

FEM modeling of structure and properties of diamond-SiC-(Al) composites developed for thermal management applications

P. Unifantowicz^{1, 2, a}, T. Boguszewski^{1, b}, Ł. Ciupiński^{1, c}, E. Fortuna^{1, d},
M. Lewandowska^{1, e}, S. Vaucher^{2, f} and K. J. Kurzydłowski^{1, g}

¹Warsaw University of Technology, Faculty of Materials Science and Engineering, Ul. Wołoska 141, 02-507 Warsaw, Poland

²EMPA - Swiss Federal Laboratories for Materials Testing and Research, Nanocomposites Processing Group, Feuerwerkerstrasse 39, 3604 Thun, Switzerland

^apaulina.unifantowicz@empa.ch, ^btboguszewski@inmat.pw.edu.pl, ^clukas@inmat.pw.edu.pl,
^delaf@inmat.pw.edu.pl, ^emalew@inmat.pw.edu.pl, ^fsebastien.vaucher@empa.ch,
^gkjk@inmat.pw.edu.pl

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Abstract

Thermal management materials frequently have multi-phase composite character with complex architecture of the constituents. As a result, design rules are needed which can be used in selection of the phases and optimizing their volume fractions. The study shows that such are provided by finite element modeling of these composites. This is demonstrated for a diamond-SiC-Si-(Al) composites, which have been optimized in terms of the volume fraction of SiC, contact area between the components and presence of open porosity.

Introduction

Worldwide research in the field of thermal management materials has led to development of high thermally conductive diamond-based composites. Among them, diamond-SiC have potentially a high thermal conductivity (>400 W/m/K), low density and, in contrast to the metal-based composites, CTE matched to the one of silicon [1].

These composites are produced in HTHP process [2], GPI or squeeze-casting [3], [4] and, more recently, by reactive microwave sintering [5]. The latter enables selective absorption of microwave energy by Si, preventing graphitization of diamond. The as-grown SiC provides a mechanical stability of the composite and a path for heat transport between the diamonds. However, the composites obtained by microwave sintering of Si and diamond powders are characterized by a complex structure, Fig. 1, which needs to be optimized for their industrial applications.

The goal of this work is to develop a model which could be used to predict the effective thermal conductivity of diamond-SiC-Si porous and infiltrated composites with varying microstructures. To this end, a finite element method (FEM) has been used with representative unit cell shown in Fig.2. The FEM is a universal tool which can be applied to problems with various types of load, including mechanical, thermal stresses [6] or heat [7] and this method was used in the current work.

Experimental

A representative cell was proposed basing on the microstructures of the diamond-SiC-Si composites. The materials were synthesised by pressure-less microwave sintering of a mixture of diamond and silicon powders at C/Si wt. ratio of 4/1. Open and closed porosity of the as-sintered composites of respectively 44 and 2 vol. % was obtained using pycnometer and the Archimedes method. The porous composites were subsequently infiltrated with aluminium by squeeze-casting. The composites microstructures are shown in Fig. 1. For verification of the phase composition energy-dispersive X-ray analysis (EDXA/EDS) was used. The SiC crystals having a cube-like

morphology occupy the diamonds faces next to remaining Si, the amount of which depends on the extent of the reaction between silicon and carbon.

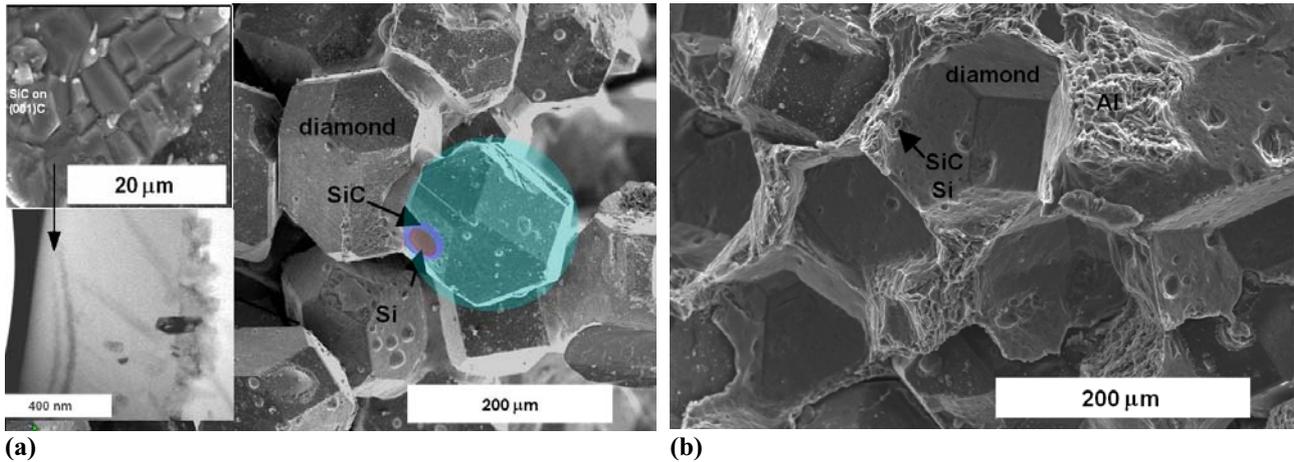


Fig. 1. SEM and TEM images of (a) porous and (b) Al-infiltrated diamond-SiC-Si composite

