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FROM DIGITAL IMAGE OF MICROSTRUCTURE TO THE SIZE OF REPRESENTATIVE VOLUME ELEMENT: B_4C/Al COMPOSITE

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Abstract: In the field of micromechanics, the notion of representative volume element (RVE) and its quantitative definition are of the paramount importance. The definitions of RVE, used by scientists for different purposes, are mathematically strict but do not quantify its size. Furthermore, all the methods of RVE size determination (available in a voluminous literature) require a large number of numerical calculations like, for instance, those of finite element or other numerical techniques. In this paper, it is shown that the size of RVE can be evaluated based only on the morphology of microstructure that is involved in the statistical microstructure descriptor, namely the two-point correlation function. A methodology is applied to the digital image of the reconstructed 2D realization of the boron-carbide/aluminum (B_4C/Al) composite. The condition for the minimum size of RVE used in the numerical procedure has been formulated in previous work of authors. The size of RVE is determined for different values of estimation error and the contrast in phase properties. The method is verified by performing numerical calculations of effective thermal conductivity coefficient.

1. INTRODUCTION

The main goal of micromechanics is to evaluate the overall properties of random heterogeneous media based on the knowledge of both geometry and mechanical properties of phases which constitute the material. Due to the rapid development of computer techniques within the last 30 years numerical calculations regarding the effective properties determination have become accepted as the ones that provide the most accurate results. In the case of numerical approach, the process of effective properties evaluation – averaging process – takes place over statistically representative finite-sized sample of the material which is referred to as the representative volume element (RVE).

The RVE is usually regarded as a volume of heterogeneous body which is small enough from a macroscopic point of view and simultaneously large enough to contain a sufficient number of inhomogeneities. Some definitions of the RVE, used by scientists for different purposes, can be found in [3], [17]. Note that these definitions are usually mathematically strict; however, none of them provides precise information on its size, in other words, the definitions do not quantify the size of RVE.

A large number of attempts have been made in order to quantify the RVE on the basis of statistical and numerical analyses. GUSEV [6] used the Monte-Carlo (MC) simulations for the generation of statistically independent realizations of periodic elastic composite consisting of disordered non-overlapping spheres. The scatter in the

results, i.e., averaged properties, has been investigated. In [17], statistical calculations of numerical experiments have been performed to quantify the size of RVE for composites that consist of particles in a matrix material. Several criteria as well as statistical tool, namely the Student's *t*-distribution, have been taken into account in order to quantify the size of RVE. GITMAN [3] has proposed to quantify the RVE on the basis of the simple chi-square statistical criterion, whereas GRUFMAN and FERNAND [5] have developed the methodology based on the Kolmogorov goodness-of-fit test.

Evaluation of the size of RVE taking into account the microstructure morphology as well as estimation of the overall properties have been extensively studied in [1], [4], [13], [22]. KANIT et al. [9] have proposed the method of numerical determination of the size of RVE on the basis of the microstructural descriptor, namely the integral range (the definition of integral range can be found in [12]). The authors claimed that the size of RVE *must be considered as a function of five parameters: the physical property, the contrast of properties, the volume fractions of components, the wanted relative precision for the estimation of the effective property and the number of realizations of the microstructure associated with computations that one is ready to carry out*. The methodology has been verified in [10] where two materials from food industry have been considered. THOMAS et al. [18] focused on the determination of RVE for anisotropic composite with high-fiber volume fraction. Three different properties (fiber area fraction, pair correlation function, effective thermal conductivity) have been considered in order to establish the size of RVE.

In the previous paper of authors [15], an innovative procedure of RVE size determination for a particular type of random microstructure (two-phase random checkerboard) has been proposed. The condition for the minimum size of RVE has been formulated based on the properties of the two-point correlation function. This condition has been then generalized for the case of any two-phase microstructure in [14], [16]. What is remarkable, the method proposed utilizes only the morphology of microstructure contained within the two-point correlation function, and therefore, it gives the possibility of RVE size determination with no large number of numerical calculations – the numerical analyses like those of FE or other methods are not necessary.

