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A comparison between different numerical methods for the modeling of polycrystalline materials with an elastic–viscoplastic behavior

Camille Robert *, Charles Mareau

Arts et Métiers ParisTech, Campus d'Angers, LAMPA, 2 bd du Ronceray, 49035 Angers Cedex 1, France

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ABSTRACT

The macroscopic behavior of polycrystalline materials is largely influenced by the shape, the arrangement and the orientation of crystallites. Different methods have thus been developed to determine the effective behavior of such materials as a function of their microstructural features. In this work, which focuses on polycrystalline materials with an elastic–viscoplastic behavior, the self-consistent, finite element and spectral methods are compared. These common methods are used to determine the effective behavior of different 316L polycrystalline aggregates subjected to various loading conditions. Though no major difference is observed at the macroscopic scale, the hardening rate is found to be slightly overestimated with the finite element method. Indeed, spatial convergence cannot be guaranteed for finite element calculations, even when fine mesh resolutions, for which the computational cost is important, are used. Also, as the self-consistent method does not explicitly account for neighborhood effects, important discrepancies between the self-consistent method and the other methods exist regarding the mechanical response of a specific grain. The self-consistent method nevertheless provides a reasonable description of the average response obtained for a group of grains with identical features (e.g. shape, orientation).

1. Introduction

The behavior of engineering materials is sometimes better described by accounting for the heterogeneous aspect of the strain and stress fields which develop during a deformation process. For the specific case of polycrystalline materials, the main reason for the fluctuations of the strain and stress fields is the anisotropy of single crystal elastic and plastic properties. These fluctuations, which may significantly impact the effective behavior of a polycrystalline aggregate, depend on the properties, the shape, the arrangement and the orientation of the different crystallites. Different methods have thus been developed to account for the polycrystalline nature of such materials when determining the effective properties.

Historically speaking, the first propositions were made by Hershey [1] and Kröner [2] who developed the self-consistent scheme to estimate the effective properties of heterogeneous materials. Since the initial propositions of Hershey [1] and Kröner [2] are restricted to constitutive models with a linear form (e.g. linear elasticity, newtonian viscosity), different extensions have been proposed to deal with heterogeneous materials with non-linear constitutive relations. For instance, the developments made by Kröner [3] and Hill [4] allow for modeling the behavior of heterogeneous materials for which the constitutive relation includes both elasticity and rate-independent plasticity. Neglecting elastic contributions, Hutchinson [5], Molinari et al. [6] and Lebensohn and Tomé [7] adapted the self-consistent model to the case of heterogeneous solids with a viscoplastic behavior. When dealing with elastic–viscoplastic constitutive relations, additional difficulties exist because constitutive relations involve different orders of time derivation. Indeed, complex space–time couplings, described by Suquet [8] as the long-memory effect, are involved and the local and macroscopic constitutive models do not have the same structure anymore. To overcome these difficulties, many approaches have been proposed. They fall into two different categories. On the one hand, hereditary models use Laplace–Carson transforms to define a single viscoelastic modulus in the Laplace–Carson space [9–12]. The self-consistent problem can then be solved in the Laplace–Carson space before proceeding to the inversion of the solution to the real time space. On the other hand, interval variable models are entirely formulated in the real-time space [13–20]. They are based on a set of internal variables whose introduction allows accounting for the interactions associated with the space–time couplings.

* Corresponding author.
E-mail addresses: camille.robert@ensam.eu (C. Robert), charles.mareau@ensam.eu (C. Mareau).

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The finite element method [21–23] is commonly used for the resolution of mechanical engineering problems. As shown by the pioneering work of Miyamoto et al. [24], the finite element method is a convenient way of investigating the local behavior of crystalline materials. Indeed, in contrast with the self-consistent method, the finite element method aims at providing stress and strain fields for which compatibility and static equilibrium conditions are locally fulfilled. The finite element method thus allows for capturing the intragranular fluctuations of the stress and strain fields. As a result, thanks to the development of computing capabilities, there has been a growing interest for the numerical simulation of polycrystalline aggregates with the finite element method [25–32].

The spectral method proposed by Moulinec and Suquet [33] is an alternative solution for the modeling of heterogeneous materials. It makes an intensive use of the Fast Fourier Transform algorithm to solve the integral equation associated with the heterogeneous problem. Though the initial applications of Moulinec and Suquet [33] were focused on composite materials, different extensions have been developed in the context of crystal plasticity [34–37]. In contrast with the finite element method, the periodicity of both the microstructure and the boundary conditions is a necessary condition for the application of the spectral method.