Thermal conductivity was modeled for a representative unit volume, RUV, of the composite in the form of a cubic cell with periodic boundaries. The diamond particles have been described as cut spheres linked by cylindrical bridges to six nearest neighbors. Fig.2 shows $\frac{1}{4}$ of the cell where a is the length of the side of the cube. This approach allows for flexibility in defining the dimensions of diamond, SiC and Si, without changing the size of the RUV. The FEM modelling of the thermal properties of RUV was carried out using Ansys. The thermal analysis was based on the heat balance equation obtained from the rule of energy conservation. The K_{eff} was obtained from the sum of heat fluxes through the voxels divided by the number of nodes. Steady state load conditions were used to obtain the temperature distribution in the modelled volume. The temperature gradient applied between the upper and lower plane of the RUV was of 2°C . The following values of thermal conductivity were assumed in the computations: $K_d = 2000$, $K_{SiC} = 420$, $K_{Si} = 130$, $K_{por.} = 0$, $K_{Al} = 230$ (W/m/K). The interfacial thermal resistance has been neglected for diamond-SiC interfaces.

The FEM model was used to study the apparent conductivity dependence on the following parameters: (1) relative amount of SiC and Si within the bridges linking diamonds ($V_d = \text{const}$), (2) volume fractions of the diamond, SiC, Si and in the porosity and (3) infiltration of the pores with aluminium.

Results and discussion

The FEM mesh of the representative cell and the temperature distribution are shown in Fig. 2. The dimensions: W , W_{SiC} and W_{Si} correspond to the diameter of the diamond face, SiC disc and absolute diameter of Si ring, respectively, Fig. 3(a). The values of effective thermal conductivity as a function of the SiC bridge width, W_{SiC} , the corresponding diamond/SiC interface area and relative volume fractions of the present phases are plotted in Fig. 4(a). Similarly, Fig. 4 (b) shows K_{eff} as a function of the width, W_{Si} , and interface area between diamond and the hybrid SiC-Si bridge. A schematic representation of Al-infiltrated composites structure with and without the SiC bridges connecting the diamonds is given in Fig. 3(b).

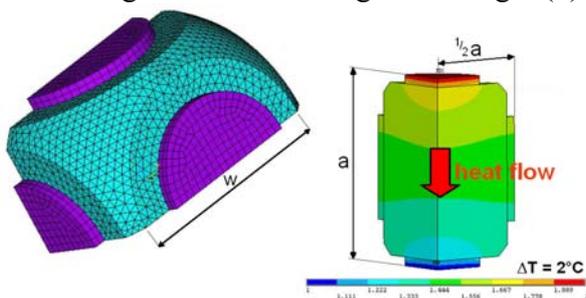
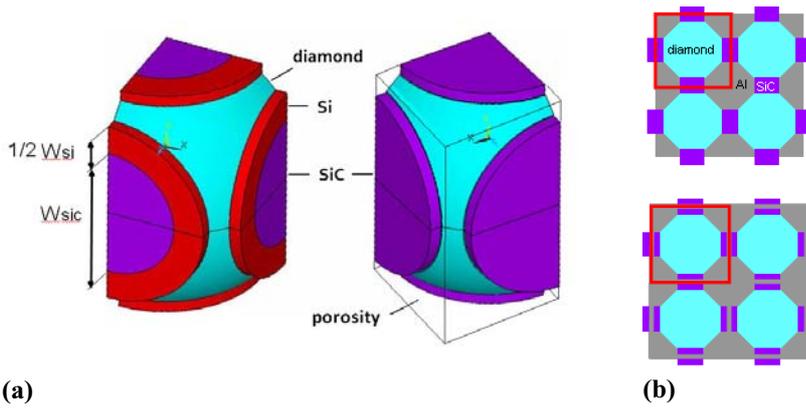
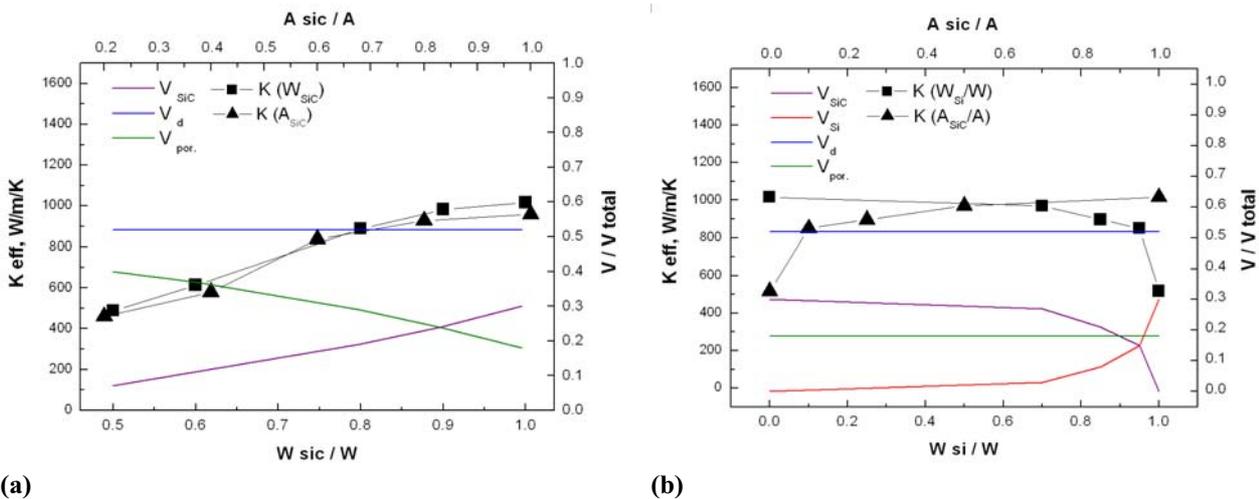


