Numerical Models of Heat Conductivity of Composite Systems

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Numerical Models of Heat Conductivity of Composite Systems

First, we consider the solution of an applied problem using machine methods of solution (BINARY COMPOSITE MODEL):

A method of computer simulation of the effective thermal conductivity of a unit cell of a composite system (CS) based on polymers has been developed. A review of methods for calculating the effective thermal conductivity of binary CSs is presented. The factors affecting the effective thermal conductivity of CSs are described, including the distribution of the filler in the matrix, the model of thermal conductivity in the interfacial layer, and the intermolecular thermal conductivity of polymers.

And then we will consider general questions and examples of the use of information methods in training (SOFTWARE IN THE EDUCATIONAL PROCESS):

Computer simulation methods in the study of physics, technical disciplines. Learning Management. Modern life, and therefore education, have become “hostages” of the undeniable successes of information formatting - mobile access via global networks to information, various tools to support routine operations of managing, storing, processing data and accessing them, time-consuming mathematical computing, solving subject problems of a scientific and industrial nature.
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BINARY COMPOSITE MODEL

By simple models of thermal conductivity of composite systems (CS) we mean models that take into account the qualitative composition, shape of particles and their fraction. Calculation of the effective thermal conductivity of CS is based on the principle of generalized conductivity. They are based on the Maxwell method. All the considered models (рисунок 1) can be used only for a preliminary assessment of the effective thermal conductivity of CS at low fractions of filler, and close coefficients of thermal conductivity of the matrix and filler.

The calculation of a larger number of factors is possible in numerical models. They are based on the solution of the heat equation, the determination of the average heat of the thermal conductivity of the filler $\lambda_1$ and matrices $\lambda_2$ flux and then the effective coefficient of heat conductivity $\lambda_{\text{eff}}$. The thermal conductivity of the filler is $\lambda_1$ and the matrices is $\lambda_2$. The filler fraction is $\rho_2$.

Fig. 1. Relative values of the effective coefficient of thermal conductivity from the filler fraction $\rho_2$ for thermal conductivity models: 1 - Maxwell, 2 - statistical, 3 - matrix, 4 - Maxwell-Burger-Aiken, 5 - percolation, 6 - linear.
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Fig. 2. Variants of particle distribution in a unit cell: 1 - random, 2 - longitudinally oriented fibers, 3 - transversely oriented fibers, 4 - fractal cluster.

**BINARY COMPOSITE MODEL**

(Modeling the distribution of filler particles in the matrix)

Technologically most often, the filler is randomly distributed in the matrix. However, it is impossible to obtain a completely uniform distribution. Even in the case of low fractions, clusters can be formed. Clusters, in turn, form cluster-cluster systems, which can lead to percolation effects [8]. The polymer matrix itself is heterogeneous in terms of structure. However, CS are of most interest when the thermal conductivity of the matrix is much lower than the thermal conductivity of the filler. From this point of view, the thermal conductivity of the composite as a whole is determined by the properties and structure of the filler.
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Binary Composite Model

(Mathematical model)

\[
\frac{\partial}{\partial x} \left( \lambda_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \lambda_y \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( \lambda_z \frac{\partial T}{\partial z} \right) = 0
\]

Boundary conditions:

\[ T = T_b, x = 0, L \geq y \geq 0, L \geq z \geq 0; \]
\[ T = T_c, x = L, L \geq y \geq 0, L \geq z \geq 0; \]
\[ \frac{\partial T}{\partial y} = 0, L \geq x \geq 0, y = 0(L), L \geq z \geq 0; \]
\[ \frac{\partial T}{\partial y} = 0, L \geq x \geq 0, L \geq y \geq 0, z = 0(L). \]

On a cubic lattice we consider a finite-difference analogue of equation. All thermal conductivity coefficients at the nodes of the lattice are not constant values, but depend on the status of neighboring nodes and temperature. The type of contact determines the status of neighboring nodes.

