Advances in Engineering Software 77 (2014) 1–12

Contents lists available at ScienceDirect

Advances in Engineering Software

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

An efficient numerical model for investigating the effects of anisotropy on the effective thermal conductivity of alumina/Al composites

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ARTICLE INFO

Article history:
Received 16 April 2014
Received in revised form 19 June 2014
Accepted 5 July 2014
Available online 1 August 2014

Keywords:
Composite materials
Thermal conductivity
Granular systems
Fast Fourier transform method
Numerical homogenization
Discrete Elements

ABSTRACT

The paper describes an efficient numerical model for better understanding the influence of the microstructure on the thermal conductivity of heterogeneous media. This is the extension of an approach recently proposed for simulating and evaluating effective thermal conductivities of alumina/Al composites. A C++ code called MultiCAMG, taking into account all steps of the proposed approach, has been implemented in order to satisfy requirements of efficiency, optimization and code unification. Thus, on the one hand, numerical tools such as the efficient Eyre–Milton scheme for computing the thermal response of composites have been implemented for reducing the calculation cost. On the other hand, statistical parameters such as the covariance and the distribution of contact angles between particles are now estimated for better analyzing the microstructure. In the present work we focus our investigations on the effects of anisotropy on the effective thermal conductivity of alumina/Al composites. First of all, an isotropic benchmark is set up for comparison purposes. Secondly, anisotropic configurations are studied in order to direct the heat flux. A transversally isotropic structure, taking benefit of wall effects, is finally proposed for controlling the orientation of contact angles. Its thermal capabilities are related to the current issue of heat dissipation in automotive engine blocks.

1. Introduction

Thermal management of automotive engine blocks is a key issue on which depends the durability of certain polymer parts, electronic devices and embedded software which are more exposed to high temperatures. Recent European Union legislations restrict pollutant emissions of light vehicles. As a result, a reshape of engine block has become necessary in order to meet the new European standards. Engine downsizing is the most natural solution for reducing CO_2 emissions but this requires a boosting device (such as a turbocharger or a supercharger) and a direct injection technology for maintaining the capacity of the engine block. Resulting heat stresses are sizeable and new materials are required for dissipating the heat flux. Recently, a manufacturing process was developed for elaborating alumina/Al composites with enhanced thermal capabilities [1]. The process is based on the method introduced by Descamps et al. [2,3] for the synthesis of organic porogen materials. Alumina/Al composites are composed of a ceramic phase which ensures the insulating character while the thermal conduction is ensured by aluminum spherical particles. Thus, such a composite could well be a potential candidate for the thermal management of engine blocks. However, the manufacturing process leads to near-isotropic materials which are not able to direct the heat flux and manage the temperature gradient. That is why some solutions have to be found for modifying the elaboration of Alumina/Al composites in such a way as to generate directional effects. Different strategies are available for this purpose including functionally graded materials [4–7], and the control of the orientation of contact angles between particles according to specific loadings or modes of deposition [8]. This paper targets the last option.

In a previous work, a numerical model was set up for predicting the effective thermal properties of alumina/Al composites [1]. On the one hand this approach uses the discrete element method (DEM) for reproducing the sedimentation process leading to the generation of granular systems composed of spherical aluminum particles. On the other hand, effective conductivities are assessed using the Finite Element Method (FEM). The model was initially used for investigating the influence of morphological and phenomenological parameters such as interconnection sizes, interfacial debonding and granulometry. Results confirmed the critical impact of the two first but no granulometry effect was exhibited. A C++ code called MultiCAMG is currently being developed for the generation and the analysis of granular systems using the numerical approach of Ferguen et al. [1]. The code satisfies some needs of efficiency, optimization and code unification, which are not met by the use of

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http://dx.doi.org/10.1016/j.advengsoft.2014.07.004
0965-9978/

a number of commercial software applications. It takes into account all steps of the numerical approach, namely the generation of granular systems, the discretization and the evaluation of the Effective Thermal Conductivity (ETC). It also permits the connection with other codes or softwares such as R one for statistical analysis purposes [9]. The lack of efficiency of the FEM leads us to consider the well-established Fast Fourier Transform (FFT) based method [10,11] as an alternative way for evaluating effective properties. Efficient voxelization methods [12] have been adapted and used for handling such an approach using the fast Eyre–Milton scheme [13].

