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P. KURTYKA*, N. RYLKO*

STRUCTURE ANALYSIS OF THE MODIFIED CAST METAL MATRIX COMPOSITES BY USE OF THE RVE THEORY

ANALIZA STRUKTURY MODYFIKOWANYCH ODLEWANYCH KOMPOZYTÓW NA OSNOWIE METALOWEJ Z WYKORZYSTANIEM TEORII RVE

The paper presents applications of a new theory of the representative volume element (RVE) based on the Mityushev-Eisenstein-Rayleigh sums (M-sums) to describe particle-reinforced composites. This theory is applied to study F3K.10S metal matrix composites reinforced SiC particles. The most important M-sum e_2 is calculated for the initial state as $e_2 = -0.00206281$. This shows considerable heterogeneity of distribution of reinforcing particles and its anisotropic properties. Further, the results are compared with the results obtained by the FSP. It is established that the use of a single FSP process causes a significant change in the distribution of particles reinforcing phase when the value e_2 becomes 3.19488. It follows from Mityushev's theory that $e_2 = \pi$ corresponds to isotropic distributions. The article confirms that the new RVE theory resolves the problem of the constructive pure geometrical description of the properties of composites. Further work requires the optimization and extension of the theory to three-dimensional models.

Keywords: Representative volume element, Mityushev-Eisenstein-Rayleigh sums, Metal Matrix Composites

W artykule przedstawiono nową teorię RVE bazującą sumach Mityushev-Eisenstein-Rayleigh (M-sums) oraz ich wykorzystanie do opisu niektórych właściwości kompozytów wzmacnianych cząstkami. Praktyczne zastosowanie prezentowanej teorii pokazano na przykładzie kompozytu na osnowie metalowej wzmacnianego cząstkami SiC (F3K.10S). Bazując na analizowanych mikrostrukturach kompozytu, obliczono wartości sum Mityushev-Eisenstein-Rayleigh'a dla stanu wyjściowego, otrzymując wartość sumy e_2 równą -0.00206281, co świadczy o dużej niejednorodności rozmieszczenia cząstek fazy wzmacniającej. Otrzymane wyniki porównano z danymi obliczonymi dla kompozytu po obróbce friction stir processing (FSP). Zaobserwowano istotny wpływ zastosowanego procesu na zmianę dystrybucji cząstek fazy wzmacniającej, co potwierdzono obliczeniowo, uzyskując wartość sumy Mityushev-Eisenstein-Rayleigh'a e_2 równą 3,19488. Obserwowana tendencja zmierzania wartości sumy Mityushev-Eisenstein-Rayleigh'a e_2 do liczby π świadczy o znacznej poprawie dystrybucji cząstek fazy wzmacniającej po procesie FSP.

W pracy pokazano, że nowa teoria RVE bazująca na sumach Mityushev-Eisenstein-Rayleigh 'a pozwala na określanie wybranych właściwości kompozytów na podstawie czysto geometrycznych czynników. Stwierdzono jednak, że konieczne są dalsze prace nad optymalizacją i rozszerzeniem teorii w celu pełnego trójwymiarowego analizowania struktur kompozytowych.

1. Introduction

The issues of modern manufacturing and testing of composite materials concerning the required distribution and particle reinforcing size in the matrix have been widely discussing in the literature for several decades. Though production of composites with the desired particle distribution is worked out, the assessment of their optimal properties often meets numerous problems. Regardless of the applied manufacturing techniques, "ex-situ" or "in-situ", getting the right structure requires additional mixing techniques for reinforcement of the matrix. Issues related to different manufacturing techniques as well as the optimization of the particle reinforcing phase distribution and their size are described among others in publications [1-7]. We apply a different approach in this work, namely, modification of the structure of already completed composites through additional processes such as plastic forming. One of the most promising processes is friction stir processing (FSP). It follows from the literature on FSP for traditional alloys [8-12,13] it is possible to use joining and processing of composite materials [8,9,14,15]. The cast composites F3K.10S reinforced with SiC particles are modified by change of the distribution of the reinforcing phase particles, hence, its structure and, thereby, the properties of the material. However, regardless of the aforementioned approach or concept of composite manufacturing, the economic factor determines their suitability. Therefore, it is advisable to develop new models and theories in order to minimize costs of complicated experimental and technological processes and to obtain more information on the properties of the new materials. Such theories to pass from geometry of the microstructure of materials to their properties has been going over years by

* INSTITUTE OF TECHNOLOGY, PEDAGOGICAL UNIVERSITY, UL. PODCHORAZYCH 2, 30-084 KRAKÓW, POLAND

several research teams. The obtained results have significant limitations. Torquato [16] discuss this problem using the correlation functions. Although they theoretically can be applied to general structures, practical applications are limited to low concentrations and weakly inhomogeneous materials [17]. Numerical computations based on the physical conception of the RVE were performed for small number of particles per a periodicity cell. Materials with higher concentrations cannot be analyzed by this theory. The paper presents a concept based on the new RVE theory developed by [18]. This theory allows to investigate systems with any number of particles per periodicity cell, hence, materials with any concentration of the particles. The objective of this study is to present a new RVE theory based on the M-sums and its application to the analysis of microstructure of the F3K.10S composite sample processed by FSP.

