Available online at www.sciencedirect.com

ScienceDirect

Defence Technology 11 (2015) 18–34

www.elsevier.com/locate/dt

Modeling mechanical behaviors of composites with various ratios of matrix–inclusion properties using movable cellular automaton method

A.Yu. SMOLIN [a,b,*], E.V. SHILKO [a,b], S.V. ASTAFUROV [a,b], I.S. KONOVALENKO [a], S.P. BUYAKOVA [a,b,c], S.G. PSAKHIE [a,c,d]

[a] *Institute of Strength Physics and Materials Science SB RAS, Tomsk 634021, Russia*
[b] *Tomsk State University, Tomsk 634050, Russia*
[c] *Institute of High Technology Physics, Tomsk Polytechnic University, Tomsk 634050, Russia*
[d] *Skolkovo Institute of Science and Technology, Skolkovo 143025, Russia*

Received 7 June 2014; revised 14 August 2014; accepted 25 August 2014
Available online 4 December 2014

Abstract

Two classes of composite materials are considered: classical metal–ceramic composites with reinforcing hard inclusions as well as hard ceramics matrix with soft gel inclusions. Movable cellular automaton method is used for modeling the mechanical behaviors of such different heterogeneous materials. The method is based on particle approach and may be considered as a kind of discrete element method. The main feature of the method is the use of many-body forces of inter-element interaction within the formalism of simply deformable element approximation. It was shown that the strength of reinforcing particles and the width of particle-binder interphase boundaries had determining influence on the service characteristics of metal–ceramic composite. In particular, the increasing of strength of carbide inclusions may lead to significant increase in the strength and ultimate strain of composite material. On the example of porous zirconia ceramics it was shown that the change in the mechanical properties of pore surface leads to the corresponding change in effective elastic modulus and strength limit of the ceramic sample. The less is the pore size, the more is this effect. The increase in the elastic properties of pore surface of ceramics may reduce its fracture energy.

Keywords: Composites; Metal ceramics; Zirconia ceramics; Gel; Modeling; Movable cellular automata; Many-body interaction

1. Introduction

Composites are widely used in industry and nature. Usually the composites consist of matrix, which constitutes the main part of the material, and a large number of small sized inclusions. Inclusions, as a rule, have higher physical and mechanical properties and are designed to improve the useful properties of composites. Typical examples are dispersion-reinforced materials and, in particular, metal–ceramic composites [1]. The availability of hard inclusions allows producing the ultra-hard materials for cutting tools, and the antifriction and protecting materials for aircraft building [2], etc. In case of porous materials, the void “inclusions” provide high heat-insulating properties and low specific density [3–5].

Composites consisting of hard matrices with soft inclusions are not practically used in industry. As an exception, we can refer to metal–ceramics for self-lubricated bearings, which are produced by sintering of mixture of iron and carbon powders followed by oil saturation. Much more such materials exist in nature, first of all as fluid-saturated geological media and bone tissues of animals and man.

* Corresponding author. Institute of Strength Physics and Materials Science SB RAS, Tomsk 634021, Russia.
E-mail address: asmolin@ispms.tsc.ru (A.Yu. SMOLIN).
Peer review under responsibility of China Ordnance Society.

http://dx.doi.org/10.1016/j.dt.2014.08.005

It has to be noted that the properties of a composite are often determined by the properties of the components and the fraction of inclusions. They also depend on the size and shape of inclusions as well as the properties of matrix–inclusion interface in a complicated way [6–8]. That is why the problem of composite modeling is very difficult and complex.

An important trend in mechanics of composite is to develop and apply the numerical methods to study the dynamics and peculiarities of mechanical behavior of heterogeneous materials and structures under complex loading conditions. The advantages of numerical modeling in comparison with analytical solutions are associated with the ability to consider complex geometry of the system, to take into account heterogeneous structure of the material as well as to study in details the dynamics of fracture and the related processes of redistribution and dissipation of elastic energy in the surroundings of the crack. At the same time, these advantages make strong demands for the formalism of applied numerical methods.

