Numerical Simulation of Temperature Field and Microwave Absorption by Carbon Nanotubes and Polymer Composites

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1. Introduction

Polymer processing methods of plastic deformation in the solid phase is the new progressive method to improve the performance of the processing equipment, reduce energy consumption of the production process of obtaining products and improve their quality.

To implement the processes of plastic deformation of polymer materials in most cases apply conductive heating to the main drawback of which is its considerable inertia.

Experimental studies on the application of electrical methods of processing materials and products in order to modify their physical and physico-mechanical properties have shown the efficiency of energy use of microwave of electromagnetic waves.

2. Problem discussion

It is now one of the most promising methods of heat treatment of various dielectric materials become the microwave heating. The effectiveness of microwave heating of dielectric materials can be greatly enhanced through the creation of composite materials with high conductivity materials: carbon, graphite, carbon-graphite fibers or metals

Important issue is to modify the structure and properties of polymeric materials ultrafine particles. Now for the modification of polymers widely used fullerenes, ultrafine carbon particles and carbon nanotubes.

Use as a modifying substance of carbon nanomaterials can be used in the microwave heating properties of nanocarbon to improve microwave processing nano-modified polymer-carbon materials.

The aim of mathematical modeling is to determine the degree of variation of the microwave absorption ABS copolymer with its modification of carbon nanomaterials "Taunit."

3. Objective and research methodologies

The object of these studies used a copolymer of acrylonitrile, butadiene and styrene (ABS copolymer) (GOST 12851-87). As a modifier used nanostructured carbon materials (CNM) "Taunit" (nanofibers, multiwall nanotubes) - dimensional nanoscale filamentary formation of polycrystalline graphite in the form of loose powder with a particle size of 40-100 nm. The investigation of the cylindrical specimens of 5 mm diameter and 15 mm long. Microwave treatment of electromagnetic waves was carried out in the microwave chamber with the radiation frequency magnetron 2450 MHz. Output power of 700W. Microwave heating time of 0-100 sec. The sample temperature during microwave heating time was determined on the surface and in the center of the axis of the sample.

The amount of applied carbon nanomaterial - 1 parts by weight per 100 parts by weight of ABS copolymer.
Medium temperature - 23 ^{0}C.
Density ABS copolymer - 1035 kg/m^3.
The heat capacity of the ABS copolymer - 1800 J / (kg * K).
Thermal conductivity of ABS copolymer - 0.214 W / (m * K).
Density CNM "Taunit" - 2200 kg/m^3.
The heat capacity of CNM "Taunit" - 840 J / (kg * K).
Thermal conductivity CNM "Taunit" - 280 W / (m * K).

Due to the significant complexity of the physical processes involved in the microwave heating of a cylindrical sample chamber of the experimental setup in the following assumptions:

- Flux density of microwave radiation through the surface of the sample is constant and the surface;
- The degree of reflection of microwave radiation from the surface of the sample is the same for the source and nano-modified materials;
- The absorption coefficient is independent of temperature;
- To change the power of the microwave radiation on the sample thickness obeys the Bouguer-Lambert-Beer;
- Heat flow along the axis of the sample available.

Non-stationary temperature field in a cylindrical specimen heated microwave field can be modeled by a solution of transient heat conduction for a solid cylinder with an unlimited volume functional heat source.

