On the validation of a crystal plasticity-based intragranular stress fields identification framework

R. Langlois[1], J. Réthoré[1] and R. Seghir[1a]

[1]Nantes Université, Ecole Centrale Nantes, CNRS GeM UMR 6183, Nantes, France

[a]rian.seghir@ec-nantes.fr

Abstract. Crystal Plasticity models are difficult to define then to calibrate as they rely on numerous internal variables, at the microscopic scale, whereas only surface kinematic data and the macroscopic load response can be measured. In this work, we propose a numerical framework to estimate intragranular stress fields from surface full-field kinematic measurements without postulating the actual form of the constitutive equation. It combines two inverse identification methods, (1) a sparse projection of the strain measurements on a relevant family of function to evaluate plastic slip magnitudes and (2) a Data-Driven Identification (DDI) strategy tuned to the physics at hand. The validation of the method on synthetically generated data is discussed. The resulting stress-strain field database could eventually be used for further parameter or model identification.

Possible Sessions Materials Testing 2.0 or (6. Data Driven Testing, 13. Metals and Microstructure, 16. Novel Experimental Techniques, 19. Optical and DIC Techniques)

Introduction

The deformation of polycrystals involves interactions between different scales of material organisation from the macroscopic scale to the atomic scale. At each scales, different tools exist to describe the core mechanisms of deformation and degradation of an initially *pristine* material. More specifically, Crystal Plasticity (CP) has been developed as a bridge between the scale of the polycrystalline aggregate and the mesoscopic *material* scale and provides a robust modeling tool [1]. In its simplest form, CP relies on the knowledge of grain orientations to define slip planes and a plastic slip evolution law to update critical resolved shear stresses (CRSS). Mesoscopic plastic strain and stress tensor can be recovered through the summation over the different systems. A large set of CP model exist allowing to recover macroscopic aggregate response. However we can not ascertain the relevance of their prediction at the intragranular scale as there is no way to locally probe, without strong assumptions, the evolution of the stress state. In particular, the proper way to introduce grain size effects, to handle grains interactions and grain boundary behavior in models remains an open question. In this talk, we propose a new numerical framework for estimating the fields of intragranular stress tensors. It relies on full-field kinematic data (e.g. obtained from digital image correlation (DIC)) and electron backscatter diffraction (EBSD) [4], as well as load measurement and original identification methods for: (1) plastic slip magnitudes (γ_i) and (2) resolved shear stress (RSS) (τ_i) identification.

Plastic slip magnitude extraction

Slip magnitude quantification methods do exist in the literature [4,5] but they are not able to extract the magnitude of all potentially activated slip systems. Indeed, in the general case the projection of 6 strain components onto a larger family of slip systems (e.g. 12 for FCC or 24 for BCC) is not unique. We propose a sparse promoting projection of the plastic strain following the seminal contributions of Brunton and his collaborators [3,6] on sparse identification. In the spirit of [6], we define a regularized least-squares projection of a measured strain onto the family of Schmid-Boas tensors T_i for each slip system i, which reads using vectorized notation as :

$$\min_{\gamma,\gamma_{sp}} \frac{1}{2}\|T\gamma - \varepsilon^{p}\|^2 + \lambda R(\gamma_{sp}) + \frac{\kappa}{2}\left\|\gamma - \gamma_{sp}\right\|^2 \quad (1)$$

Where T is the vectorized Schmid-Boas tensors, γ is the regularized least-squares solution, γ_{sp} is a sparse representation close to γ in the sense of the norm L2, ε^{p} is an estimation of the plastic strain tensor (see next part), R is a sparsity promoting metric and finally λ and κ are regularization weights which promote (or cancel) respectively the degree of sparsity in γ_{sp} and the closeness between the two outputs. This problem can be efficiently solved using a prox-gradient descent algorithms proposed in [6].

Stress fields identification

Second, we propose a modification of the DDI method developed by Leygue and co-authors [7] to be consistent with Crystal Plasticity. Therefore, a new constitutive space is introduced using $\{(\tau_i, \gamma_i)\}_{\forall i \in [1,N_s]}$leading to a problem of the form:

$$\min_{\tau,\gamma^*,\tau^*} \frac{1}{2} \sum \int \int (\gamma_i(t) - \gamma_i^*)\, G(\gamma_i(t) - \gamma_i^*) + (\tau_i(t) - \tau_i^*) G^{-1} (\tau_i(t) - \tau_i^*) dV dt$$

$$\text{under the constraint of mechanical quasi-static equilibrium:}$$

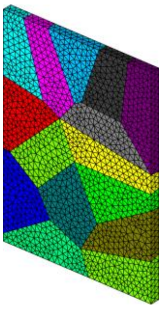
$$\forall t: \begin{cases} \text{div}\left(\sum \tau_i\,(t) T_i\right) = 0 \text{ in } \Omega \setminus \partial\Omega_F \\ \int \sum \tau_i\,(t) T_i . n = F(t) \text{ on } \partial\Omega_F \end{cases} \quad (2)$$

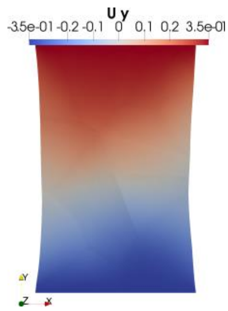
Where N_s is the number of slip systems of the crystal(s), Ω the domain defined by the sample comprised of multiple crystals and $\partial\Omega_F$ the boundary where the load is measured, G a scaling operator akin to a shear modulus, (τ_i^*, γ_i^*) a collection of discrete point sampling the material response in the constitutive space (τ_i, γ_i). This problem is solved using a staggered scheme alternating between updating the plastic slip magnitudes (Eq. 1) and computing the RSS (Eq. 2) until convergence on slips and RSS.

Results

The presentation will focus on the validation of the methods developed, using synthetic data generated with *code_aster* and *NEPER* [8]. The test consists in a quasi-2D coarse grain structure shown in Fig. 1 loaded in uni-axial tension up to 5% of strain. For this proof of concept, the underlying CP model is a Méric-Cailletaud with kinematic and isotropic hardening. The CPFE simulation will be used as ground-truth and compared to the "experimentally" identified plastic slip magnitudes and RSS, FE strain being considered as DIC data (Fig. 1). This work fall well within the framework of Materials Testing 2.0 where full-field measurements and inverse methods are used to capture complex material responses in a more efficient way, and using a small number of tailored tests.

Table 1: Example of microstructure and CPFE displacement used to feed the methods.





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