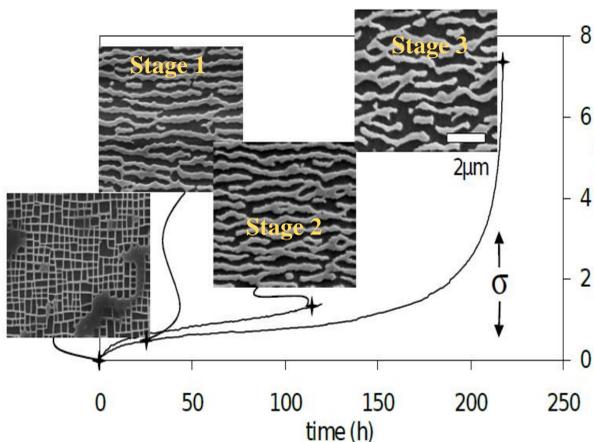


Figure 1a : Microstructure evolution during creep

Lattice misfit calculation during creep

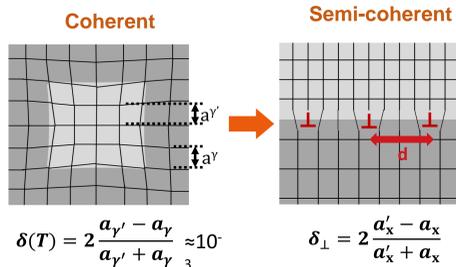


Figure 1b : Lattice misfit calculation during creep

Diffraction peaks acquisition during creep experiment

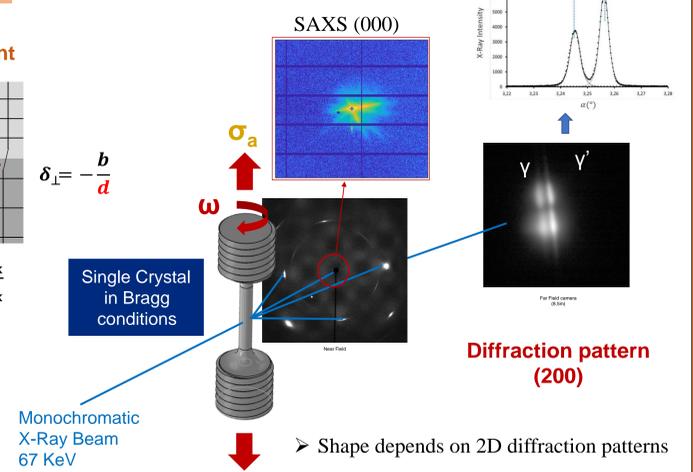


Figure 2 : Experimental setup for diffraction acquisition

Objectives :

- Simulation of Small Angle X-ray Scattering of Nickel based superalloy to get insight on the shape / distribution effects of precipitates on (000) diffraction profiles
- Automatic detection of microstructures by training neural networks based on diffraction pattern database

Microstructure Generation

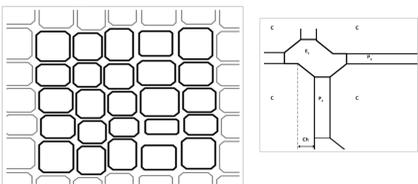
In house Code (Jacques, 2016)

Length RVE : 2 μ m, periodic

Volume fraction of precipitates γ' : 0,65

Composition

- 125 precipitates γ' in the form of cuboids
- 3 x 125 platelets (Px, Py, Pz) between cube faces
- 3 x 125 prisms along edges (Ex, Ey, Ez)
- 125 prisms at the corners of cuboids



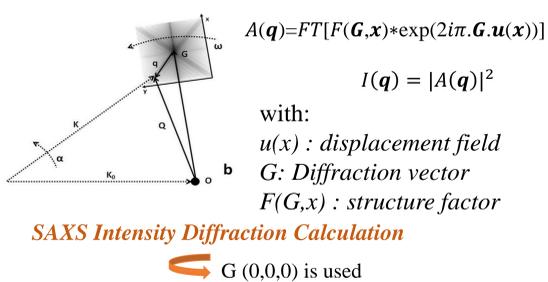
Phase field Code : In progress (coll. Sandia National Labs, USA)

- To simulate more realistic microstructure (Zhou et al. 2010, Stewart and Dingreville, 2020)

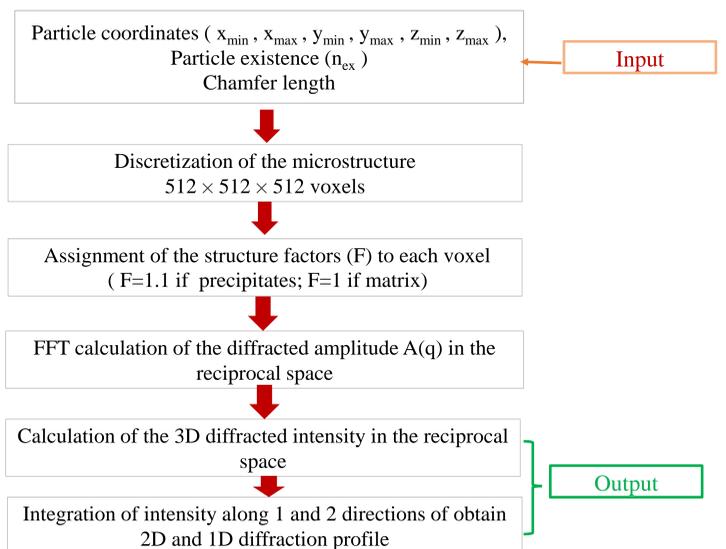
Geometrical Parameters of microstructure