Statement of the problem of heat conduction:

$$\frac{\partial t(r,\tau)}{\partial \tau}=a\left(\frac{\partial^2 t(r,\tau)}{\partial r^2}+\frac{1}{r}\frac{\partial t(r,\tau)}{\partial r}\right)+\frac{q(r)}{c\rho};\quad 0\le r\le R;\qquad \tau>0; \tag{1}$$

$$t(r,0)=f(r); \tag{2}$$

$$\frac{\partial t(0,\tau)}{\partial r}<\infty; \tag{3}$$

$$\lambda\frac{\partial t(R,\tau)}{\partial r}+\alpha\,(t(R,\tau)-t_c)=0. \tag{4}$$

The problem (1) - (4) is:

$$t(r,\tau)=\sum_{n=1}^{\infty}\frac{U(\mu,\tau)\,W(r,\mu)}{S}+t_c; \tag{5}$$

where:

t(r, τ) – The temperature field of the cylindrical sample, ^{0}C, as a function of radial coordinate *r*, м, and the time *τ*, s,
R – radius of the cylindrical sample, m;
a – thermal diffusivity of the sample material, m^2 / s;
c – specific heat of the sample material, J / (kg * K);
ρ – density of the sample material, kg/m3;
λ – thermal conductivity of the sample, W / (m * K);
$\nu=\sqrt{a}$, m/s^{0,5};
f (r) – The temperature distribution within the sample at the initial time as a function of radial coordinate, ^{0}C;
α – coefficient of heat transfer from the sample to the environment, W / (m^2 * K);
t_c - Ambient temperature, ^{0}C.

In accordance with the assumption,

$$I(r)=I_0\,Exp(-k\,(R-r)) \tag{6}$$

where
- $I(r)$ – the current intensity of the microwave radiation in the sample, W/m^2;
- I_0 – intensity of the penetrating component of microwave radiation on the sample surface, W/m^2;
- k – the absorption coefficient, 1 / m.

Capacity of the heat source in the sample, caused by the absorption of microwave radiation, is defined as:

$$q(r)=\frac{dI(r)}{dr}=I_0\,k\,Exp(-k\,(R-r)) \tag{7}$$

Effective density and heat capacity of the modified model can be defined additively:

Since the inclusion of nano-carbon clusters in the polymer can be considered as isolated, to calculate the effective thermal conductivity of such a system can use Odelevsky formula:

$$\lambda_{effect}=\lambda_n\left(1-m\left(\frac{1}{1-\lambda_c/\lambda_n}-\frac{1-m}{3}\right)^{-1}\right) \tag{8}$$

The indices *n* and *c* relate to the characteristics of the polymer and nanocarbon respectively, *m* – mass fraction of nanocarbon in the modified polymer sample.

With a uniform initial temperature distribution in the sample, ie, at $f(r)=Const=t_0$

$$F=(t_0-t_c)\frac{\nu R}{\mu}J_1\left(\frac{\mu}{\nu}R\right) \tag{9}$$

By achieving agreement between the calculated temperature field with the experimental data (Table 1) are given numerical values of I_0 and *k*.

Table 1. The experimental and calculated data on the microwave heating of the sample ABS copolymer modified with carbon nanomaterials "Taunit".

Time, s	Temperature, ^{0}C			
	Center of the sample		The sample surface	
	Experimental	Calculated	Experimental	Calculated
0	23	23,0	23	23,0
10	28	24,3	30	27,5
20	30	27,2	32	30,4
30	30	30,1	33	33,2
40	32	33,0	34	35,9
50	33	35,7	36	38,5
60	37	38,3	39	40,9
70	40	40,8	41	43,3
80	42	43,2	42	45,5
90	45	45,5	46	47,7
100	48	47,7	49	49,8

The minimum value of I_0, corresponding to total absorption of microwave radiation pattern for a given heating rate is determined based on the total heat balance for a given point in time: the total heat source of heat equal to the change of heat content of the sample, less heat loss from the sample surface to the environment.

$$\tau R\int_0^R q(r)\,dr=\frac{2c\rho}{\tau}\int_0^{\tau}\int_0^{r} r\,(t(r,\tau)-t_c)\,dr\,d\tau-2R\alpha\int_0^{\tau}(t(R,\tau)-t_c)\,d\tau \tag{10}$$

The value of *k* is determined by iteration to match the calculated temperature difference in the sample with the experimental ones.