It has been shown in [14]–[16] that in the methodology proposed, the size of RVE is directly associated with the number of random microstructure realizations. In other words, for the evaluation of the overall property, say effective thermal conductivity coefficient K^{eff}, a set of n independent microstructure realizations has to be considered. Therefore in what follows we introduce the notion of a sample. The sample is treated as a set of finite number n of RVE elements, each having the same finite size (figure 1). Then, the effective property K^{eff} can be estimated as the mean value averaged over the sample, i.e.:

$$K^{\text{eff}} \approx \overline{K} = n^{-1} \sum_{j=1}^{n} K_j, \tag{1}$$

where K_j is the property determined from the solution of the appropriate boundary value problem stated for the RVE_j, whereas n is the sufficient number of realizations (the size of the sample).

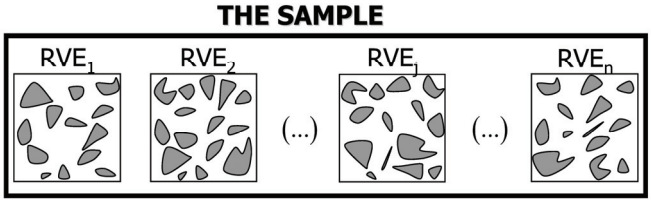

Fig. 1. The graphical illustration of the notion of the sample

In this paper, based on the condition proposed in [14], [16], a numerical procedure of RVE size determination from a digital image of microstructure is proposed. It has to be emphasized that the procedure of RVE size evaluation is devoted to the case of thermal conductivity. The methodology is applied to the digital image of the reconstructed 2D realization of the B_4C/Al composite. The digital image is obtained by the two-point probability reconstruction procedure. It is shown in the paper that the size of RVE depends on the value of estimation error, the volume fraction of phases as well as the contrast in phase properties (conductivities). The methodology proposed is verified by performing numerical calculations of effective thermal conductivities for different values of both estimation error and the contrast in phase properties.

The paper is organized as follows. In Section 2, a short description of the boron carbide/aluminum composite microstructure is provided. Next, the condition for the minimum size of RVE with respect to overall thermal conductivity is presented. Section 4 describes the procedure of the two-point correlation function evaluation. A Monte Carlo approach of the two-point correlation function integration is outlined in Section 5. The general scheme of RVE size determination procedure is outlined in Section 6. The RVE sizes for the microstructure of the B_4C/Al composite are provided in Section 7. Next, the results of numerical calculations validating the methodology proposed are presented. Final conclusions end the paper.

2. THE MICROSTRUCTURE OF BORON CARBIDE/ALUMINUM COMPOSITE

As mentioned in Section 1, the methodology of RVE size determination is applied to the digital image of the reconstructed 2D realization of the B_4C/Al composite. This microstructure has been obtained via the two-point correlation function reconstruction procedure – for more details the reader is referred to [20], [21].

Roughly speaking, the reconstruction process consists in finding such a realization for which the calculated two-point correlation function $S_2^{(i)}$ best matches the "target" two-point correlation function $\widetilde{S}_2^{(i)}$ (note that $S_2^{(i)}$ is two-point correlation function of the phase *i* [19]). The target function can be established, e.g., in the way of laboratory experiments or theoretical models.

Starting from some initial realization, preserving volume fractions of phases, the microstructure is evolved into $\widetilde{S}_2^{(i)}$ by minimizing the energy *E* which at any time step is defined as:

$$E = \sum_r [\widetilde{S}_2^{(i)}(r) - S_2^{(i)}(r)]^2, \tag{2}$$

where *r* is the distance between two arbitrary points in the microstructure. In the case of digital images, *r* is the distance in pixels. The procedure of minimizing *E* (at any time step) is performed by simulated annealing algorithm [11].

It has been shown by JIAO et al. [8] that in the case of the B_4C/Al composite, the target two-point correlation function for aluminum phase can be approximated by the following relation:

$$\widetilde{S}_2^{(i)}(r) = (0.81\exp(-r/3) + 0.19\exp(-r/10)\cos(0.22))\phi_1\phi_2 + \phi_1^2, \tag{3}$$

where $\phi_1 = 0.353$ and $\phi_2 = 0.647$ are the volume fractions of aluminum and boron carbide phases, respectively.