Then, the finite-difference analogue of equation is solved by the relaxation method. All internal nodes are scanned and the temperature in the node is calculated. Iterations are repeated until a stationary temperature distribution is established. Based on this model, an algorithm is compiled and a computer implementation is performed.
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**BINARY COMPOSITE MODEL**

*(Computer implementation)*

Experiments to determine the effective thermal conductivity were performed for composites based on polyethylene and polyamide with a filler of particles of silicon carbide with sizes of 60-50 μm and 0.9 - 1 μm with mass fractions: 0.5%, 20% и 60%. Tables 1 and 2 show the thermal conductivity coefficients of the compositions “polyethylene silicon carbide” (PE) and “polyamide 6-silicon carbide (PA)”.

Computer simulation was performed for various concentrations of filler and various configurations of its distribution in the matrix. Based on these experiments, factors that influence the effective coefficient of thermal conductivity of the composite system are analyzed.
Numerical Models of Heat Conductivity of Composite Systems

- The thermal conductivity of the PE composition at low fractions, $W/mK$

<table>
<thead>
<tr>
<th>$t, \degree C$</th>
<th>Experiment $\lambda_{eff}$, $W/mK$</th>
<th>Calculation $\lambda_{eff}$, $W/mK$</th>
<th>$\rho_c$, %</th>
<th>Particle size, microns</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0,269</td>
<td>0,267</td>
<td>0,5</td>
<td>50 – 63</td>
</tr>
<tr>
<td>80</td>
<td>0,181</td>
<td>0,180</td>
<td>0,5</td>
<td>50 – 63</td>
</tr>
<tr>
<td>25</td>
<td>0,275</td>
<td>0,272</td>
<td>0,5</td>
<td>0,9 – 1,5</td>
</tr>
<tr>
<td>80</td>
<td>0,204</td>
<td>0,203</td>
<td>0,5</td>
<td>0,9 – 1,5</td>
</tr>
</tbody>
</table>

**BINARY COMPOSITE MODEL**
*(Calculation and experiments)*

Computer simulation was performed for various concentrations of filler and various configurations of its distribution in the matrix. Based on these experiments, factors that influence the effective coefficient of thermal conductivity of the composite system are analyzed. Let us consider the factors that determine the thermal conductivity of CS: thermal conductivity of the matrix, thermal conductivity of the filler, modification of the boundary layers, clustering of the filler, interfacial thermal resistance and contact resistance of the filler particles.
The clusters considered above were formed naturally because of a random distribution of the filler in the matrix. Of great interest are the distribution structures of the filler associated with their preventive formation (see Figure 2). Figure 4 shows the results of numerical calculations of the effective thermal conductivity for different variants of the distribution of filler particles under the same other conditions. The most favorable particle arrangement is the flow orientation and the fractal structure of the filler distribution. The fractal dimension at the selected concentrations of the filler was in the range from 1.62 to 2.75.

Fig. 4. The calculated dependences of the effective thermal conductivity of the CS “polyethylene-silicon carbide” at a temperature of \( t = 25^\circ C \) and a particle size of the filler 50 – 60 μm for various structures of the distribution of the filler: 1 - random, 2 - longitudinal, 3 - transverse, 4 – fractal.
Numerical Models of Heat Conductivity of Composite Systems

**BINARY COMPOSITE MODEL**
*(Calculation and experiments)*

Figure 5 shows the calculated and experimental data of the CS “polyethylene-carbamide silicon” and “polyamide 6-carbamide silicon” at a temperature of $t=25 ^\circ C$ and a particle size of the filler 50 to 60 microns.

Calculation methods have been used to study the effect of clustering on the effective thermal conductivity coefficient of CS. The dependence (Ff full surface of filler particles) from the mass concentration of the filler is obtained.

Fig.5. The calculated and experimental dependences of the CS “polyethylene-silicon carbide” and “polyamide 6-silicon carbide” at a temperature $t = 25 ^\circ C$ and a particle size of the filler 50 - 60 μm.
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**BINAR Y COMPOSITE MODEL**

*(Calculation and experiments)*

Based on experimental data and calculations, significant factors determining the effective thermal conductivity were determined.