2. Materials and research methods

The research material be a foundry alloy F3K.10S reinforced with SiC particles. Its chemical composition is shown in TABLE 1. Strengthening phase of the reinforce particles has the average size 15 um, and its volume fraction is 10%. The material is thermomechanical treated using a friction stir processing. This process consists of mixing the melt in the solid state when the material is placed on the rotating pin linearly sliding. The temperature of the process provides ability for freely thermomechanical treatment of the material. Details of the process, terms and phenomena occurring during friction stir processing were described extensively in [8-15].

The results of microscopic examination are based on the light microscopy (Olympus GX51) and on the scanning electron microscopy (JEOL JSM 6610). Microscopic examination is supplemented by calculation the M-sums in the framework of the RVE theory.

TABLE 1

The chemical composition of the composite matrix (wg %)

Materials	Si	Fe	Cu	Mg	Ni	Ti	Other	Al
F3K.10S	9.5	0.3	2.8	0.8	1	0.2	0.03	balance

3. New RVE theory and its application

Geometric classifications of particle-reinforced composites can be based on the representative volume element (RVE). A physical definition of this term can be given in the following way. RVE is a part of material which is small enough from a macroscopical point of view and can be thus treated as a typical element of the heterogeneous medium. On the other hand, it is sufficiently large in the microscopical scale, and it represents typical microstructure of the material under consideration. It is difficult to directly follow this description to determine the RVE and to classify composites. Fortunately, a simple algorithm was proposed in [18] to describe composites. The new RVE theory [18] resolves the transformation problem from geometry to physics, i.e., constructively answers the question how to classify composites by the macroscopic behaviour based on the locations of inclusions and their sizes. It was established in [18] that the effective property tensors of fibre–reinforced composites has the form of double series on the concentration of inclusions and on "basic elements" which depend only on locations of the inclusions. These basic elements are written in terms of the M-sums (generalized Eisenstein–Rayleigh sums by Mityushev's terminoloigy). This observation was also extended to general particle–reinforced composites. The RVE theory [18] complemented by computer simulations [17] yields a simple straight-forward method to describe the mechanical macroscopic properties of composites by locations of inclusions.

Following [18-24] we present constructive formulae for the Eisenstein-Rayleigh sums corresponding to the lattice Q. Consider a lattice Q which is defined by two fundamental translation vectors expressed by complex numbers ω_1 and ω_2 on the complex plane $\mathbb{C}$. For the definiteness we assume that $Im\tau > 0$, where $\tau = \omega_2/\omega_1$. Introduce the section (0, 0) -cell $Q_{(0,0)} := \left\{z = t_1\omega_1 + t_2\omega_2 : -1/2 < t_j < 1/2\,(j = 1, 2)\right\}$. The lattice Q consists of the cell $Q_{(m_1,m_2)} := \{z \in \mathbb{C} : z - m_1\omega_1 - m_2\omega_2 \in Q_{(0,0)}\}$, where m_1 and m_2 run over integer numbers.

The M-sums S_m can be easily calculated through the rapidly convergent series

$$S_2 = \left(\frac{\pi}{\omega_1}\right)^2 \left(\frac{1}{3} - 8\sum_{m=1}^{\infty} \frac{mq^{2m}}{1-q^{2m}}\right), \quad q = \exp\left(\pi i \frac{\omega_2}{\omega_1}\right) \tag{1}$$

$$S_4 = 60\left(\frac{\pi}{\omega_1}\right)^4 \left(\frac{4}{3} + 320\sum_{m=1}^{\infty} \frac{m^3q^{2m}}{1-q^{2m}}\right) \tag{2}$$

$$S_6 = 1400\left(\frac{\pi}{\omega_1}\right)^6 \left(\frac{8}{27} - \frac{448}{3}\sum_{m=1}^{\infty} \frac{m^5q^{2m}}{1-q^{2m}}\right) \tag{3}$$

$S_{2n}\,(n \geqslant 4)$ can be calculated by the recurrent formula

$$S_{2n} = \frac{3}{(2n+1)(2n-1)(n-3)} \sum_{m=2}^{n-2} (2m-1)(2n-2m-1)\, S_{2m} S_{2(n-m)} \tag{4}$$

The rest of the sums vanishes.