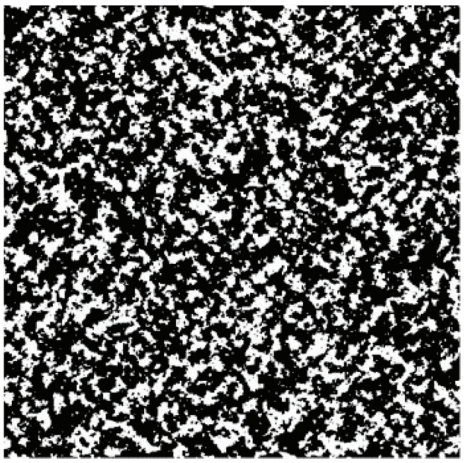

Fig. 2. The digital image (500×500 pixels) of the reconstructed 2D realization of the B_4C/Al composite

Adopting the methodology presented in [20], [21] the microstructure of the B_4C/Al composite has been reconstructed. Figure 2 shows the digital image of 2D recon-

structed realization of the composite considered. The resolution of the digital image is 500×500 pixels. The aluminum phase is shown in white, whereas black pixels are associated with boron carbide phase.

3. THE CONDITION FOR THE MINIMUM SIZE OF THE REPRESENTATIVE VOLUME ELEMENT

The condition for the minimum size of RVE (proposed by authors in [14], [16]) with respect to effective thermal conductivity reads:

$$\| \Omega \|_{\mathrm{RVE}} \geq \max[\| \Omega \|_1; \| \Omega \|_2; \| \Omega \|_3], \tag{4}$$

where

$$\| \Omega \|_1 = \frac{2|1-\Theta|}{(\phi_1 + \phi_2 \Theta)} \sqrt{\frac{\int_0^a \int_0^b (S_2^{(1)}(r) - \phi_1^2)(a-x)(b-y)dxdy}{\varepsilon}}, \tag{5}$$

$$\| \Omega \|_2 = \frac{2|1-\Theta|}{(\phi_2 + \phi_1 \Theta)} \sqrt{\frac{\int_0^a \int_0^b (S_2^{(1)}(r) - \phi_1^2)(a-x)(b-y)dxdy}{\varepsilon}}, \tag{6}$$

$$\| \Omega \|_3 = 4 l_p^2(\Theta, \varepsilon). \tag{7}$$

In the relations above, Θ stands for the contrast in phase properties, ε is the value of the error tolerance assumed and l_p is the so-called correlation length defined as:

$$\forall r \geq l_p(\Theta, \varepsilon) \Rightarrow \frac{(1-\eta(\Theta))^2 \phi_1^2}{(\phi_1 + \eta(\Theta)\phi_2)^2} \left| \frac{S_2^{(1)}(r) - \phi_1^2}{\phi_1^2} \right| \leq \varepsilon, \tag{8}$$

where

$$\eta(\Theta) = \min\left\{\Theta, \frac{1}{\Theta}\right\}. \tag{9}$$

Note that in the case of digital images, the size of RVE is associated with the number of pixels contained within the image. Furthermore, assuming that the image is a square composed of N^2 pixels, the size of RVE can be treated as $\|\Omega\|_{\mathrm{RVE}} \geq N^2$. Therefore, utilizing the properties of equation (9) relations (5) and (6) can be rewritten and interpreted as below:

Find N such that $N^2 = \dfrac{2(1-\eta(\Theta))}{(\phi_1+\eta(\Theta)\phi_2)}\sqrt{\dfrac{\int_0^N\int_0^N (S_2^{(1)}(r)-\phi_1^2)(N-x)(N-y)dxdy}{\varepsilon}}$. (10)

Observing relations (10) one can simply notice that in order to determine the size of RVE, first, the two-point correlation function $S_2^{(1)}(r)$ has to be calculated. The methodology of $S_2^{(1)}(r)$ determination is presented in the next section.

