Computers and Structures 200 (2018) 11–20

Contents lists available at ScienceDirect

Computers and Structures

journal homepage: www.elsevier.com/locate/compstruc

Dynamic analysis of three-dimensional polycrystalline materials using the boundary element method

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ARTICLE INFO

Article history:
Received 24 August 2017
Accepted 12 February 2018

Keywords:
Dynamic analysis
Boundary element method
Anisotropy
Polycrystalline materials

ABSTRACT

A new computational framework to analyse the microscale dynamic behaviour of three-dimensional polycrystalline materials with different lattice structures is presented. The absence of analytical solutions for these stochastic materials has been a challenge in validating the numerical results. In macroscale analysis, when the number of crystal aggregates in the microscale is large, polycrystalline aggregates exhibit an effective isotropic nature. To model the elastodynamic effects, random crystalline orientations and morphology configurations are used for each polycrystalline aggregate. The recently proposed fundamental solution based on double Fourier series for general anisotropy coupled to the dual-reciprocity boundary element method is used. A drastic reduction in the degrees of freedom is achieved owing to the nature of the boundary mesh. The stochastic time-dependent displacement wave under various boundary conditions is evaluated, and the validation is carried out using homogenisation over the grain surfaces. An assessment of the effective macroscopic properties of the available analytical isotropic models is proposed, wherein the convergence is evaluated using statistical samples. Numerical results are presented using a large number of simulations to obtain a good confidence interval.

1. Introduction

The analysis of constitutive behaviour of polycrystalline materials under various load conditions is essential to improve the performance in applications at macro- and micro-scales. The presence of flaws in the microstructure causes a reduction in the effective overall mechanical properties at macroscale. The analyses of behaviour and failure using the boundary element method (BEM) were carried out by Sfantos and Aliabadi [1] in 2D polycrystalline materials, and the 3D grain boundary formulation for the microstructural modelling of polycrystalline materials was performed by Benedetti and Aliabadi [2]. Furthermore, a multiscale quasi-static analysis of polycrystalline materials using the BEM was presented by Benedetti and Aliabadi [3]. The lattice structure, crystalline orientations, and morphology of the polycrystalline aggregate are considered in the microscale constitutive model. Therefore, heterogeneous behaviour of mechanical fields at microscale is produced.

Meshing methods have been developed for the simulations of polycrystalline materials. Different schemes of volumetric and surface mesh generators [2–6] for finite element method (FEM) and BEM simulations have been presented. Process image reconstruction from experimental data [7–9] and Voronoi and Laguerre tessellation-based meshing and remeshing are necessary for polycrystalline aggregates. Random and homogeneous morphologies are required to avoid singularity problems and reproduce the results from these simulations more accurately. BEM three-dimensional triangle element meshes were generated by Benedetti and Aliabadi [2,5] based on the methodology presented by Fritzen et al. [4] for FEM analysis, and this methodology was applied in this work.

The application of dynamic loads with a rapid rate of change over time leads to other physical considerations, when compared with static or quasi-static models. The inertial force dependency of the mechanical fields is caused by the dynamic loads, which resist accelerations of the structure. These physical effects are the main characteristics of dynamics problems [10]. Further, the dynamic deformation owing to high-rate loads should be analysed. In this case, there is a high strain gradient in a part of the body, and the remaining parts do not yet experience stresses. Strain and stress waves propagate through the solid at a specified velocity [11]. Dynamic loads play an important role in failure analysis, as the material is more susceptible to failure under impulsive or high-strain-rate loads, which affect the fracture behaviour [12]. Therefore, dynamic fracture mechanics should be applied [13].

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https://doi.org/10.1016/j.compstruc.2018.02.009
0045-7949/

BEM is a powerful numerical method to model high stress and strain gradients using surface discretisation. Therefore, crystal aggregates can be modelled only using the grain boundaries. The interface analysis is conducted using the multidomain algorithm. The 3D fundamental solution and its derivatives based on double Fourier series were proposed by Tan et al. [14]. To the best of the authors' knowledge, this is the most recent development of efficient evaluation of these quantities. This fundamental solution has been applied to generally anisotropic solids by Shiah et al. [15–17]. Dynamic displacement and traction fields were evaluated using the dual reciprocity boundary element method (DRBEM), as presented by Kögl and Gaul [18] and Gaul et al. [19] for three-dimensional problems of anisotropic elastodynamics. This method uses a set of radial functions and transforms the domain integral into a boundary integral using the dual reciprocity method. Time integration is carried out using Houbolt's algorithm [20]. Notably, other numerical formulations have been used to treat dynamic problems using BEM, such as dual reciprocity in the Laplace domain [21]. Comparisons among the Laplace transform, dual reciprocity, and time-domain methods using isotropic materials can be found in [22], which reported accurate results. The applications of dynamic fracture mechanics were developed for 3D isotropic models in Laplacian space [21,23,24], where the authors computed the dynamic stress intensity factors. Furthermore, problems of modal analysis could be solved using this Laplace formulation.

