



## Full length article

# Study of lattice strain evolution during biaxial deformation of stainless steel using a finite element and fast Fourier transform based multi-scale approach



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## ABSTRACT

A multi-scale elastic-plastic finite element and fast Fourier transform based approach is proposed to study lattice strain evolution during uniaxial and biaxial loading of stainless steel cruciform shaped samples. At the macroscale, finite element simulations capture the complex coupling between applied forces in the arms and gauge stresses induced by the cruciform geometry. The predicted gauge stresses are used as macroscopic boundary conditions to drive a mesoscale elasto-viscoplastic fast Fourier transform model, from which lattice strains are calculated for particular grain families. The calculated lattice strain evolution matches well with experimental values from in-situ neutron diffraction measurements and demonstrates that the spread in lattice strain evolution between different grain families decreases with increasing biaxial stress ratio. During equibiaxial loading, the model reveals that the lattice strain evolution in all grain families, and not just the 311 grain family, is representative of the polycrystalline response. A detailed quantitative analysis of the 200 and 220 grain family reveals that the contribution of elastic and plastic anisotropy to the lattice strain evolution significantly depends on the applied stress ratio.

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## 1. Introduction

Metals and alloys used for engineering applications often experience biaxial stress states during their fabrication or under service conditions. Their macroscopic yield and subsequent plastic behavior significantly depends on this applied biaxial stress state. However, most of our knowledge on material behavior is derived from uniaxial deformation tests. Relying solely on uniaxial tests may result in an erroneous description of biaxial mechanical behavior for these materials.

The past few decades have seen an increasing trend towards the development and use of biaxial mechanical testing techniques (see Ref. [1] and references within). Biaxial testing on cruciform shaped samples has proven to be particularly useful in characterizing the

macroscopic behavior of materials [2–7]. The cruciform shape has the advantage of applying any arbitrary stress ratio in both tension and compression. This allows access to a large portion of the 2-dimensional stress space without changing the experimental setup. However, Makinde and co-workers [8–10] noted that an analytical computation of the gauge stresses in a cruciform sample is not simply the force divided by area. Hoferlin et al. [11] used finite element (FE) simulations to show that the cruciform geometry results in a coupling between the forces in the arms and the gauge stresses. For instance, FE simulations of Bonnard et al. [12] and Claudio et al. [13] showed that for a cruciform geometry similar to the one used in this study a uniaxial load in the arm results in biaxial gauge stresses with a compressive component normal to the loading direction. Based on this, FE modeling has been used to study the evolution of gauge stresses in different cruciform geometries [14,15] and optimize the cruciform geometry shape [16]. Foecke and co-workers proposed to use an x-ray diffractometer to measure multiaxial stresses and corresponding yield loci [17–19].

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At the microstructural level, elastic and plastic anisotropy of polycrystalline aggregates result in a heterogeneous distribution of internal stresses and strains. In recent years, in-situ synchrotron x-ray and neutron diffraction have become well established techniques to measure the lattice strain evolution for differently oriented grain families [20]. This is achieved by tracking changes in lattice spacing through diffraction peak position shifts. Collins et al. [21] used in-situ synchrotron x-ray diffraction to study lattice strain and texture evolution during biaxial tensile deformation of cruciform samples made from cold rolled low carbon ferritic steel. They showed that the lattice strain evolution as a function of the azimuthal angle is highly dependent on the applied biaxial stress ratio. The role of cruciform geometry on the macroscopic stress state was however not addressed. Recently, a unique biaxial testing rig was designed and installed in the POLDI neutron beamline at the Paul Scherrer Institute in Switzerland [22]. Using this machine, a series of in-situ neutron diffraction measurements were performed on 316L stainless steel cruciform samples (also used in this work) subjected to biaxial monotonic loading and strain path changes [22,23]. It was found that lattice strain evolution under monotonic equibiaxial tension is significantly different from uniaxial tension. Furthermore, the lattice strain evolution differs when deforming uniaxially a cruciform sample or a dog-bone sample. However, a quantitative analysis of the applied stress ratio on the lattice strain evolution was not performed.

A quantitative understanding of the relation between the applied stress ratio and the lattice strain can be achieved by combining in-situ diffraction studies with crystal plasticity modeling. In this regard, a number of advanced polycrystal plasticity models are available: the small strain elasto-plastic self consistent [24], the finite strain elasto-plastic self consistent [25,26], the elasto-viscoplastic self consistent [27], the elasto-viscoplastic fast Fourier transform (EVPFFT) [28,29] and the crystal plasticity FE [30] models. In this work, the EVPFFT model of Lebensohn and co-workers [28,29] is used. In contrast to mean field self-consistent approaches, EVPFFT is a full field approach that accounts for elastic and plastic grain neighborhood interactions. Furthermore, it is computationally faster than the crystal plasticity FE model. However, EVPFFT is designed to study representative cubic volume elements of polycrystals subjected to strain rate or stress boundary conditions; capturing directly the macroscopic biaxial stress evolution in the cruciform gauge region under the action of experimental forces or displacements is therefore beyond the scope of this model.