The most of research on computational mechanics are performed using finite element method. This method belongs to continuum concept in mechanics, i.e., it assumes that the state controlling variables distribute in space continuously. At the same time for modeling the severe distortion and failure of a material, converting finite elements into particles is more effective and promising [9]. In Ref. [10], so-called meshless (or mesh free) method were used for this purpose (namely smoothed particle hydrodynamics and generalized particle algorithms). Strictly speaking, meshless methods are not pure particle ones. They just use the scattered nodes associated with the centers of finite volumes to discretize the continuum mechanics equations in space, i.e., they are really based on continuum approach. Concerning the problem of modeling heterogeneous media, it should be noted that at least 3–5 meshless particles are required to represent a matrix–inclusion interface. A true particle method can describe this interface using just one particle. The principal difference of particle methods from computational methods in continuum mechanics is to replace the continuous representation of a material with an ensemble of interacting particles (at micro-, meso- or macroscopic scale) or point masses (at the atomic scale within the framework of molecular dynamics or Monte-Carlo method). This in turn determines the difference in governing equations as well. In particular, the conventional partial differential equations of continuum mechanics are replaced by Newton–Euler equations governing the motion of discrete ensemble. Constitutive laws for the considered material in tensor form, which conventionally describes the relationship between local stress and strain or their time derivatives, therewith are replaced by the potentials/forces of inter-particle interaction. One of the most important consequences of these features of particle-based methods is an inherent capability of the discrete objects (particles) to change their surroundings (interacting neighbors). This feature makes "discrete" methods extremely attractive for direct modeling of complicated fracture-related processes including multiple fracture accompanied by formation and mixing of large number of fragments [11–17].

The key points determining the behavior of an ensemble of simple deformable discrete elements are the structural form of the expressions for central and tangential interaction between elements and the relationship between these expressions and constitutive law of the modeled material. A conventional approach is based on the use of pair-wise elastic interaction forces which can be treated as springs between elements. Corresponding value of the spring stiffness is derived on the assumption that strain energy stored in a unit cell of deformed element ensemble is equal to the associated strain energy of the equivalently deformed continuum [18,19]. An approximation of pair-wise interaction has a number of important limitations, among which are the following: i) maximum value of Poisson's ratio of element ensemble depending on packing of elements; ii) packing-related artificial anisotropy of mechanical response of the ensemble; iii) fundamental problems in correct simulation of irreversible strain accumulation in ductile materials.

Our research shows that many of these problems can be solved by using many-particle interaction [20–22]. Note that the construction of such relations becomes possible due to using a hybrid computational technique to combine the mathematical formalisms of discrete elements and cellular automata [23]. Many-body formulation of inter-element forces is adopted from the Wiener–Rosenblueth model of cellular automaton interaction [23,24]. This hybrid technique is referred to as movable cellular automaton method (MCA) [21,22,25,27]. The proposed generalized expression for inter-element forces is the ability to establish the relationship between vector parameters of the interaction and tensor parameters of the material constitutive law. It makes possible to implement different models and criteria of elasticity, plasticity and fracture within the mathematical formalism of MCA.

This paper is devoted to the computational study of composite materials consisting of matrix and equiaxial inclusions using MCA method. The main peculiarity of the considered composite is the ratio of mechanical properties of the matrix and inclusions that varies in a wide range. First, we study the classical dispersion-reinforced material based on the example of metal ceramics. Then the porous ceramics with soft gel inclusions are considered. In the last case, the inclusion rigidity is much less than the matrix one. The main attention of the study is paid on the influence of properties and width of inter-phase boundaries on the effective mechanical properties of the composites.

2. Method of movable cellular automata

Within the frame of MCA, it is assumed that any material is composed by a certain amount of finite size elementary objects (automata) which interact among each other and can rotate and move from one location to another, thereby simulating a real deformation process. The automaton motion is governed by the Newton–Euler equations