Institut de Recherche en Génie Civil et Mécanique

UNIVERSITÉ DE NANTES

Title: *Identification of the statistical parameters of polycrystalline materials from wave field measurements*

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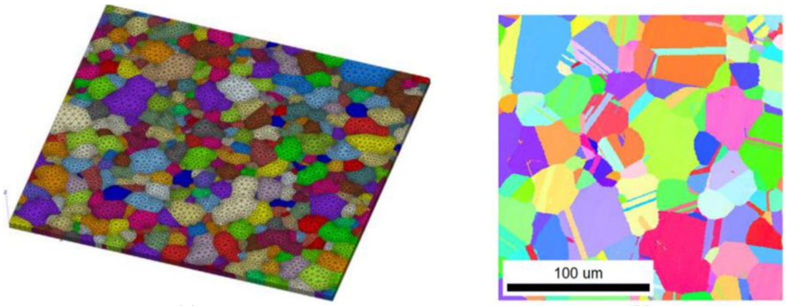
Abstract :

The non-destructive probing of polycrystalline aggregates using waves is a vast research topic. These materials are composed of discrete grains with different shapes, sizes and crystallographic orientations (Fig 1a, [1]). This strongly heterogeneous and anisotropic microstructure comes, among others, from metallurgical manufacturing processes such as rolling, forging or isothermal annealing. As a result, adjacent grains present strongly heterogeneous mechanical properties, as well as incompatibilities of strains that yield fields of internal (residual) stresses which could induce cracks within the material. These individual fractures may also induce locally anisotropic behavior. The prediction of durability of structural parts requires to be able to (i) localize these cracks; (ii) gather a wide knowledge of mechanical behavior of the material at the mesoscopic (grain) scale as well as (iii) understanding how grains interactions occur.

The characterization of the mechanical properties of polycrystals (and their evolutions) at the grain scale is very complex and is a subject of industrial interest. One of the main applications of this study is that it allows us to more precisely monitor the evolution of the material properties during the manufacturing process. The main objective of this project is to identify the statistics of the mechanical parameters of polycrystalline materials. These parameters are for instance the grain size (in terms of its probability density function (PDF)), the correlation distance of the grain size (the mathematical expectation of the grain size random variable), the grain form (in terms of the PDF of its sphericity), its average (the background medium) and dispersion level (variance), its spatial correlation function (covariance function) and the anisotropy level of the medium which also is a random variable that should be statistically characterized.

Stochastic approaches being capable of describing very complex spatial variations are naturally suited for the probabilistic representation of crystallographic orientations [2,3]. Thus, the aforementioned identifications will be done based on (i) a probabilistic modeling of the polycrystalline medium based on the Euler angles characterizing local grain orientations, and (ii) measurements of the scattered wave field in the medium. A probabilistic model will therefore be used to describe the realizations of the heterogeneous field of the Euler angles. In order to feed this probabilistic model, the experimental data obtained by an electron backscatter diffraction (EBSD) or X-ray diffraction test will be used (Fig 1b, [1]). We will need to have a database with different types of grain morphologies, and different textures (from highly textured to texture-less). The elasticity tensor of each grain $C^g(\boldsymbol{x})$ will thus be equal to a random rotation matrix applied to the stiffness tensor of the single crystals C^{cr}.



(a) (b)

Figure : (a) 3D finite element mesh of a polycristalline material, (b) EBSD mapping of a Nickel-based supperalloy sample (from [1])

Indeed, when the wave propagates through a polycrystalline medium, its interaction with the heterogeneities in mechanical properties as well as density of the crystallites creates a scattered wave field. As of today, we know that the energy content of the multiply scattered waves carries information related to the statistical parameters of the propagation medium. These energies are theoretically described by the Radiative Transfer Equations (RTE) that were mainly developed for locally isotropic materials [4] and often applied for concrete and geophysical materials [5,6,7]. These equations have recently been developed for the general case of continuous anisotropic heterogeneous materials [8]. The RTEs are characterized by the scattering operators which depend on the statistical characteristics of the underlying medium. These operators are often developed for isotropic random media with low scattering degrees and for the frequencies below the geometrical optics regime [9,10]. In contrast, in this project we are interested in polycrystals being intrinsically strongly heterogeneous and strongly anisotropic and the identification will be done using high frequency waves. For this purpose, we recently derived the scattering operators for a texture-less anisotropic (of cubic type) polycrystal in which the grains have no preferred orientation (uniform distribution) and the macroscopic behavior is statistically isotropic [11]. Further developments for more complicated anisotropy types are to be considered in this project. In this regard, the main theoretical difficulty is that the scattering operators become extremely complex when the number of independent parameters describing the elasticity matrix becomes significantly large. Regarding the identification of the covariance function of the medium parameters, the influence of this function is analytically studied for different propagation regimes (frequencies) [12]. This contribution aims at drastically reduce the complexity of the inverse problem to be solved in order to achieve the identification of the correlation function.

Another approach to identify the background medium (first-order statistics) along with the foreground statistics is to use the asymptotic diffusion regime at long propagation times during which the ratio of the energies of the compression (P) and shear (S) waves becomes stable. Having recourse to the software package SPECFEM3D, we simulated the wave propagation in randomly heterogeneous media and estimated the energy densities. Large scale simulations performed in [13] and [11] respectively for locally isotropic and locally anisotropic media have shown that the setting up of a stabilization regime occurs regardless of the local behavior of the medium. An example of the wave propagation simulation performed in a locally anisotropic texture-less randomly heterogeneous medium recently done by the coordinator of the project can be found here: https://www.youtube.com/watch?v=srDblKJxZ-M. Furthermore, since the time beyond which the ratio of the energy densities becomes stable is also a function of the first and second-order statistics of the medium, its estimation, especially in some particular propagation regimes, could reveal some statistical information about the medium.

The main steps of the project are the following: (1) numerical generation of a polycrystal using open source codes such as NEPER and then meshing it; (2) numerical modeling of the random Euler angles based on the experimental EBSD maps in order to be able to calculate the stiffness tensor for each element; (3) using the open source software package SPECFEM3D to simulate the wave propagation in the generated medium; (4) analyzing the obtained wave field at the surface along with the energies to obtain the statistical parameters of the medium; (5) extending the results obtained in [11] to the case of a textured random medium; (6) taking into account the presence of cracks on the one hand and the multiple phases on the other hand are other aspects that will be treated during the project. (7) study how the existing uncertainties, for instance on the average equivalent diameter of grains, propagates through the system and transforms to the uncertainty of the quantities of interest (maximum local stress, average stress, …). We will use different uncertainty quantification methods as introduced in [14].

The main scientific bottlenecks to achieve these goals are as follows: (1) Both the generation of the medium and simulation of the wave propagation are strongly time consuming so that we should definitely use a supercomputer (HPC) and develop parallelized codes. Moreover, the algorithms required to generate the medium and the Euler angles random fields should be optimized. This item is one of the main novelties of the project since the mean-field based methods are often used in the related literature [15,16,17]; (2) The classical tessellation generates sharp edges which should be regularized in order to be more efficient regarding the mesh size. (3) Taking into account the anisotropy, since the latter will complexify the analytical form of the scattering operators. Recently, we derived these operators for the case of cubic local anisotropy [11]. During this project, we need to do a profound mathematical study on the scattering operators and try to simplify the final equations as far as possible for more complex anisotropy scenarios.

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