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Multiscale dynamic transition of 2D metallic materials using the boundary element method

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ABSTRACT

In this paper, a multiscale dynamic transition is analyzed for metallic materials. The boundary element method (BEM) is used in order to model macro and micro domains, being considered isotropic and anisotropic properties respectively. To connect both scales, a displacement field is obtained from the macroscale, and it is imposed to a micro domain. Thus, assuming polycrystalline structures at a lower level, the dynamic response is found. The transient analysis is implemented by the dual reciprocity method (DRM) to evaluate the non-linear and time-dependent problem. Furthermore, the Houbolt algorithm is applied to solve the time integration scheme. Finally, numerical examples are presented demonstrating the validation of the dynamic transition between the macro and micro scales.

1. Introduction

Nowadays, some of the primary goals of science and technology are to understand and control the behavior of materials on different space and time scales. The reason is the relevance of the microstructure and how it affects the macro-domain. There are several engineering materials that present a granular structure at the microscale, e.g. metals, alloys, and ceramics. The constitutive behavior is related to the homogeneous properties at the macroscale and heterogeneous properties at the microscale, see Fig. 1. Under those circumstances, it is necessary to consider both scales inside a hierarchical modeling [1].

The multiscale analysis has emerged as a research area to evaluate and connect the physical response of materials under operational conditions. This analysis is determined by a hierarchy process and three categories can be distinguished. In the first category, a high resolution is applied to a small part inside the macro-domain, in which particular details of the morphology need to be solved (e.g. dislocations, cracks, etc.). In the second, the category relies on a macroscopic description that has to be resolved from an essential microscale analysis. In the third category, parts of the macro-domain are fully resolved at the microscale, and other parts are probed at the microscale only through the effective macroscopic response [2]. These types of analyses present a hierarchy process, and not only connect theories and experiments but also is a feasible and non-expensive tool to be used in the laboratory [3]. However, there are some obstacles to overcome when the information is being transferred between scales. The first one is the continuum and classical model used to approximate the geometry of the problem, and second the computational cost [4].

Recently, analyses of polycrystalline materials have been developed in order to obtain the mechanical response in a multiscale framework. To study the influence of micro defects on a macroscopic domain and under static loads, the extended finite element method (XFEM) has been used by Liu et al. [5] and Fu et al. [6]. To describe the crack propagation in polycrystalline domains, the variational multiscale method (VMM) has been incorporated with enrichment functions to represent the microscale, while a generalized finite element method (FEM) has been applied to model the macroscale [7]. In most of the works about multiscale transition, the FEM has been widely used [8–12]. However, using this numerical technique, the mesh refinement at the microscale needs to be much higher. Owing to the high gradients and internal force concentration over small regions, the BEM has been applied as an alternative computational method to model metallic materials. Sfantos and Aliabadi [13] introduced a 2D macro and micro analysis of polycrystalline materials under static loads. The authors considered the representative volume elements (RVEs) to transfer the mechanical response between macro and micro scales. However, in this type of transition, the information is constrained by the size of elements that are required to be much smaller than in the microscale. A transient analysis using BEM was presented by Galvis and Sollero [14]. The authors related the mechanical behavior of polycrystalline materials under dynamic loads.

This work presents the first 2D dynamic approach to couple macro-

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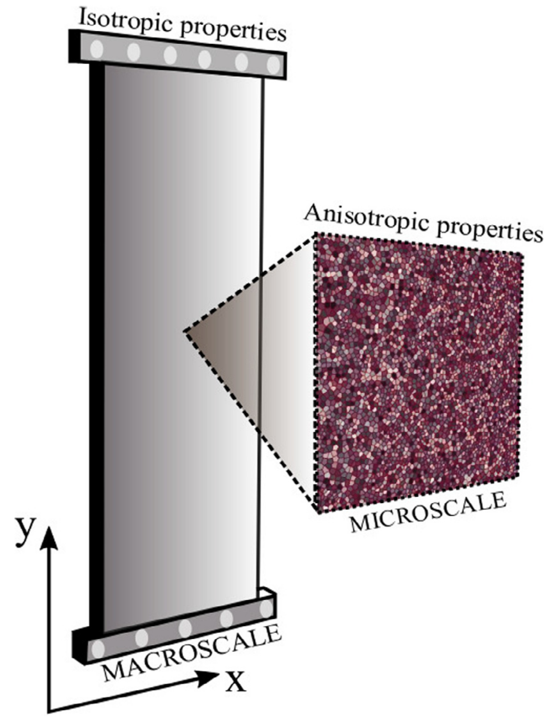

Fig. 1. Multiscale visualization for macroscopic and microscopic domains.

micro scales using BEM, to the author's knowledge. In order to consider the relevance of material properties at different scales, both isotropic and anisotropic media are considered. Furthermore, internal points are evaluated at the macroscale to obtain the prescribed boundary conditions to be applied at the microscale. A parallelization on a shared memory architecture, using Fortran-OpenMP, is applied to evaluate the BEM matrices. Finally, the results are presented with analytical solutions to validate the multiscale transition, showing the displacement field at different space and time scales.