4. DETERMINATION OF THE TWO-POINT CORRELATION FUNCTION

Consider a binary ($M\times M$ pixels) image of random microstructure. We assume that each pixel has only one of two possible values: 0 or 1. Hence, the digital image can be interpreted as the matrix $\mathbf{A}_{[M\times M]}$ – each element of the matrix $\mathbf{A}$ is equal to 0 or 1, i.e.: $A[i, j] = 1$ if pixel represents the phase for which the two-point correlation function is calculated. Furthermore, the indices i and j correspond to the localization of the pixel within the image – they denote the number of a row and a column, respectively. Then, the two-point correlation function for phase 1 can be expressed as:

$$S_2^{(1)}(r) = \frac{1}{M^2}\sum_{j=1}^{M}\sum_{i=1}^{M}\frac{A[i, j](A[i, j+r]+A[i+r, j])}{2}, \quad r = 1, 2, ... \tag{11}$$

A procedure of $S_2^{(1)}(r)$ determination has a specific geometrical interpretation: the two-point correlation function is evaluated by translating a line segment of the length r (in pixels) at a distance of one pixel at a time and by spanning the whole image (each time the end points of r are located at the pixel centers), see figure 3. The number of events, such that two-end points of line segment of the length r are found in phase 1, are counted and divided by the total number of trials. Note that by assuming the system isotropy, the sampling is performed only along two orthogonal directions: rows and columns.

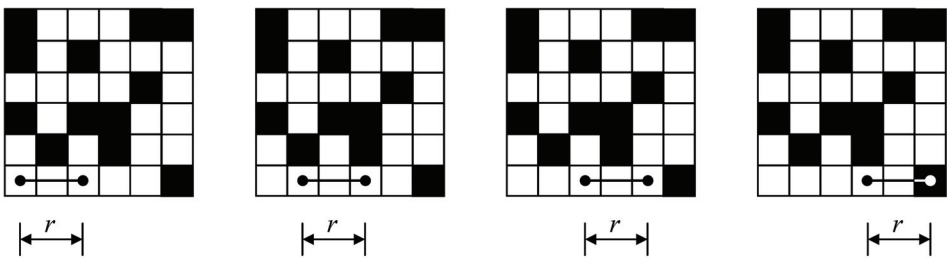

Fig. 3. Geometrical interpretation of numerical evaluation of the two-point correlation function

5. INTEGRATION OF THE TWO-POINT CORRELATION FUNCTION

In order to evaluate the integral of the two-point correlation function, we propose the MC integration approach. In what follows, we introduce the function g given in the following form:

$$g(N) = \frac{4}{\| \Omega \|^2} \int_0^N \int_0^N (S_2^{(1)}(\sqrt{x^2 + y^2}) - \phi_1^2)(N - x)(N - y) dx dy. \tag{12}$$

One can simply notice that:

$$\frac{4}{\| \Omega \|^2} \int_0^N \int_0^N (N - x)(N - y) dx dy = \left[\frac{2}{N^2} \int_0^N (N - x) dx \right] \left[\frac{2}{N^2} \int_0^N (N - y) dy \right] = 1. \tag{13}$$

Therefore the function:

$$p(x, y) = p(x) p(y), \tag{14}$$

where

$$p(x) = \frac{2}{N^2}(N - x) \quad \text{and} \quad p(y) = \frac{2}{N^2}(N - y), \tag{15}$$

can be treated as the probability density functions in Ω.

If we introduce additionally the function $h(x, y)$ defined as:

$$h(x, y) = (S_2^{(1)}(\sqrt{x^2 + y^2}) - \phi_1^2), \tag{16}$$

then by inserting (15) into relation (12) we can express g as an expectation of the function h, i.e.:

$$g = \int_0^N \int_0^N h(x, y) p(x) p(y) dx dy = \langle h(X, Y) \rangle, \tag{17}$$

where $\langle * \rangle$ is the expected value operator. Therefore, the estimation of the integral considered consists in generating random numbers X_i and Y_i from the density functions $p(x)$ and $p(y)$ and then computing the mean of $h(x, y)$, i.e.:

$$g \approx \frac{1}{n} \sum_{i=1}^{n} h(X_i, Y_i). \tag{18}$$

Note that in order to evaluate the MC estimator (18), pseudorandom numbers from a non-uniform distribution have to be drawn. Following [7] this problem is divided into two steps. First, a simple generator is used to generate uniformly distributed ran-

