



HAL
open science

Simulation in situ of X-ray diffraction peaks of single crystal superalloys

Ablam Massa, Thomas Schenk, Stephane Berbenni

► **To cite this version:**

Ablam Massa, Thomas Schenk, Stephane Berbenni. Simulation in situ of X-ray diffraction peaks of single crystal superalloys. International Conference on Strength of Materials, Jun 2022, Metz, France. 2023. hal-04574544

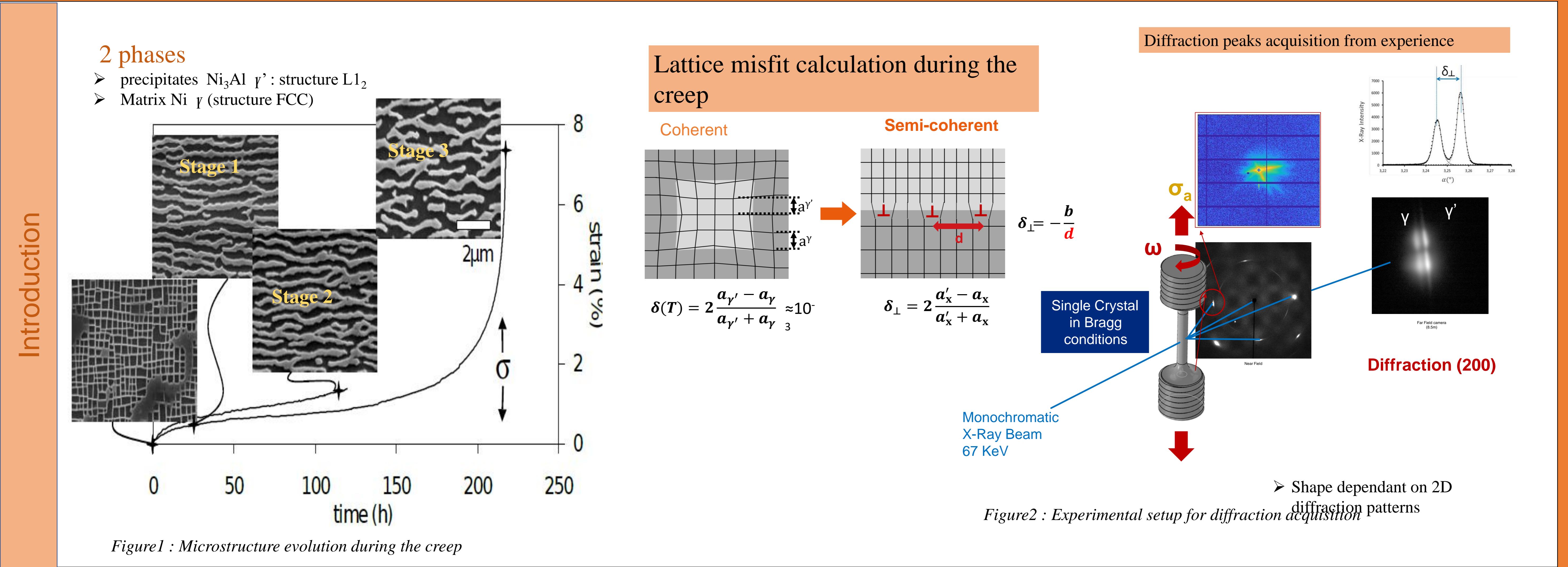
HAL Id: hal-04574544

<https://hal.science/hal-04574544>

Submitted on 14 May 2024

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Objectives : 1) Simulation of diffraction patterns of Nickel based superalloy in Small Angle X-ray Scattering Mode in a way to understand the shape effect of precipitates;
2) Automatic detection of microstructure from training with diffraction pattern

Methodology

Microstructure Generation

In house Code

Length RVE : 2µm, periodic

Volume fraction of precipitates γ' : 0,65

Composition

- 125 Précipités γ' sous forme de cuboïdes
- 3*125 platelets (Px, Py, Pz) between cube faces
- 3*125 prisms along edges (Ex, Ey, Ez)
- 125 prisms at the corners of cuboids

Geometrical Parameters of microstructure

- Chamfered value of precipitates : X_{ch}
- Surface fraction of précipitates f_{xy}
- Spatial cos function amplitude Ampli
- Fraction of Random distribution of precipitates in the matrix : F_{rad}

Figure 3 : Experimental setup for diffraction acquisition

Phase field Code : In progress

- To simulate more realistic microstructure

Diffraction peaks calculation

particules cordantes (x_{min}, x_{max}, y_{min}, y_{max}, z_{min}, z_{max}), Particles existence (n_{ex}) Chamfered value

Input

Voxelization of the microstructure Into 512*512*512 voxels

assignment of the structure factors to each voxels (f=1,1 if precipitates; f=1 if matrix)

FFT calculation of the diffracted amplitude A(q) in reciprocal space

Calculation of the 3D diffracted intensity in the reciprocal space,

Intragation of intensity along 1 and 2 directions of obtain 2D and 1D diffraction profil

Output

Diffraction Intensity Calculation

$$A(q) = FT[F(G,x) * \exp(i \cdot 2\pi \cdot G \cdot u(x))]$$

$$I(q) = |A(q)|^2$$

U(x) : displacement field ; G : Diffraction vector
F(G,x) : structure factor

SAXS Intensity Diffraction Calculation

G (0,0,0) used

$$A(q) = FT[F(G,x)] ; I(q) = |A(q)|^2$$

