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A GENERALIZED FINITE ELEMENT METHOD FOR GRAIN-BOUNDARY SLIDING IN POLYCRYSTALS

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Summary. *We present a Generalized Finite Element Method for the analysis of grain-boundary sliding in polycrystals. Grain boundaries are represented by means of elements with embedded displacement discontinuities through the partition of unity property of finite-element shape functions. Consequently, the finite-element mesh does not need to conform to grain boundaries.*

1 INTRODUCTION

In many polycrystalline materials, grain boundary sliding is one of the main mechanisms behind anelastic deformation. In this contribution, we consider novel developments in the field of Generalized Finite Element Methods [2, 5] and present a model for the analysis of polycrystals in which grain boundaries are represented by means of elements with embedded displacement discontinuities. A cohesive constitutive law for grain boundary sliding is applied across grain boundaries which are described using the GFEM formulation presented in Section 2. Simple applications illustrate the potential of the proposed model. More specifically, the effect of grain boundary sliding [3] and the influence of grain size, shape and distribution on anelasticity of polycrystals are assessed.

We also discuss an extension of the model for the description of grain refinement, a phenomenon which is believed to be a key ingredient in the development of superplastic flow in some coarse-grained materials.

The proposed GFEM approximation for polycrystals can also be used for branched and intersecting cohesive cracks in two or three dimensions. We demonstrate that the two-dimensional case of our approach produces the same approximation spaces as techniques making use of the eXtended Finite Element Method [1, 4]. However, the choice of enrichment functions is simplified, thus making it an appealing alternative to the XFEM.

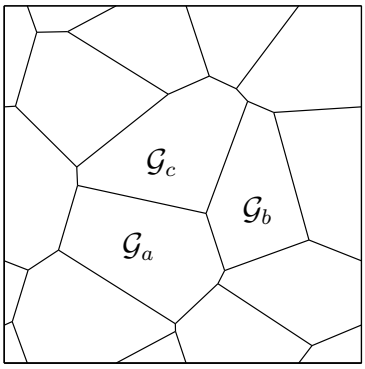

Figure 1: Unit cell for a polycrystal

2 GFEM FOR POLYCRYSTALS–MAIN IDEAS

The model relies on novel developments in the field of GFEM. The displacement field in a polycrystal comprising $N_{\mathcal{G}}$ grains (see Figure 1) is decomposed according to

$$\boldsymbol{u} = \hat{\boldsymbol{u}} + \sum_{\alpha=1}^{N_{\mathcal{G}}} \mathcal{H}_\alpha \tilde{\boldsymbol{u}}_\alpha, \tag{1}$$

where the field $\tilde{\boldsymbol{u}}_\alpha$ is an enhancement, related to grain $\mathcal{G}_\alpha$, to the standard displacement field $\hat{\boldsymbol{u}}$ and

$$\mathcal{H}_\alpha(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \boldsymbol{x} \in \mathcal{G}_\alpha \\ 0 & \text{otherwise.} \end{cases} \tag{2}$$

The resulting field equations are discretized by using the finite-element method.

The analysis of the polycrystal unit cell depicted in Figure 1 is accomplished by defining a structured background finite-element mesh on which the polycrystal topology is superimposed as schematically depicted in Figure 2. It is worth noting that the analysis of the polycrystalline region depicted in Figure 1 can be performed without recourse to mesh generators (see e.g. [6]). This is specially important for three-dimensional models since the grain topology, in this case, is in general difficult to mesh. However, as in standard finite-element methods, the quality of the GFEM approximation depends on the level of refinement of the background mesh. Alternatively, the GFEM approximation can also be improved through p-type enrichment of the approximation spaces defined on a course background mesh.

References

[1] C. Daux, N. Moës, J. Dolbow, N. Sukumar, and T. Belytschko. Arbitrary branched and intersecting cracks with the extended finite element method. *International Journal for Numerical Methods in Engineering*, 48:1741–1760, 2000.

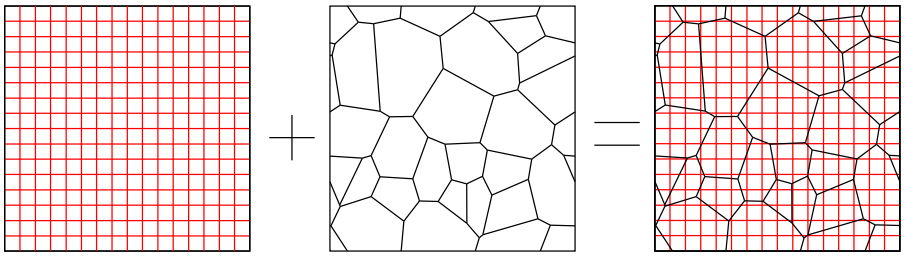

Figure 2: GFEM approximation of a polycrystal unit cell

[2] C. A. M. Duarte and J. T. Oden. Hp clouds – an hp meshless method. *Numerical Methods for Partial Differential Equations*, 12(6):673–705, 1996.

[3] F. Ghahremani. Effect of grain boundary sliding on anelasticity of polycrystals. *International Journal of Solids and Structures*, 16:825–845, 1980.

[4] N. Moës, J. Dolbow, and T. Belytschko. A finite element method for crack growth without remeshing. *International Journal for Numerical Methods in Engineering*, 46 (1):131–150, 1999.

[5] J. T. Oden and C. A. Duarte. Clouds, cracks and fem's. In B. Daya Reddy, editor, *Recent Developments in Computational and Applied Mechanics*, pages 302–321, Barcelona, Spain, 1997. International Center for Numerical Methods in Engineering, CIMNE.

[6] N. Sukumar, D. J. Srolovitz, T. J. Baker, and J.-H. Prévost. Brittle fracture in polycrystalline microstructures with the extended finite element method. *International Journal for Numerical Methods in Engineering*, 56:2015–2037, 2003.