The Eisenstein functions E(z) are related to the Weierstrass function $\wp(z)$ by the identities

$$E_2(z) = \wp(z) + S_2, \quad E_m(z) = \frac{(-1)^m}{(m-1)!} \frac{d^{m-2}\wp(z)}{dz^{m-2}}, \; m = 3, 4, \ldots \tag{5}$$

Following [7] we introduce the M-sums. Let $a_k (k = 1, 2, ..., N)$ be a set of points. Let q be a positive integer; k_t runs over 1 to N; $m_j = 2, 3, ...$ Let C be the operator of complex conjugation. Introduce the following sum of multi-order $(m_1, ..., m_q)$

$$\begin{aligned} e_{m_1 \ldots m_q} &:= N^{-\left[1+\frac{1}{2}(m_1+\ldots+m_q)\right]} \sum_{k_0 k_1 \ldots k_q} E_{m_1}(a_{k_0} - a_{k_1}) \\ &\times \overline{E_{m_2}(a_{k_1} - a_{k_2})} \ldots C^q E_{m_q}\left(a_{k_{q-1}} - a_{k_q}\right). \end{aligned} \tag{6}$$

Here, it is assumed for convenience that

$$E_m(0) := S_m \tag{7}$$

The theoretically computed values of the M-sums for randomly distributed non–overlapping inclusion are presented in TABLE 2 obtained by Czapla et al. [17].

TABLE 2

Theoretical basic elements ekk for various concentrations ν. Data are from [4]

ν	$\langle e_{22}\rangle$	$\langle e_{33}\rangle$	$\langle e_{44}\rangle$	$\langle e_{55}\rangle$	$\langle e_{2222}\rangle$	$Re(\langle e_{3322}\rangle)$	$\langle e_{2332}\rangle$
0.05	54.4562	-382.333	4190.05	-50427.7	9643.33	-66675.3	-64221.9
0.1	30.3341	-94.6858	554.766	-3416.08	2135.82	-5660.96	-5548.78
0.15	22.346	-41.9403	174.956	-739.574	974.611	-1463.18	-1476.22
0.2	18.2159	-23.2581	76.7296	-252.174	576.092	-573.461	-591.867
0.25	15.7966	-14.6562	41.6043	-114.382	395.838	-286.93	-303.729
0.3	14.2628	-9.88543	25.2077	-61.0286	297.019	-163.827	-178.244
0.35	12.8822	-6.46391	15.3884	-33.213	223.286	-91.9693	-102.209
0.4	12.1174	-4.69994	10.8078	-22.0623	186.765	-60.5965	-68.9144
0.45	11.5527	-3.49796	7.93768	-15.7805	161.768	-41.8831	-48.5197
0.5	11.0934	-2.57665	5.94659	-11.9023	142.964	-28.9071	-34.1006
0.55	10.766	-1.90511	4.49997	-9.38056	129.983	-20.3632	-24.4439
0.6	10.4837	-1.38498	3.38179	-7.58524	119.44	-14.1216	-17.1713
0.65	10.2755	-0.911354	2.37488	-6.06037	111.759	-8.97626	-11.1578
0.7	10.0566	-0.402342	1.07512	-3.85177	103.82	-3.64061	-5.11471
0.75	9.96082	-0.198966	0.52554	-2.16478	100.567	-1.72926	-2.54225
0.8	9.90916	-0.0839384	0.216754	-0.982389	98.7614	-0.713257	-1.07474
0.85	9.8814	-0.0222027	0.0588841	-0.267471	97.7665	-0.187318	-0.284677
0.9	9.86974	-0.00031838	0.000867687	-0.0038436	97.414	-0.00267407	-0.0040697

Computations [17] were performed by generations of the uniform random walks of non–overlapping disks for high concentrations and by direct simulations of the uniformly distributed disks for lower concentrations.

The verification of the model is carried out on the cast composite F3K.10S microstructures obtained in two cases. First, the initial state is investigated immediately after casting. The second one is a composite modified by friction stir processing. This choice is done due to the previously obtained results devoted to adequate structure and the specific nature of FSP processing ensuring very high values of composite deformation and, consequently, complete reconstruction of the structure. It is expected that the application of friction stir processing in the first place improves the distribution of reinforcing particles in the composite, as well as it leads to their fragmentation. This will obviously have a considerable influence on changing the properties of the obtained material. Different structures are used in the FSP-modified material [10-12]. Only one variant of the structure with the highest degree of deformation is selected for further study. Clearly marked distinction of reinforcing particles on the background of the matrix is the key condition for the usefulness of the obtained microstructures. Therefore, after initial trials, microstructures with an optical microscope are given up to obtain microstructures with scanning electron microscopy. These microstructures are processed by special software in order to create a model of the RVE cell containing only 20 particles of the reinforcing phase. Due to the optimized algorithms [17] it will be possible to analyze much larger cells. 20 particles per RVE is more than sufficient to confirm the accuracy of the developed model. Properly prepared microstructure images further computer-process are applied to give only the boundaries of the SiC particles at the final stage, as shown in Fig. 1a and Fig. 1b.

