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A domain decomposition approach for the simulation of fracture phenomena in polycrystalline microsystems

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Highlights

- Fracture processes in polycrystalline solids under dynamic loading are considered.
- A new domain decomposition algorithm is proposed.
- Strategies for the spatial domain decomposition are proposed.
- The proposed algorithm is validated through the numerical simulation of known results.
- Real cases of microsystems fracture processes are simulated and discussed.

Abstract

In this work, a domain decomposition technique is proposed to reduce the computational burden of three-dimensional numerical analyses of fracture processes in polycrystalline solids under dynamic loads. The material considered is polysilicon, which is the most widely employed structural material for Micro-Electro-Mechanical Systems (MEMS).

The algorithm extends the proposal of Gravouil and Combescure (2001) to fracture processes involving the presence of discrete cracks propagating both inside the sub-domains and across the interfaces between neighbouring sub-domains. The case of brittle or quasi-brittle fracture is addressed by means of a cohesive approach. Alternative choices for the spatial subdivision strategy are compared. Numerical examples concerning known fracture tests are used for validation. Two applications to real MEMS are presented.

Keywords: Quasi-brittle fracture; Polysilicon; Cohesive crack; MEMS; Domain decomposition

1. Introduction

This work focuses on a domain decomposition approach to the 3D finite element simulation of crack initiation and propagation in polycrystalline materials via a cohesive methodology. The main application is the numerical modelling

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of the mechanical behaviour of polycrystalline silicon in microsystems. Polysilicon displays indeed a quasi-brittle behaviour at room temperature: consequently, as underlined in [1] and [2], the reliability of microsystems is often affected by rupture phenomena, due for instance to impacts or accidental shocks. In particular, the analysis refers to the microscale level, i.e. to the microstructural parts composing the MEMS device, which may be subjected to local failure phenomena.

Polysilicon is an aggregate of mono-crystalline silicon grains, whose overall behaviour is sensibly influenced by the mechanical properties of the grains and of the grain boundaries, by their shape and orientation. At this scale, the overall behaviour is strongly influenced by the material microstructure and the models have to take into account the presence of heterogeneity, interfaces between grains and micro-cracks. Consequently, any computational model for the prediction of its microscale behaviour must properly reproduce the grain morphology and the grain boundaries, which strongly influence the resulting mechanical response. As a result, a very refined discretization is required to reproduce the grain geometry. The computational burden of a traditional finite element simulation of the mechanical response of polycrystalline solids, under impact dynamics and in the presence of crack-propagation, is indeed very high, especially in the three dimensional case: the explicit time step is ruled by the Courant–Friedrichs–Lewy (CFL) condition and it could be very small, since a very refined spatial discretization is often required to properly mesh the grain boundaries and to solve the cohesive process zone.

A domain decomposition technique, described in the following section, is proposed in this work to overcome this limitation. The basic idea of domain decomposition techniques, as suggested by the name itself, lies in the subdivision of the global domain into subdomains to be solved separately and then reconnected by interface conditions. These approaches naturally apply to the solution of problems of great size; their goal is indeed to significantly increase the computational efficiency of the numerical simulations. The algorithm here described starts from the dual Schur's domain decomposition method for the solution of the dynamic problem, developed by Gravouil and Combescure [3] and Mahjoubi et al. [4], as an extension of the Finite Element Tearing and Interconnecting Method (FETI), originally proposed by Farhat and Roux [5] for the multi-domain and parallel solution of the elastostatic problem. In the literature, domain decomposition techniques have been recently applied e.g. by Lloberas-Valls et al. [6] and by Pebrel et al. [7] to the study of localized damage phenomena under static loading conditions and by Kerfriden et al. [8] to the analysis of delamination in composite materials. A survey of the state of the art on domain decomposition methods can be found in [9] and in [10]. The introduction of a domain decomposition approach allows for a sensible reduction of the number of degrees of freedom for each subdomain with respect to those of the whole domain and for a more efficient handling of the time integration, thus reducing the computational burden. The aims are to exploit smaller sub-problems and to overcome the time-step limits encountered with the standard description in an explicit dynamic scheme (i.e. the CFL condition).

The present paper contains a comprehensive description of the domain decomposition approach for fracture propagation in polycrystalline solids that has already been partially described in [11] with specific reference to microsystems applications. The proposed approach includes: the use of a Voronoi tessellation algorithm for the reproduction of the polycrystalline micro-structure; interface, cohesive laws for the description of fracture processes; dynamic insertion of interface Finite Element (FE) and relevant topology modification of the FE mesh; a new domain decomposition multi-time step strategy that allows for fracture propagation inside, at the boundary at across sub-domains; various strategies for domain partition. In the literature, cohesive models were extensively used for the numerical simulation of the mechanical fracture properties of microstructured materials with different numerical techniques [12–18].

The paper is organized as follows. In Section 2 the reference problem is introduced; Section 3 is devoted to the description of the proposed algorithm. Various partition techniques are discussed in Section 4. Section 5 contains a collection of numerical examples; closing remarks are proposed in Section 6.

2. Reference problem

The reference problem, shown in Fig. 1, can be formulated considering a continuum three-dimensional body Ω crossed by a propagating discontinuity surface Γ_c and subjected to dynamic loading conditions. The outer boundary of the body is partitioned into two portions $\partial\Omega_f$ and $\partial\Omega_d$, such that $\partial\Omega_d \cap \partial\Omega_f = \varnothing$ and $\partial\Omega_d \cup \partial\Omega_f = \partial\Omega$: surface forces $\mathbf{f}$ and displacements $\bar{\mathbf{u}}$ are assigned respectively on $\partial\Omega_d$ and $\partial\Omega_f$. Body forces, collected in the vector $\mathbf{b}$, are assigned in $\Omega\backslash\Gamma_c$. The two flanks of the crack are referred to as Γ_c^+ and Γ_c^-.