This new computational framework is based on related publications. The pre-processing is performed using an in-house C++/C code based on [2,4], the Voro++ library by Rycroft [25] and the Triangle mesh generator by Shewchuk [26]. We applied the 3D elastostatic fundamental solution for anisotropic media based on double Fourier series proposed by Tan et al. [14] and used by Rodriguez et al. [17]. The dynamic BEM analysis is carried out using the DRBEM, using the particular solutions presented by Gaul et al. [19]. The displacement field in the time domain is obtained using Houbolt's time integration algorithm [20]. Owing to the large number of degrees of freedom (DOFs), an Message Passage Interface (MPI) implementation is required in the critical sections of the in-house BEM code. Therefore, a MUltifrontal Massively Parallel Sparse direct solver (MUMPS) [27,28] is used to solve the resulting block sparse system of equations.

This work presents the first approach to model polycrystalline materials under dynamic boundary conditions using BEM. Kögl and Gaul [29–31] introduced works treating the dynamic behaviour of 3D anisotropic materials, where 3D piezoelectric materials were analysed using DRM and the dynamic behaviour and free vibration of anisotropic elastic solids were presented. In these publications, the authors used a fundamental solution based on the Radon transform and DRBEM formulation. They presented examples with a domain of anisotropic media and compared the solution with the analytical models. Extensive static analysis on modelling polycrystalline materials was presented by Benedetti and Aliabadi in [2,5] using the anisotropic elastostatic Greens functions based on Fourier transform, as presented by Wilson and Cruse [32]. The two main differences are presented herein: first, the application of dynamic boundary conditions on artificial polycrystalline materials with randomly oriented grain crystal planes; second, the use of an anisotropic fundamental solution based on double Fourier series, as proposed by Tan et al. [14].

In this paper, a new computational framework for the dynamic analysis of 3D hexagonal (HCP) and cubic (BCC/FCC) anisotropic polycrystalline materials is presented. Dynamic simulations using step, ramp, and harmonic loads are carried out. In order to validate these dynamic models, in the absence of analytical solutions for anisotropic media, comparisons with isotropic macroscale dynamic models are presented, using the effective Youngs moduli. These isotropic models and effective elastic properties are available in the literature. The convergence of this model depends on the (large) number of crystal aggregates included in the microscopic model. In the case of polycrystalline materials, isotropic behaviour is achieved when the number of grains is large. This leads to high computational requirements for the simulations. Owing to the large number of DOFs of this physical model, distributed memory architecture is used with MPI parallelisation.

2. Material modelling

Polycrystalline materials are composed of random morphology grains or crystals with each grain having an individual crystalline orientation at microscale. The grain medium is modelled as a linear elastic anisotropic material such as metallic or ceramic crystalline materials. Artificial polycrystalline morphologies are generated and discretised to model the overall dynamic behaviour from a set of stochastic distributed material properties [1–3,33]. In this work, a boundary element mesh was generated following the scheme initially proposed in [2] using three-node discontinuous boundary elements to discretise the structure; the C++/C description algorithm can be found in detail in [33].

Dynamic simulations are carried out for zinc, copper, and iron. The anisotropic elastic constants and mass density values of these materials at microscale are presented in Table 1.

As suggested by Fritzen et al. [4], Euler rotation angles and convention $(z-x-z)$ are implemented to obtain stiffness tensor $\mathbf{C}$ at specific orientation, and the angles are generated using a uniform distribution from 0° to 360°.

3. Dynamic BEM formulation

Three-dimensional anisotropic problems of elasticity are analysed using the boundary element formulation for dynamic loading. General anisotropic solids are modelled using the displacement fundamental solution based on double Fourier series proposed by Tan et al. [14]. In this case, a multidomain algorithm is used to assemble the overall system of equations of the polycrystalline structure. The boundary integral equation expresses the relationship between displacements u_i and traction t_i on a surface Γ using known fundamental solutions for displacements $U_{ik}(\mathbf{x}',\mathbf{x})$ and traction $T_{ik}(\mathbf{x}',\mathbf{x})$. For a homogeneous elastic body, the boundary integral equation (BIE) considering the body forces on the domain Ω is given by

$$c_{ik}(\mathbf{x}')u_i(\mathbf{x}') + \int_\Gamma T_{ik}(\mathbf{x}',\mathbf{x})u_i(\mathbf{x})\,\mathrm{d}\Gamma = \int_\Gamma U_{ik}(\mathbf{x}',\mathbf{x})t_i(\mathbf{x})\,\mathrm{d}\Gamma - \int_\Omega \rho\ddot{u}_i U_{ik}(\mathbf{x}',\mathbf{x})\,\mathrm{d}\Omega, \tag{1}$$

where $(\mathbf{x}')$ and $(\mathbf{x})$ are the source and field points, respectively; $c_{ik}(\mathbf{x}')$ is $\delta_{ik}/2$ for a smooth surface boundary at the source point; ρ is the mass density. For transient analysis, the body forces are caused by the acceleration field $\ddot{u}_i$.

3.1. DRBEM formulation

To model the dynamic effects, the response of the displacement field is obtained in the time domain. In order to develop this dynamic analysis, it is necessary to transform the domain integral into a boundary integral by applying the dual reciprocity formulation as presented by Kögl and Gaul [18,19]. The domain integration in Eq. (1) can be represented as

$$\rho\ddot{u}_i = \sum_{m=1}^{M} f_{ik}^m(x)\alpha_i^m, \tag{2}$$