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

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

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

[b]*LEM3, 7 rue Félix Savart F-57070 Metz Technopôle, France*

[a]*ablam.massa@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.

Acknowledgment: LabeX Damas, Metz, France

References:

[1] R. Tréhorel *et al.* Real-time study of transients during high-temperature creep of an Ni-base superalloy by far-field high-energy synchrotron X-ray diffraction. Journal of Applied Crystallography, 51(5) 2018, 1274-1282.
[2] A. Jacques, From Modeling of Plasticity in Single-Crystal Superalloys to High Resolution X-rays Three-Crystal Diffractometer Peaks Simulation. Metallurgical and Materials Transactions A, 47(12), 2016, 12, 5783-5797
[3] K. S. Eloh *et al.* The Effect of Crystal Defects on 3D High-Resolution Diffraction Peaks: A FFT-Based Method, Materials Vol. 11(9), 2018, 1669