- Chamfer length for precipitates: X_{ch}
- Surface fraction of precipitates f_{xy}
- Spatial function amplitude **Ampli** (periodic: **cos. function**)
- Fraction of Random distribution of precipitates in the matrix: F_{rad}

Diffraction Intensity Calculation

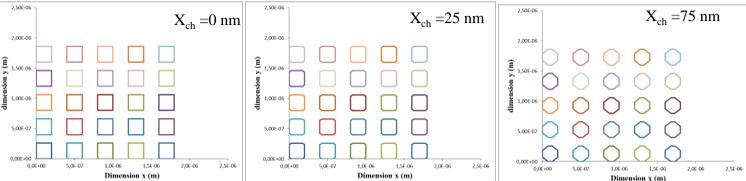


Diffraction peaks calculation

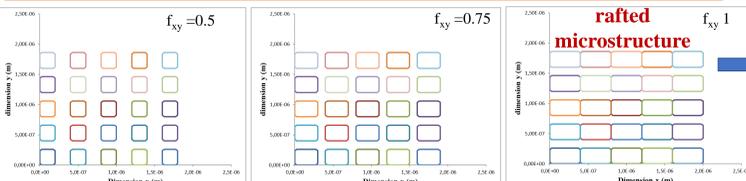


Examples of microstructures

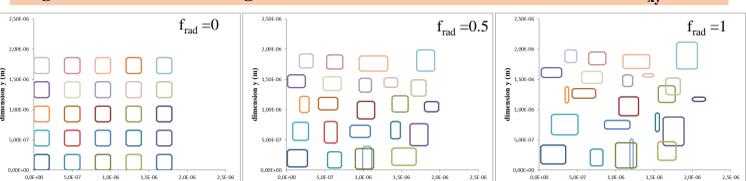
Cuboidal microstructure



Regular microstructures generated with different chamfer lengths X_{ch}

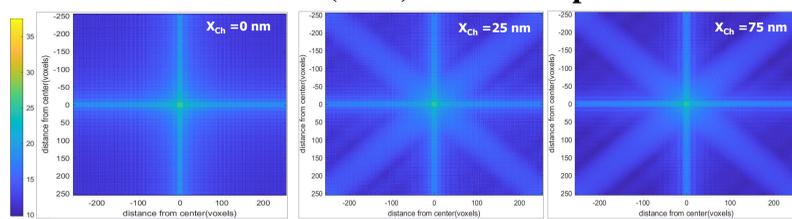


Regular microstructures generated with different surface fraction f_{xy}

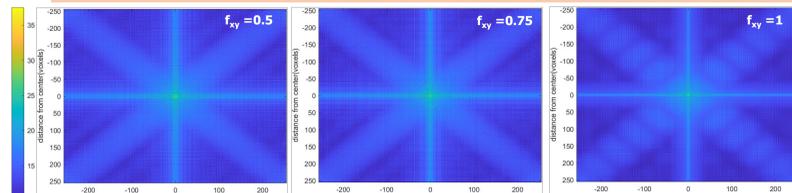


Microstructures generated with different random fraction f_{rad}

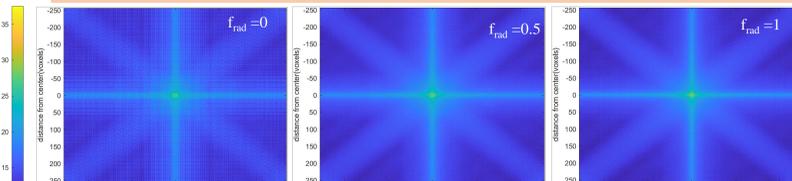
Numerical results: 2D(0 0 0) diffraction patterns



2D diffraction patterns of a microstructure with different chamfer lengths

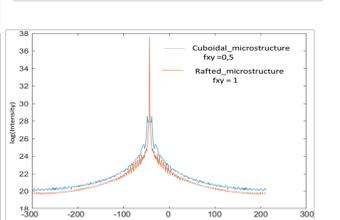
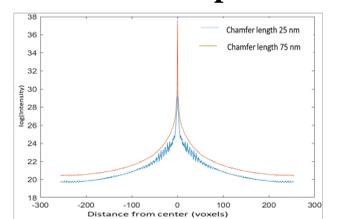


2D diffraction patterns of a microstructure during rafting



2D diffraction patterns of a microstructure with different random fraction f_{rad}

1D diffraction profiles



Automatic detection of diffraction peaks (pattern recognition) using neural networks

Perspectives: Database of 2D, 1D diffraction peak profiles for many microstructures generated by phase field model, training using a neural network (CNNs, ...)

References

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- Zhou, N., Shen, C., Mills, M., & Wang, Y. (2010). Large-scale three-dimensional phase field simulation of γ' -rafting and creep deformation. *Philosophical Magazine*, 90(1-4), 405-436
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- Ratel-Ramond, N. (2007). Investigation of the strain induced rafting of the gamma prime precipitates in single crystal nickel based superalloys. Université Joseph-Fourier-Grenoble I.