In the present work, our objectives are twofold. First, we extend the numerical approach of Ferguen et al. [1] to FFT-based methods and statistical analysis using MultiCAMG. Two kinds of systems are considered, namely random packings composed of unpenetrable hard spheres, and granular systems composed of partially penetrable spheres for which overlappings are enabled and controlled. We investigate effects of the volume fraction of spherical particles, the orientation of contact angles and the distribution of particles on the ETC of alumina/Al composites. An isotropic configuration is set up for comparison purposes. We assume the material to be isotropic when the distribution of particles and the orientation of contact angles are statistically independent of the orientation of chosen axes [8]. Furthermore, in the case of random packings, the volume fraction of spherical particles is set to 0.64 which approximately corresponds to the random close packing (or maximally random jammed packing) for monodispersed spherical particles [14–18]. Several numerical and statistical tools such as the covariance [19] and the radial plot [8,20] are set up and used for better characterizing the granular system in such a context. ETC are estimated by FFT and reference graphs are plotted as well. Secondly, anisotropic configurations are studied with the same numerical and statistical tools. Some lattice structures are investigated and compared to the isotropic system. A composite composed of chains of aligned particles is also described and analyzed. Such a structure is transversally isotropic and thus has a higher thermal conductivity along the preferred axis. However this is particularly difficult to design. That is why, finally, a more realistic methodology is proposed for controlling the orientation of contact angles using inner walls in order to take benefit of wall effects [21]. Parametrization, ETC and capability to direct the thermal flux in this framework are discussed, and related to the issue of thermal management in engine blocks.

The paper is outlined as follows. First, we list the various steps in the manufacturing process. A third section is then dedicated to the numerical approach and MultiCAMG code. The fourth section describes the setting up and the investigation of isotropic granular systems. The last part deals with anisotropic configurations and gives the results of the proposed approach for controlling the orientation of contact angles.

2. Manufacturing process

The process used for manufacturing a composite with graded microstructure is based on the porogen organic agents method developed by Descamps et al. [2,3] for the synthesis of macroporous β-tricalcium phosphate. The main idea of the technique consists of creating an alumina foam with controlled macroporosity, and infiltrate it with a melt aluminum alloy. Pore and interconnection sizes are critical in determining the properties of the final composite material. The main steps of the process are described below.

2.1. Producing of the organic frame

A polymeric scaffolding composed of polymethylmethacrylate particles (PMMA) is used as precursor foam. The granular system is composed of spherical particles with fixed granulometric distribution. Particles are chemically stuck within a metallic mold using a solvent and by squeezing the particle skeleton. The applied pressure slightly deforms the particles so that necks appear between PMMA particles [2,3]. Thus, the resulting network of spherical particles seems to be interconnected at contact points but no real overlapping arises here. The shrinkage of the granular system is measured by Scanning Electron Microscope (Hitachi S-3500N) in order to correlate the height of the bed to the pore interconnectivity of the organic frame.

2.2. Synthesis of the ceramic foam with controlled macroporosity

Before starting the impregnation, an alumina slurry is made from mixed powder with varied concentrations in the range of 65–75 wt.%. When the organic frame and the alumina slurry are ready the impregnation process is carried out. After drying, a debinding treatment is then used at low temperature (1 °C/min, 30 h at 200 °C). This allows PMMA particles to be removed and generate macroporous foam with open pores whose dimensions depend on interconnection sizes of PMMA particles. Subsequently, the ceramic foam is sintered (5 °C/min, 1 h at 1670 °C) until consolidation of the ceramic walls occurs [2,3].

2.3. Infiltration of the ceramic foam

The infiltration process of the melt aluminum inside the ceramic foam is achieved in vacuum condition with temperature held at 720 °C. The fluidity of the melt aluminum inside the foam strongly depends on the wetting properties of the ceramic surfaces. Magnesium is added to the aluminum alloy in order to enhance the fluidity of the melt alloy and improve the filling of pores.

Steps of the manufacturing process discussed above are summarized in a flowchart as shown in Fig. 1.

3. Numerical modeling

A C++ based code called MultiCAMG (Multifunctional Code for the Analysis and the Modeling of Granular Packings) has been implemented for simulation purposes. This enables the generation and the study of random systems composed of spherical particles using the Discrete Element Method (DEM) on the one hand. The program also estimates the ETC of composites using either FEM or FFT approach.

3.1. Generation of granular systems

The architecture of the alumina/Al composite is simulated considering a granular system composed of spherical particles. The particle skeleton is generated using the DEM which is a well-established approach to take into account both velocity of particles and inter-particle collisions [22,23]. A spring and dash-pot contact model is used to describe particle–particle and particle–wall collision. The normal force between two particles i and j in contact is given by Eq. (1) which allows small overlappings of rigid particles to occur at contact points. In Eq. (1) the shear component is neglected and no tangential displacement is considered.

$$F_n = K_n U_n + 2\sqrt{mK_n}V_n \tag{1}$$

where n is the unit normal vector to the contact plane. K_n and U_n are respectively the normal stiffness and the displacement in the normal direction. $2\sqrt{mK_n}$ is the critical damping constant and V_n is the relative velocity at the contact between particles i and j. In the case of a particle–particle contact, m is given by Eq. (2).

$$m = \frac{m_i m_j}{m_i + m_j} \tag{2}$$