Fig. 2. FEM mesh and the temperature distribution across the representative unit volume.



(a) (b)
Fig. 3. (a) The representative cell with and without Si and (b) schematic illustration of the structure of diamond-SiC-Al composite with SiC bridges linking the diamonds and with disconnected diamonds

It has been computed that the effective conductivity of the diamond-SiC composite, D-SiC, gradually increases with the W_{SiC} and with the area of the SiC/diamond interface, A_{SiC} , Fig. 4(a). On the other hand, an increase of the volume fraction of Si substituting the SiC causes a decrease of the thermal conductivity in the Si-containing diamond-SiC composite, D-SiC-Si, Fig. 4(b). The low conductivity of silicon is limiting the effective conductivity of the composite. This implies that the content of Si must be minimized for heat sink applications.



(a) (b)
Fig. 4. Dependence of the thermal conductivity of K_{eff} on the width of SiC, W_{SiC} , and Si bridge, W_{Si} , the SiC-diamond interface area, A_{SiC} , and the volume of diamond, V_d , silicon carbide, V_{SiC} , silicon, V_{Si} , and porosity, V_{por} for: (a) diamond-SiC and (b) diamond-SiC-Si composite; $V_{total} = V_{cell} = a^3$

The K_{eff} calculated for the infiltrated and porous composites with varying amount of Si in the SiC-Si bridges are plotted in Fig. 5. One can see a decrease of K_{eff} with the Si volume in both composites. In the case of SiC comprising 100 vol. % of the bridge, the thermal conductivity of the porous diamond-SiC is similar to the conductivity of the infiltrated diamond-SiC-Al composite, Fig. 5.

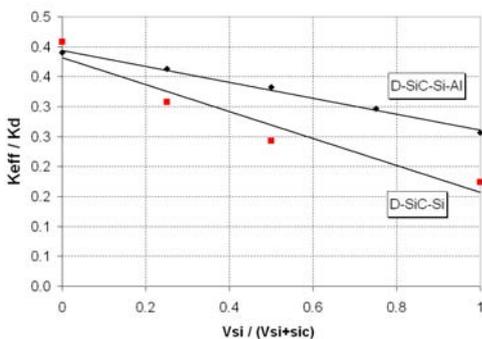


Fig. 5. Relative K_{eff} for the non infiltrated and Al-infiltrated diamond-SiC-(Si) composites as a function of Si content

SiC % bridge	Si % bridge	Al % cell	K_{eff} W/m/K
100	-	55, without SiC bridge	510
100	-	20, with SiC bridge	870
-	100	non infiltrated	600
50	50	non infiltrated	950

Table 1. The effective thermal conductivity of diamond-SiC-Si-(Al) composites for different RUV parameters

The results of the calculation reveal a strong contribution of high thermally conductive SiC to the total conductivity of the composite. The conductivity values obtained for various types of RUV are listed in Table 1. It can be noted that for disconnected diamond particles in aluminum matrix, Fig. 3(b), the conductivity is significantly lower than in the case where SiC is linking the diamonds. This rationalizes the design of a skeleton-like structure comprising diamonds connected by a well-conducting SiC rather than diamonds in a continuous Al matrix having a moderate thermal conductivity.

Summary

The FEM model allows for estimation of effective thermal conductivity of the diamond-SiC-(Si) composites as a function of the width of SiC bridges and interface area between diamond and SiC. The un-reacted silicon lowers the effective conductivity due to a three times lower thermal conductivity of Si (130 W/m/K) with respect to SiC (420 W/m/K). The K_{eff} obtained for the composite with bridges built of Si approaches 500 W/m/K. The same value of K_{eff} is obtained for the composites with bridges built of SiC with two time smaller volume. Infiltration with Al does not contribute to the increase the K_{eff} . The SiC on diamond works as an efficient heat path only when it percolates the entire structure. Finally, it can be pointed out that the results obtained here can be used to design new types of composites for industrial applications.

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