Determination of the parameter *k* for the nano-modified ABS copolymer is in the same manner at a fixed flow of microwave radiation through the external surface of the sample from the experimental data presented in Table 2.

Table 2. The experimental and calculated data on the microwave heating of samples ABS copolymer, initial and modified carbon nanomaterials "Taunit."

Time, s	Temperature of the center of samples,^{0}C			
	ABS copolymer original		ABS copolymer modified	
	Experimental	Calculated	Experimental	Calculated
0	23	23,0	23	23,0
10	29	24,4	29	24,3
20	29	27,0	30	27,2
30	29	29,6	30	30,1
40	30	32,1	32	33,0
50	31	34,5	33	35,7
60	33	36,8	37	38,3
70	35	39,0	40	40,8
80	39	41,2	42	43,2
90	41	43,2	45	45,5
100	45	45,1	48	47,7

The calculation results
Calculation program written in algorithmic language C++.

The calculations, the following indicators:
1. The minimum value of the intensity I_0 = 580 W/m^2.
2. The actual value of the intensity I_0 = 830 W/m^2.
3. The absorption coefficient for the initial sample k = 2,0 * 10^3 1 / m
4. The absorption coefficient for the nano-modified sample k = 4,5 * 10^3 1 / m
5. Characteristics of nano-modified ABS copolymer:
- Density 1046 kg/m^3 (1.1% change);
- Heat capacity of 1790 J / (kg * K) (change 0.5%);
- Thermal conductivity of 0.220 W / (m * K) (3.0% change)

From these data suggest that the efficiency of microwave heating increases when making CNM. The experimental study of the process by the example of solid formation ram extrusion using high-pressure cell (Fig. 1) showed a reduction of the required pressure formation nano-modified materials of pre-short microwave heating by 15-20% (Fig. 2).

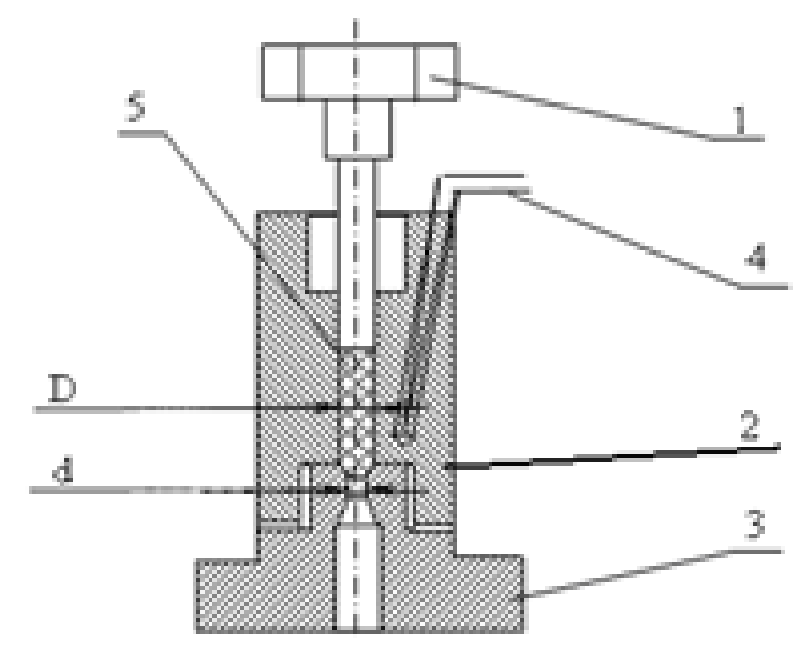

Figure 1. High-pressure cell:
1 - punch 2 - matrix; 3 – base;
4 - thermocouple; 5 - storage material.
D - diameter of the initial sample,
d - diameter of the spinneret.

