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

Alain Jacques\textsuperscript{a,cf}, Komlavi Elo\textsuperscript{a,b,c}, Stéphane Berbenni\textsuperscript{b,c}, Ablam Massa\textsuperscript{a,b,c}, Thomas Schenk\textsuperscript{a,b,c}

\textsuperscript{a}Institut Jean Lamour, 2 rue André Guinier, 54011 Nancy Cedex, France
\textsuperscript{b}Université de Lorraine, CNRS, Arts et Métiers ParisTech, LEM3, F-57000 Metz, France
\textsuperscript{c}Laboratory of Excellence on Design of Alloy Metals for low-mAss Structures (LabEx DAMAS), University of Lorraine, Metz, France

Single crystal superalloys are two phased alloys, where hard cuboidal γ' precipitates (L\textsubscript{1\textsc{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 \(\delta(T) = 2(a_{\gamma'} - a_\gamma)/(a_{\gamma'} + a_\gamma)\), 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 \textit{in situ} far field diffractionometry [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 \((2\mu\text{m})^3\) 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 \(G\) can then be computed as the FFT of \(\exp[2i\pi G \cdot \mathbf{u}(r)]\) with the displacement field \(\mathbf{u}(r)\) 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: