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Overcoming the limitations of distinct element method for multiscale modeling of materials with multimodal internal structure ☆

Evgeny V. Shilko [a,b,*], Sergey G. Psakhie [a,c,d], Siegfried Schmauder [e], Valentin L. Popov [f], Sergey V. Astafurov [a,b], Alexey Yu. Smolin [a,b]

[a] Institute of Strength Physics and Materials Science SB RAS, Tomsk 634055, Russian Federation
[b] Tomsk State University, Tomsk 634050, Russian Federation
[c] Tomsk Polytechnic University, Tomsk 634050, Russian Federation
[d] Skolkovo Institute of Science and Technology, Skolkovo 143025, Russian Federation
[e] Materials Testing Institute, University of Stuttgart, Stuttgart D-70569, Germany
[f] Institute of Mechanics, Berlin University of Technology, Berlin D-10623, Germany

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ABSTRACT

This paper develops an approach to model the deformation and fracture of heterogeneous materials at different scales (including multiscale modeling) within a discrete representation of the medium. Within this approach, molecular dynamics is used for the atomic-scale simulation. The simply deformable distinct element method is applied for simulating at higher length scales. This approach is proposed to be implemented using a general way to derive relations for interaction forces between distinct elements in a many-body approximation similar to that of the embedded atom method. This makes it possible to overcome limitations of the distinct element method which are related to difficulties in implementing complex rheological and fracture models of solids at different length scales. For an adequate description of the mechanical behavior features of materials at the micro- and mesoscales, two kinds of models that consider grain and phase boundaries within the discrete element framework are proposed. Examples are given to illustrate the application of the developed formalism to the study of the mechanical response (including fracture) of materials with multiscale internal structure. The examples show that the simply deformable distinct element method is a correct and efficient tool for analyzing complex problems in solid mechanics (including mechanics of discontinua) at different scales.

1. Introduction

Currently, the design of advanced materials is in many respects based on theoretical results obtained with computer simulation. The necessity for computer simulation in modern materials science and mechanical engineering has promoted a rapid development of numerical methods and generated a need for the development of methodologies and approaches of multiscale modeling of material deformation and fracture. In the last years, multiscale modeling has evolved into an independent line of computer-aided research and design of materials, which has greatly influenced the development of computational methods and led to the development of various combined numerical techniques [1–4]. Despite a significant difference in various multiscale modeling approaches, all of them are similar in that they take into account (explicitly and implicitly) the contribution of deformation mechanisms of spatial and structural scales, lower with respect to the considered one, to the mechanical response of the material at the considered scale (this assumption is called the structure–property paradigm [1]). This actually means the requirement for taking into account the internal structural and rheological features of basic structural elements at different scales, first of all, at the nano- and microscale. The basic elements of the internal structure are not only grains and inclusions of other phases but also interfaces between them and discontinuities whose deformation ability and evolution play a crucial role for a wide range of materials, primarily, nanostructured materials.

The whole family of various methods that take into account the hierarchy of structural scales on the mechanical response of the material can be arbitrarily divided into two types (methodologies). The first one is based on decomposing a problem into fine and

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* Corresponding author at: Institute of Strength Physics and Materials Science SB RAS, Tomsk 634055, Russian Federation. Tel.: +7 3822 286971; fax: +7 3822 492576.
E-mail address: shilko@ispms.tsc.ru (E.V. Shilko).

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coarse scales [2]. The practical implementations of this methodology as a rule reduce to two-scale methods and models. These are, particularly, the variational multiscale method proposed by Hughes et al. [5] and different multigrid methods including combined techniques in which a system is divided into domains with different discretization step modeled with the use of different numerical methods (finite element method, molecular dynamics method, discrete element method, etc.) [6–9]. The second, most widely adopted methodology implies the determination of a hierarchy of basic structural scales in the modeled material and determination of a representative volume or a system of representative volumes with qualitatively different structural and phase composition on each scale [10–14]. The representative volume of a considered scale must contain a sufficient number of structural elements of this scale for correct subsequent homogenization. Numerical results on the mechanical response of the representative volume are used to determine its integral mechanical properties, including the equation of state and its parameters, the fracture criterion and fracture parameters, and so on. These parameters are taken as input parameters (response parameters of discretization units) on a higher scale. Consistent implementation of the given procedure starting from the atomic or nanoscale yields the construction of micro-, meso- and macroscale models of solids with multiscale internal structure. It should be noted that this methodology is based on two essential approximations. The first one implies a unique relation between characteristic sizes of the internal structure elements on a considered scale and characteristic times of accommodation/relaxation processes of this scale. The second approximation implies that energy thresholds of activation of deformation mechanisms depend uniquely on their spatial scales. Today, there are different practical implementations of the discussed methodology. The most rigorous and advanced implementations take into account the kinetics of deformation, including relaxation, processes on lower scales through the introduction of additional input parameters (internal variables) governed by special evolution equations [13,15].

Despite different formalisms of different approaches, a common problem of multiscale modeling is the different representation of the medium in numerical methods applied for modeling at different scales. For example, the integral properties of the atomic and nanoscale representative volumes are determined using molecular dynamics and molecular mechanics methods, Monte-Carlo method and others. These methods are based on a discrete description of solids. At the same time, multiscale modeling of materials on higher spatial and structural scales is conventionally performed using continuum mechanics methods (finite element and finite difference methods). Different concepts of the medium representation result in qualitatively different formalisms of these numerical methods, particularly, different formulation of equations of motion and state. The question naturally arises whether it is possible and efficient to perform numerical modeling of material deformation and fracture on all scales using numerical methods that refer to a unified (discrete) concept of the medium representation. The importance of this question is particularly related to the necessity of taking into account the evolution of different-scale initial discontinuities (cracks and damages) and new discontinuities formed under deformation. A large group of problems in which a direct description of discontinuous (discrete) structure of a considered medium at different scales is crucial for obtaining an adequate solution has been called the mechanics of discontinua [16]. The necessity of describing a solid as a multiscale discontinuous (discrete) system led to the development of a broad class of "discrete" numerical methods based on the representation of the medium as an ensemble of interacting particles (currently these methods are called particle-based) [17–24]. The principal difference of these methods from computational methods in continuum mechanics is the replacement of a continuous representation of the material or medium by an ensemble of interacting point masses (at the atomic scale within the framework of molecular dynamics or Monte-Carlo method) or by an ensemble of interacting particles of finite size (at higher spatial scales). The difference in the medium representation within continuum and discrete concepts determines differences in governing and balance equations. In particular, in explicit formulation conventional equations of motion of continuum are replaced by ordinary differential equations (for translations and rotations) governing the evolution of a particle ensemble. Relations between local stresses and strains or their time derivatives are replaced by expressions for potentials/forces of particle–particle interaction. One of the most important consequences of these features of particle-based methods is an inherent ability of discrete domains (particles) to change surroundings. This makes "discrete" numerical methods extremely attractive for direct modeling of complicated fracture-related processes at different spatial and structural scales up to the macroscale [16,18,22,25–27].

Well-known numerical methods widely applied for problem solving in the mechanics of discontinua are discrete element methods (DEM). The term DEM implies a large group of modeling techniques that treat a solid as an ensemble of deformable or rigid bodies of arbitrary shape [16–21,24,27–31]. The main differences between various representatives of the DEM group are in the principles of formulation of motion equations and in the approximations to the description of element deformability. There are two approaches to formulate the motion equations of discrete elements: implicit (represented by discontinuous deformation analysis) and explicit [29,31]. In the framework of the first approach motion equations are written for all the elements in matrix form and solved simultaneously using corresponding methods for solving of sets of linear/nonlinear algebraic equations. In the second approach, which is used in this paper, motion equations are written and solved "individually" for each element.

Various representatives of the group of explicit discrete element methods differ in the approximations used to describe (i) strain distribution in the bulk of discrete element, and (ii) influence of shape/geometry of the element on its kinematics and interaction with surrounding [31]. In particular, for discrete elements of complex shape, conventionally approximated by generally shaped polygons or polyhedrons, the motion equations for rotational degrees of freedom has a complex form. Besides, presence of vertices and edges for such elements lead to separation of the interaction with surrounding into several types (vertex–vertex, vertex–face, vertex–edge, edge–edge, etc.) [31]. Such details are of principle for modeling blocky and granular materials and media. At the same time, use of polygonal shape of discrete elements in modeling consolidated materials with complex internal structure (polycrystals, composites) at the mesoscopic scale results in some limitations for spatial discretization. In particular, a polygonal element is correct structural model for separate grain or phase inclusion. However, modeling grain/inclusion by ensemble of interacting polygonal elements may lead to generation of artificial effects. That is why simplified elements are mainly used in DEM-based modeling of consolidated polycrystal and multiphase materials at mesoscopic scale. In the framework of this approach it is assumed that interaction between discrete elements occurs on plane faces (face–face interaction). The size of face is chosen based on the local packing of elements so that imaginary polygons (obtained by connecting the vertices of the plane faces) fill the space without voids (or produce required fraction and shape of the voids). The effect of vertices and edges is usually neglected here. One representative of such simplification of element geometry is its interpretation as equivalent circular disc (in 2D problem statement) or sphere [29–31] (obviously, that is applicable for