Because of their design, the self-consistent, finite element and spectral methods are based on different assumptions. As a result, the choice of an appropriate method for a given problem requires being aware of how these assumptions may influence the estimate of effective properties. The present work thus aims at comparing these methods in the context of the determination of the effective properties of polycrystalline aggregates with an elastic–viscoplastic behavior. The paper is structured as follows. In the first part, the equations associated with the heterogeneous problem are presented and the different methods are briefly described. In the second part, some applications are proposed and the results determined with the different methods are compared. The results are obtained for 316L polycrystalline aggregates subjected to different loading conditions: uniaxial tension, cyclic tension–compression and some multiaxial loading paths allowing for the determination of yield surfaces.

2. Model description

2.1. Field equations

In this work, a volume element V with boundary ∂V, which is representative of a polycrystalline material, is considered. The volume element consists of many subdomains with homogeneous properties (i.e. crystallites) being perfectly bonded across their interfaces. The effective properties are determined from the macroscopic stress and strain tensors (denoted by Σ and E) which are related to the local stress and strain fields (denoted by σ and ε) through the classical averaging relations of homogenization theory[1]:

$$\Sigma(t) = \frac{1}{V}\int_V \sigma(x,t)dV = \langle\sigma(t)\rangle_V \tag{1}$$

$$E(t) = \frac{1}{V}\int_V \varepsilon(x,t)dV = \langle\varepsilon(t)\rangle_V \tag{2}$$

Within the infinitesimal strain framework, kinematical compatibility relations are given at any point x and any time t by:

$$\varepsilon(x,t) = \mathrm{sym}(u(t)\otimes\nabla_x) \tag{3}$$

$$\dot{\varepsilon}(x,t) = \mathrm{sym}(\dot{u}(t)\otimes\nabla_x) \tag{4}$$

where u is the displacement field. Also, when no volume forces are present, the stress field σ should satisfy the static equilibrium conditions:

$$\nabla_x\cdot\sigma(t) = 0 \tag{5}$$

$$\nabla_x\cdot\dot{\sigma}(t) = 0 \tag{6}$$

Assuming an elastic–viscoplastic behavior, the local strain and strain rate fields are decomposed into elastic (subscript e) and viscoplastic (subscript p) contributions:

$$\varepsilon(x,t) = \varepsilon_e(x,t) + \varepsilon_p(x,t) \tag{7}$$

$$\dot{\varepsilon}(x,t) = \dot{\varepsilon}_e(x,t) + \dot{\varepsilon}_p(x,t) \tag{8}$$

Within a rate-dependent framework, the viscoplastic strain rate $\dot{\varepsilon}_p$ is a non-linear function f of the stress tensor σ and some internal variables v_k whose detail does not need to be known at this stage:

$$\dot{\varepsilon}_p(x,t) = f(\sigma, v_k) \tag{9}$$

The introduction of the elastic stiffness tensor c allows for connecting the stress and stress rate tensors to the strain and strain rate tensors:

$$\sigma(x,t) = c(x) : \left(\varepsilon(x,t) - \varepsilon_p(x,t)\right) \tag{10}$$

$$\dot{\sigma}(x,t) = c(x) : \left(\dot{\varepsilon}(x,t) - \dot{\varepsilon}_p(x,t)\right) \tag{11}$$

In order to close the above problem, which consists of Eqs. (3)–(11), the boundary conditions have to be specified. The boundary conditions prescribed on ∂V should reflect as better as possible the in situ state of the representative volume element. However, in most cases, only partial information regarding the exact in situ state is available. Therefore, depending on the method, different strategies have been adopted to circumvent this difficulty.

In the general case, no analytical solution exists for the heterogeneous problem which is uniquely defined from field equations and boundary conditions. Consequently, different methods, which are briefly described in the following sections, have been developed to obtain numerical solutions to this problem. These methods aim at finding the stress and strain fields (or equivalently the stress rate and strain rate fields) satisfying both compatibility, equilibrium and boundary conditions.

In the following, unless otherwise specified, the dependence with time t and position x will be omitted.

2.2. Finite element method

The finite element method aims at finding approximate solutions to boundary value problems such as the heterogeneous problem described earlier. The first step consists of writing the heterogeneous problem in its weak form. The weak formulation is obtained by introducing a virtual displacement field v which allows for transforming Eq. (5) into:

$$\int_V (\nabla_x\cdot\sigma)\cdot v dV = 0 \tag{12}$$

Integrating by parts the above relation and using the divergence theorem leads to the weak formulation of the heterogeneous problem:

$$\int_V \sigma : \epsilon dV - \int_{\partial V}(\sigma\cdot n)\cdot v dS = 0 = R(u) \tag{13}$$

[1] These relations hold if and only if the volume element is submitted to homogeneous boundary conditions or periodic boundary conditions. Only these specific (but rather common) situations are considered in the present work.