dom numbers, which in a second step are transformed to follow the distribution required. Then the MC estimator of the integral (18) can be presented as:

$$g \cong \frac{1}{n}\sum_{i=1}^{n}(S_2^{(1)}(\sqrt{X(Q_i)^2 + Y(Q_i)^2}) - \phi_1^2, \tag{19}$$

where the values of Q_i are obtained from the uniform distribution on the interval [0, 1], while $X(Q_i)$ as well as $Y(Q_i)$ are the non-uniformly distributed random numbers determined via the following relations:

$$X(Q) = N(1-\sqrt{1-Q(X)} \quad \text{and} \quad Y(Q) = N(1-\sqrt{1-Q(Y)}). \tag{20}$$

6. A GENERAL SCHEME OF RVE SIZE DETERMINATION PROCEDURE

In order to determine the minimum size of RVE from the digital image of microstructure, one should follow these steps:

- having a digital image of microstructure, determine – using relation (11) – the two-point correlation function for phase 1,
- assume the value of the error tolerance ε and determine the correlation length l_p defined by relation (8),
- calculate the value of $||\Omega||_3$ – use expression (7),
- using MC integrating procedure (equation (19)) find such N that satisfies the following inequality:

$$\frac{(1-\eta(\Theta))^2}{(\phi_1 + \eta(\Theta)\phi_2)^2} g(N) \le \varepsilon, \tag{21}$$

- determine the minimum size of RVE, i.e., N_{RVE} as:

$$N_{\mathrm{RVE}} \ge \max[N; N_3] \tag{22}$$

where $N_3 = 2l_p = \sqrt{||\Omega||_3}$.

7. NUMERICAL RESULTS

The aluminum phase two-point correlation function for the digital image of the B_4C/Al composite has been determined utilizing the method presented in Section 4 (equation (11)). This function is graphically presented in figure 4. Based on the values of $S_2^{(1)}(r)$ the correlation length has been determined for different values of both error

tolerance ε and the contrast in phase properties Θ – the results are summarized in table 1. One can observe that the greater the value of the contrast Θ, the greater the value of the correlation length and, as a consequence, the value of the size N_3. Furthermore, for a fixed value of Θ, as error ε is decreasing, the size N_3 is increasing.

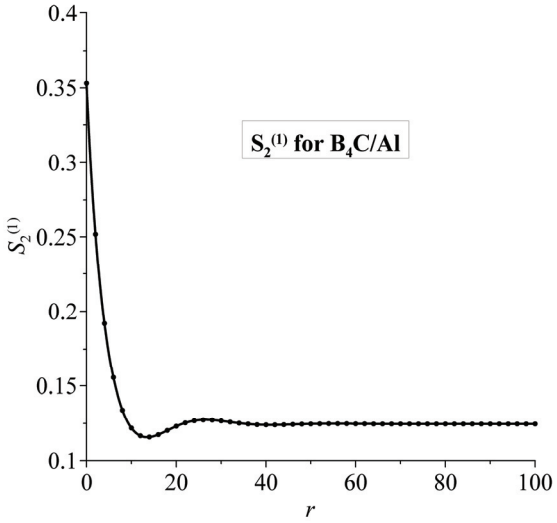

Fig. 4. The two-point correlation function for the B_4C/Al composite (the distance r in pixels)

Table 1

The correlation length l_p and the size N_3 for different values of both ε and Θ

Θ	ε	l_p	N_3
5	3%	8	16
10		14	28
50		18	36
100		19	38
1000		19	38
5	1%	19	38
10		26	52
50		32	64
100		32	64
1000		33	66

Next, using the MC integration procedure, i.e., relation (19), the integral of the two-point correlation function, given by equation (12), has been calculated. In figure 5, the

values of the function g, plotted against the size N, are graphically presented. Note that as N is increasing, the function g is decreasing.