This paper is organized as follows. Section 2 introduces the multiscale implementation. The elastodynamic BEM formulation is described in Section 3. Numerical examples and the multiscale transition are provided in Section 4. Finally, some conclusions are presented in Section 5.

2. Multiscale approach

In order to develop the multiscale transition of metallic materials, this work analyzes the influence of the macroscopic conditions on a microscopic structure. It is known that both scales can be modeled by continuum methods. The range of simulations begins at a length and time of about 10^{-6} m and 10^{-6} s, respectively [3].

At the macroscale, the aforementioned materials present homogenous properties. In this scale, the material is typically assumed as an isotropic medium. Here, the BEM is implemented to model the time-space domains, where Kelvin's fundamental solutions are used to evaluate the mechanical response. On the other hand, such materials at the microscale, where polycrystalline structures are found require another formulation. Thereby, the BEM must be implemented applying anisotropic fundamental solutions. In addition, a multizone framework must be considered due to a large number of crystals to be analyzed.

Standard methods are presented in the literature to normalize the number of crystals that are contained within an area of 1.0 mm^2. The American Society for Testing and Materials (ASTM) specified the average number of grains for metallic materials [15]. Iron at room temperature, whose properties are used in this work, contains around 2000 to 5000 grains per square millimeter.

Regarding the mesh discretization, Fig. 2 illustrates the BEM boundary modeling to both macro and micro scales. At the microscale is useful to model each grain as a continuum body applying displacement compatibility and traction equilibrium at the grain interfaces. Furthermore, the polycrystalline structure can be reproduced by the Voronoi tessellation algorithm [16]. This algorithm has been extensively used to represent a grain morphology, e.g. [14,17,18].

In the context of the macro-micro transition, this work intends to consider all the requirements to treat an enhanced multiscale approach. First, the internal points are evaluated from the macroscale to obtain the dynamic displacement response. Consequently, the microstructure is conditioned by the macro results as prescribed boundary conditions, and the use of RVEs is avoided. Second, owing to the larger number of regions to be evaluated, the critical sections of the BEM code are parallelized. The sections to be parallelized correspond to the computation of BEM matrices and the solver of the linear system of equations. The solution of this system is carried out using the Pardiso solver [19,20], which is a thread-safe, high-performance, robust memory efficient for solving large sparse unsymmetric linear systems equations on a shared-memory architecture. The Fig. 3 describes a general flowchart of this multiscale process.

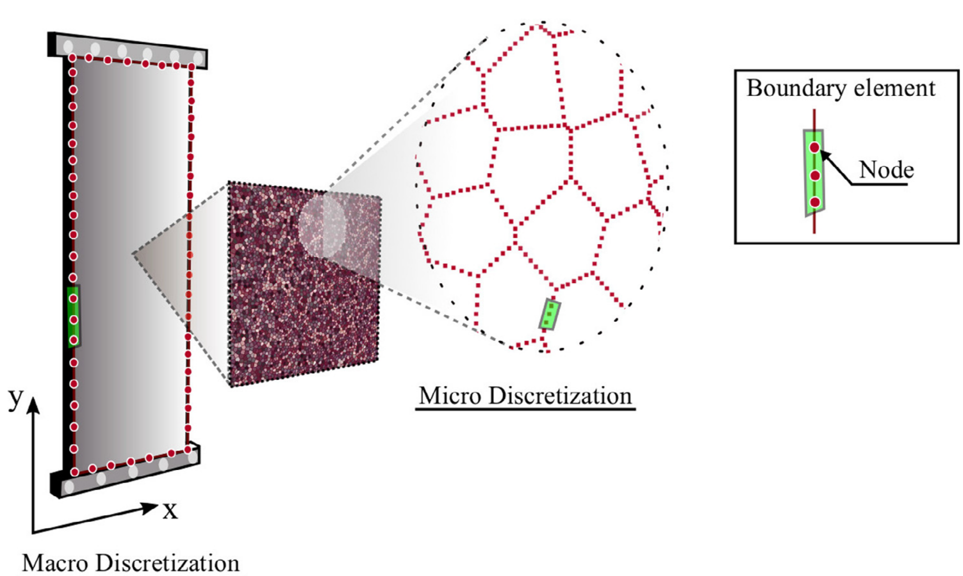

Fig. 2. 2D multiscale discretization for macro and micro domains.

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