Proper Generalized Decomposition (PGD) for numerical calculation of polycrystalline aggregates under cyclic loading

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One of the most challenging task in mechanics of materials is to get access to the mechanical response at the grain scale of a polycrystalline aggregate especially when it is subjected to a fatigue loading [1]. Indeed, local plasticity, microstructural heterogeneities and the crystal orientations play an essential role in the birth and growth of cracks. With regard to this matter, it is necessary to know the history of the various mechanical quantities in fatigue initiation site. From a numerical point of view, it is not enough to perform a simple monotonic calculation, but we must simulate the entire load history. The numerical modeling of materials at the microstructural scale has been greatly developed over the last two decades. Different numerical methods have been used to explicitly model a polycrystal : finite elements method (FE), spectral method (FFT). The finite element method is the most commonly used for numerical simulation of polycrystalline aggregates [2] and its resolution is usually performed by the incremental method. However, to ensure a better convergence, the overall evolution is not resolved globally in one problem, but the study interval is discretized in time increment and loading. For each increment, a Newton-Raphson type resolution scheme is applied. This method is taken as a reference and is very fluently used in commercial and academic computation code. Unfortunately, problems with large number of degrees of freedom, the resolution of the linear system is very costly because of the prohibitive calculation times [3]. The tangent stiffness matrix is recalculated in every iteration and creates a significant computational cost for a high number of degrees of freedom. Moreover, this calculation time is proportional to the time discretization and therefore the number of cycles simulated.

This study aims at the developing of a numerical method for the resolution of the finite element for nonlinear viscoplastic problems. For this, two ideas are used. The first is to maintain a constant stiffness matrix [4] to do only one factorization. The second concerns the use of a model reduction method to decouple the dimensions of space and time. PGD [5] has been selected. This method, which is based on radial approximation [6], has shown its effectiveness in solving problems with a large number of degrees of freedom [7]. The general principle is to calculate the solution defined on the entire space/time field, in the form of a sum of products functions of each variable. PGD method has been implemented in a computation code developed at the LAMPA [8]. The simulations have been made on a polycrystalline aggregation as the geometry of the grain is cubic and the

aggregate is composed of 512 grains. Several mesh densities are composes, from 1 to 512 elements in grain. The crystalline behavior law used in this work was introduced by Meric and Cailletaud [9]. The material is a stainless steel 316L and the parameters of the elastoviscoplastic behavior law were identified by [10]. The results are compared with the incremental method conventionally used in commercial computation codes at the macroscopic values (aggregate averages) and mesoscopic (grains averages). The analyses show a good precision between the two methods of resolution with a significant time savings for PGD method but with more memory usage. In particular we can see that the differences are most important at the mesoscopic deformation but still quite acceptable (maximum relative gap less than 0.1%). These differences can be attenuated by decreasing the tolerance, but in this case, the computation time increases significantly.

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