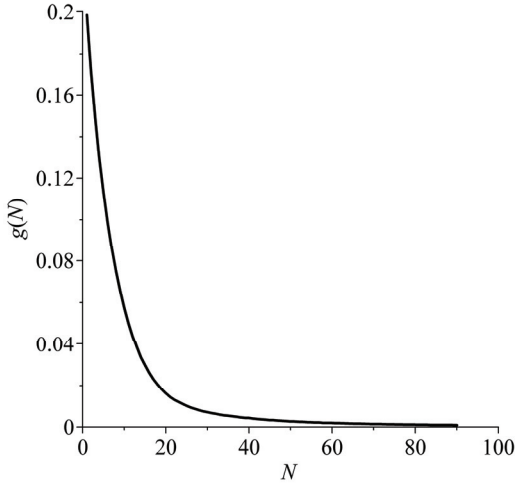

Fig. 5. The function g (equation (12)) plotted against the size N

Following the procedure presented in previous section, the size N has been determined by making use of relation (21). The results are summarized in table 2. Once again, the sizes have been evaluated for different values of both error tolerance ε and the contrast in phase properties Θ. It can be seen that the same dependence as in the case of N_3 can also be observed for the size N, i.e., the size N is increasing with the increase in the value of Θ. Furthermore, lower values of error ε correspond to larger values of N.

Table 2

The sizes N determined by making use of relation (21)

Θ	ε	N
5	3%	25
10		30
50		40
100		42
1000		44
5	1%	44
10		54
50		70
100		75
1000		77

As has been mentioned in Section 6, the final size of RVE is treated as the maximum value of two quantities (see relation (22)). Comparing the results summarized in tables 1 and 2, we see that for all values of Θ and ε

$$\max[N; N_3] = N \tag{23}$$

and therefore, in the case of the microstructure under consideration, the size of RVE is $N_{\mathrm{RVE}} = N$.

8. NUMERICAL VALIDATION OF METHODOLOGY

As mentioned in the Introduction, it was shown in our previous works [14]–[16] that the size of RVE, i.e. N_{RVE}, is directly associated with the size of the sample n. Therefore, in order to determine the overall thermal conductivity coefficient, one has to consider a sufficient number of microstructure realizations and the effective property is then estimated as the mean value averaged over all realizations (entire sample n) – see equation (1). The sample size n can be estimated based, e.g., on the Central Limit Theorem (for more details see [2]). Then, the number of the realizations n is given by the following inequality [14], [16]:

$$n \geq \frac{(1-\eta(\Theta))^2}{(\phi_1 + \eta(\Theta)\phi_2)^2} \left(\frac{\Phi^{-1}(1-\alpha/2)}{\varepsilon} \right)^2 g(N_{\mathrm{RVE}}), \tag{24}$$

where Φ is the cumulative distribution function of the standard normal random variable, α denotes the significance level and ε is the relative error of estimation.

Table 3

Mean values of thermal conductivity coefficients corresponding to various values of both estimation error ε and the contrast in properties Θ

Θ	ε	N_{RVE}	n	$\overline{K}$ [W/mK]	K^{eff}[W/mK]
5	3%	25	144	2.893	2.803
10		30	128	4.485	4.403
50		40	140	13.807	13.550
5	1%	44	439	2.852	2.803
10		54	398	4.480	4.403
50		70	452	13.681	13.550

The methodology proposed has been verified by performing numerical calculations for the different values of the estimation error and the contrast in properties Θ. For previously estimated RVE sizes, i.e., $N_{\mathrm{RVE}} = N$, the mean values have been evaluated and compared with the effective property (thermal conductivity coefficient corre-

sponding to RVE size for which only one realization is sufficient). The results are summarized in table 3.

It should be noted that the values of n have been determined for the significance level $\alpha = 5\%$. Furthermore, the numerical calculations of the effective properties have been performed only for the case of periodic boundary conditions prescribed at the peripheries of each RVE_j.