<table>
<thead>
<tr>
<th>Factor/filler concentration</th>
<th>$\rho_c = 0.5%$</th>
<th>$\rho_c = 20%$</th>
<th>$\rho_c = 60%$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix thermal conductivity</td>
<td>$+$</td>
<td>$+$</td>
<td>$-$</td>
</tr>
<tr>
<td>Thermal conductivity of the filler</td>
<td>$-$</td>
<td>$+$</td>
<td>$+$</td>
</tr>
<tr>
<td>Modification</td>
<td>$+$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>Filler Clustering</td>
<td>$-$</td>
<td>$+$</td>
<td>$+$</td>
</tr>
<tr>
<td>Interfacial thermal resistance</td>
<td>$+$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>Thermal contact resistance of the filler particles</td>
<td>$-$</td>
<td>$+$</td>
<td>$+$</td>
</tr>
</tbody>
</table>
SOFTWARE IN THE EDUCATIONAL PROCESS

It is important that manufacturability is ensured — ease of use at the level of teacher and student — is ensured by the maximum automation of development, management, analysis, and control tools; intelligence - a variety of didactic tools; motivation - formed by the learning algorithm; regularization - is ensured by strict observance of the sequence and deadlines for completing tasks. At the Physics and Technology Faculty of the Yanka Kupala State University of Grodno, the concept of using information technologies in education is implemented based on the CACTUS system (an office for automated control of students' current academic performance). The system is a cloud resource that provides a full cycle of the use of electronic tools in education and provides them: creation, editing, assembly, presentation, testing, statistics, assignment of tasks, remote dialogue between student and teacher. We will consider applications developed by us that we use in the educational process.
SOFTWARE IN THE EDUCATIONAL PROCESS

T-physics stands for our way of looking at the learning process when studying the physics topic. We think that the learning process involves theory, problem solving, testing and training. In short, T-physics.

Surely, realizing these issues in one project is a difficult task. Therefore, we decided to begin with problem solving and practice. The learning process involves using high visibility, accessibility and simplicity of the computer model interpretation of the physical processes.

We have set the goal of teaching students problem-solving skills by standard methods as well as computer modeling and simulation. All problems in the book have a common structure: clearly defined problem conditions, formulas and solution examples. Most of the problems described, have computer models for demonstrating the physical processes described. The dataset for the problems is randomly generated, allowing for the effective training of students.
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SOFTWARE IN THE EDUCATIONAL PROCESS

(Physics)

Three point charges $q_i = 1, 2, 3$, a test charge $q$, and their coordinates $(x_i, y_i, z_i)$ are specified. Find the electric field strength and the electric potential due to these charges at the point $P$.

$$q_i = 8.85 \times 10^{-10} \text{C} \cdot \text{m}^2 / \text{V} \cdot \text{m}$$
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SOFTWARE IN THE EDUCATIONAL PROCESS

(Laboratory physics)

I. Zeylikovich
A. Nikitin
N. Matetsky

Entry

Exit
SOFTWARE IN THE EDUCATIONAL PROCESS

(Technology)

3. The stationary problem. Ball
4. Unsteady task. Endless plate
6. Non-stationary task. Ball
7. Unsteady task. Parallelepiped
9. Convective heat transfer.
SOFTWARE IN THE EDUCATIONAL PROCESS
(Conclusion)

The topic of informatization of education, as well as education in general will always be relevant from the point of view of “what to teach and how to teach.” The didactic aspect that determines the content and presentation of educational information is fundamental in the implementation of effective training, regardless of whether we use information technology or not. Are teachers ready to use all the computer “benefits”? We do not mean interactive whiteboards, multimedia opportunities – these are an old way. We are talking about new forms and possibilities of presenting educational material. Despite the thirty-year period of development of the application of information technology in education, it still remains a transition. The foregoing suggests that one should not seek to unify the use of computer technology in education and develop any theoretical platform for this. Each didactic problem is solved specifically.

It is important to ensure manufacturability. Ease of use at the level of teacher and student is provided by the maximum automation of development, management, analysis and control tools. Intelligence is provided by a variety of didactic tools. Motivation is formed by the learning algorithm. Regularization is ensured by strict observance of the sequence and timing of tasks. It is important that manufacturability is ensured — ease of use at the level of teacher and student — is ensured by the maximum automation of development, management, analysis, and control tools; intelligence - a variety of didactic tools; motivation - formed by the learning algorithm; regularization - is ensured by strict observance of the sequence and deadlines for completing tasks.
Thank you for attention!

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