To circumvent this limitation, we propose using the following multi-scale approach. The experimental biaxial load and displacement boundary conditions on cruciform samples are supplied to the commercial finite element simulation software ABAQUS [31]. The predicted surface strains are compared with those obtained from digital image correlation (DIC) measurements. The predicted macroscopic field variables are averaged over the neutron irradiated gauge volume and supplied as macroscopic boundary conditions to the meso-scale EVPFFT model. Lattice strains calculated using the EVPFFT model are then compared with those obtained from in-situ neutron diffraction measurements. The proposed synergetic combination of multi-scale FE and EVPFFT, henceforth known as FE-FFT, modeling and experiments is shown in Fig. 1. To the author's knowledge such an FE-FFT approach has not yet been used to study lattice strain evolution during uniaxial or biaxial loading using experimental boundary conditions. Note that recently Kochmann et al. [32] proposed an integrated FE-FFT and phase field approach to study austenite to martensite transformation.

The main objective of this work is to use the FE-FFT approach to obtain a quantitative understanding of the load dependence of

lattice strain evolution during uniaxial and equibiaxial monotonic loading tests performed on 316L stainless steel cruciform samples [22]. The paper is divided into sections as follows. In Section 2 the relevant properties of 316L stainless steel are recalled along with the in-situ neutron diffraction technique to measure lattice strains. Then the cruciform sample geometry studied in this work is presented along with the details of the monotonic loading tests performed. Section 3 presents the multi-scale FE-FFT model and the passage of information between experiments and simulations. The simulation procedure and material parameters used at both length scales are described. Section 4 compares the FE-FFT model with the experimental observations. In Section 5, a detailed analysis of the lattice strain evolution of 200 and 220 grain families is performed to obtain a quantitative understanding of their load dependence. Section 6 presents the main conclusions from this study. A biaxial stress ratio dependent expression for the directional elastic compliance is proposed in the appendix. Throughout this document, upper case letters will be used to denote macroscopic mechanical field variables and lower case letters will be used to denote meso-scale mechanical field variables.

## 2. Material and experimental method

In a recent work involving the authors [22], a series of in-situ neutron diffraction experiments were performed during biaxial loading of cruciform shaped samples of 316L stainless steel. In the following, we briefly recall the details of these tests that are relevant to this work.

### 2.1. Material properties

The material is a warm rolled face centered cubic (fcc) 316L stainless steel composed of: Cr-17.25, Ni-12.81, Mo-2.73, Mn-0.86, Si-0.53, C-0.02 (weight %). Electron backscattering diffraction (EBSD) analysis reveals a mild texture with an average grain size of  $\sim 7 \mu\text{m}$ . The mechanical properties of the material are tested using dog-bone samples prepared along the rolling and transverse direction. The mechanical response is similar for both type of samples, confirming a negligible role of the mild texture [22]. The von Mises (VM) stress v/s strain curve from a monotonic uniaxial tensile loading test is shown with a black line in Fig. 2.

### 2.2. Biaxial testing on cruciform sample geometry

Fig. 3 shows the cruciform geometry used in this work. Directions 1 and 2 in this figure represent the horizontal and vertical directions of the rig, respectively. All samples are prepared such that direction 1 is along the rolling direction. The sample has a circular gauge area of diameter 24 mm with a through thickness of 3 mm. Surface strains in the gauge area are measured in-situ using DIC. The biaxial tension, compression and torsion rig described in Ref. [22] is used to deform these cruciform shaped samples. Two types of monotonic loading are studied in this work: (a) uniaxial loading along the horizontal direction such that  $F_2:F_1 = 0:1$ , and (b) equibiaxial loading i.e.  $F_2:F_1 = 1:1$ . The results are compared with tensile loading tests on dog-bone samples [22]. All the tests are performed under load control at a rate of 40 N/s along each arm.

### 2.3. In-situ neutron diffraction

Neutron diffraction experiments were performed at the time-of-flight neutron strain scanner POLDI beamline located at the SINQ neutron facility of the Paul Scherrer Institut, Switzerland. Detailed information on the setup can be found in Refs. [33,34]. The incoming beam has a square cross-section with a side of 3.8 mm

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