The results summarized in table 3 prove that for all values of Θ there is a good agreement between the mean value $\overline{K}$ and the effective property K^{eff}. In figure 6, the mean value of thermal conductivity coefficient is plotted against the size of RVE. The results correspond to the case of $\Theta = 10$ and the estimation error $\varepsilon = 3\%$. Moreover, the effective property K^{eff} and the bounds of Voigt–Reuss as well as Hashin–Shtrikman are also provided. We see that the value of $\overline{K}$ corresponding to the case of $N_{\mathrm{RVE}} = 30$ is between the error bounds assumed (see figure 6). In other words, the following inequality is fulfilled:

$$K^{\mathrm{eff}}(1-\varepsilon) < \overline{K}(N_{\mathrm{RVE}}) < K^{\mathrm{eff}}(1+\varepsilon)\,. \tag{25}$$

What is most important, relation (25) is also valid for all remaining values of ε and Θ.

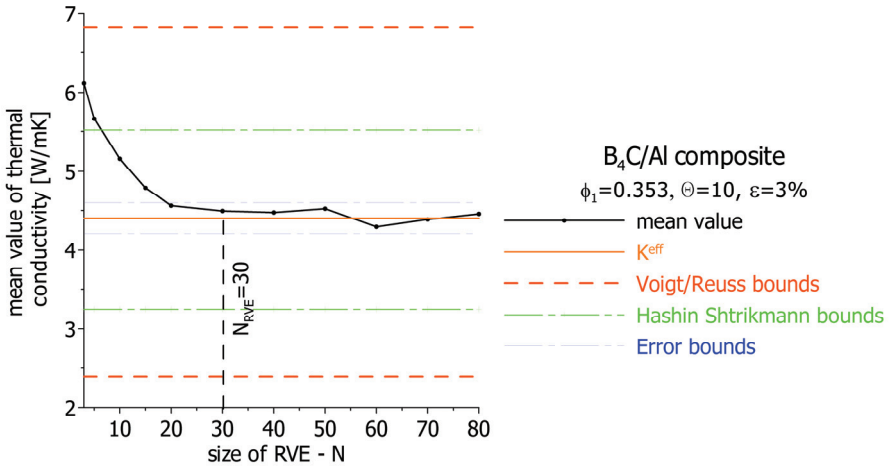

Fig. 6. The mean value of the thermal conductivity coefficient (W/mK) plotted against the size of RVE; the Voigt–Reuss and Hashin–Shtrikman bounds

9. CONCLUSIONS

In this paper, the numerical algorithm of RVE size determination from the digital image of microstructure has been formulated. The methodology utilizes the minimum

RVE size condition proposed in our previous works [14], [16]. As has been mentioned before, this condition is based on the statistical microstructure descriptor, namely the two-point correlation function, and is devoted to the case of effective thermal conductivity.

In general, the procedure proposed consists of several simple steps. First, one has to evaluate the two-point correlation function $S_2^{(1)}$ for the digital image. It has been proposed to calculate $S_2^{(1)}$ by simple procedure based on translating a line segment over the whole image. Note that assuming the system isotropy, the sampling is performed only along two orthogonal directions: rows and columns. Then $S_2^{(1)}$ can be determined by making use of equation (11). Next, the particular integral of $S_2^{(1)}$ has to be determined. This integral is represented by the function g and is proposed to be calculated by making use of the Monte Carlo approach (equation (19)).

Assuming the value of the error tolerance ε, we have to determine the correlation length l_p which is defined by relation (8) – then the value of $N_3 = 2l_p$ is simply evaluated. Furthermore, having the values of the function g one has to find such N that satisfies condition (21). Finally, the size of RVE is the maximum value of N_3 and N, see (22).

The methodology has been verified by applying to the digital image of the boron carbide/aluminum composite. The microstructure of B_4C/Al composite has been obtained via the two-point correlation function reconstruction procedure. Using the algorithm provided in Section 6, the RVE sizes have been evaluated for different values of the estimation error ε and the contrast in properties Θ. The method proposed has been validated by calculating the mean values of effective thermal conductivity coefficients. The validity of relation (25) for all the values of Θ and ε confirms that the numerical procedure presented in the paper is proper and can be successfully applied to the case of digital images. What is most remarkable, the procedure formulated offers the possibility of determining the size of RVE (for the case of thermal conductivity) with no large number of numerical calculations – the numerical analyses like those of FE are not necessary. Compared to other methods available in the literature, the one proposed in this paper allows a high computational cost to be decreased.

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