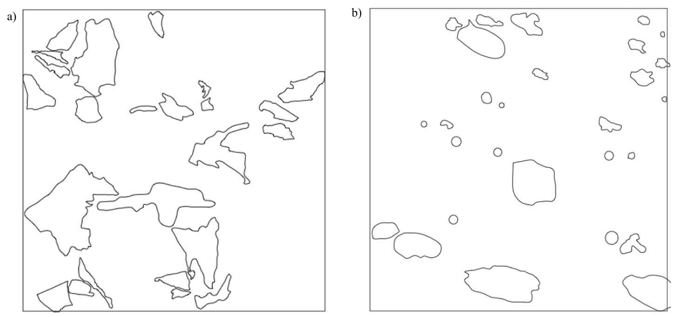

Fig. 1. Reinforcement distribution in composite: a) initial state b) modified by FSP

Microstructures prepared by this method are analyzed in order to determine the center of gravity of each particle and the prepared data are computationally processed by use of Mathematica 8.0.4. Calculations are carried out for the both variants of the materials previously described, the initial state and the state treated by FSP.

Calculations are performed with the use of the collected experimental data, applying the M-sums. The obtained result include the values of the M- sums and the model distribution of SiC particles, as shown in Fig. 2a and Fig. 2b for the both test variant. The results are analyzed by the sum e_2 calculated for the variants.

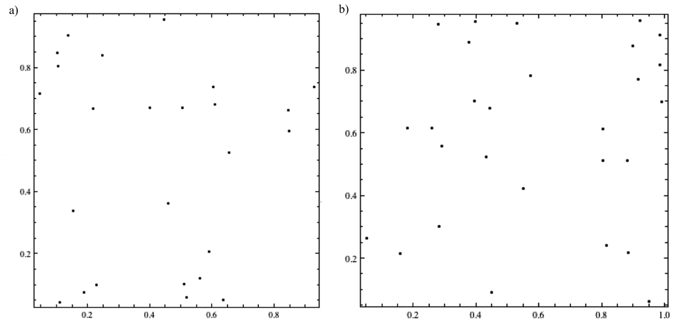

Fig. 2. Reinforcement distribution in composite: a) initial state b) modified by FSP with RVE theory

The e_2 sum is obtained by Eq. (8) where N denotes the number of inclusions per cell

$$e_2 = \frac{1}{NN^2} \sum_{k=1}^{NN} \left(\sum_{m=1}^{NN} \mathbb{E}\left[2, a[k] - a[m]\right] \right) \tag{8}$$

The sum e_2 for the initial state material is equal to -0.00206281, and for the material processed by FSP e_2 = 3.19488. It is known that for a perfectly isotropic material $e_2 = \pi$. This implies that the starting material is anisotropic, while in the friction stir modified material processing we arrive at the isotropic material. The observed trend suggests that further subjecting of the material to the next thermomechanical processes will impact onto the optimization of the distribution of reinforcing elements.

The anisotropy coefficient can by calculated by Eq. (9) obtained from Eq. (8)

$$\kappa = \frac{Abs\left[\mathrm{Re}\left(e_2 - \pi\right)\right]}{\pi} \tag{9}$$

The initial state material anisotropy coefficient $\kappa = 0.500328$ and $\kappa = 0.016961$ for the material after the process of thermomechanical treatment. The coefficient κ vanishes for isotropic materials.

4. Summary

A new RVE theory based on the M-sums is applied to the analysis of microstructures of composites. It is established that the proposed model describes the distribution of the reinforcing phase particles in the matrix of the composite. This allows us to accurately determine the degree of anisotropy of the distribution of reinforcing particles. The article shows, that the new RVE theory resolves the problem of the constructive pure geometrical description of the mechanical properties of composites. This gives hope to extend the model to determine the properties of composite materials of general structures. It requires extension of the theory to three-dimensional structures. It is found that the uniform distribution of reinforcing particles of the conducted process can be identified by the value e_2. The M-sums show, with high probability, that the longer use of processes thermomechanical deformation like FSP will further improve the distribution of reinforcing particles in the matrix.

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