# Simulation of in situ X-Ray Diffraction peaks of single crystal Superalloys

Alain Jacques[a,c†], Komlavi Eloh[a,b,c], Stéphane Berbenni[b,c], Ablam Massa[a,b,c], Thomas Schenk[a,b,c]

[a] *Institut Jean Lamour, 2 rue André Guinier, 54011 Nancy Cedex, France*

[b] *Université de Lorraine, CNRS, Arts et Métiers ParisTech, LEM3, F-57000 Metz, France*

[c] *Laboratory of Excellence on Design of Alloy Metals for low-mAss Structures (LabEx DAMAS), University of Lorraine, Metz, France*

*thomas.schenk@univ-lorraine.fr*

Single crystal superalloys are two phased alloys, where hard cuboidal γ' precipitates ($L1_2$ structure) are embedded within a softer *fcc* γ matrix. During high temperature creep, the precipitates evolve into platelets (rafts). Both phases bear a complex stress state, resulting from the temperature dependent lattice mismatch $\delta(T) = 2\left(a_{\gamma'} - a_{\gamma}\right)/\left(a_{\gamma'} + a_{\gamma}\right)$, the distribution of alloy elements between dendritic and interdendritic zones, and the different plastic strain states of both phases. Using the symmetry around the [001] tensile axis and following the evolution of the (200) diffraction peaks during creep by *in situ* far field diffractometry [1] (ESRF, DESY) it is possible to compute the stress and plastic strain state of each phase. However, the (200) diffraction peak also contains information: the actual shape of cuboids and mobile dislocations densities, which can be retrieved only by modelling the microstructure, and compare the experimental diffraction peak to a simulated one [2]. A major hurdle is to build an efficient method to compute the mechanical fields (stress, strain, and displacement) within a $(2\mu m)^3$ 3D representative element of the microstructure containing dislocations divided in $512^3$ voxels. We use a method based on the Fast Fourier Transform (FFT) well adapted to materials with heterogeneous elastic constants [3]. The scattered amplitude in the vicinity of a reciprocal lattice vector $\boldsymbol{G}$ can then be computed as the FFT of $exp[2i\pi\boldsymbol{G}.\boldsymbol{u}(r)]$ with the displacement field $\boldsymbol{u}(r)$ at point $r$. Intensities generated at different points can be summed to get whole diffraction peaks. Further correction [3] is needed to remove oscillations of the displacement field in the vicinity of dislocation. The effect of various microstructural features is discussed and compared to experimental results.

*Keywords: SX superalloys; FFT method; load transfer; dislocations.*

**References:**

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