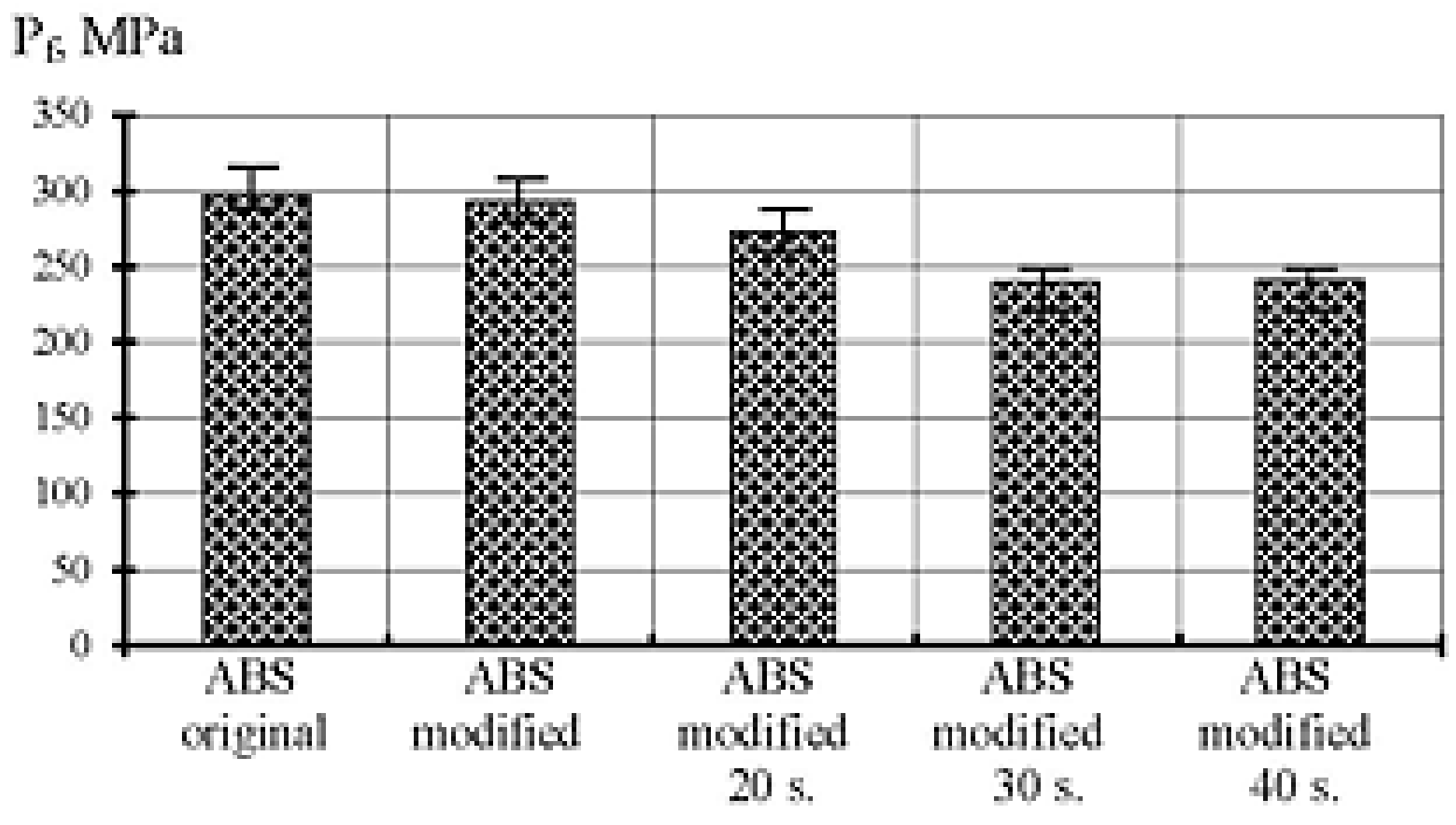

Figure 2. Diagrams of dependence of necessary pressure of formation from microwave processing time. λ_{extr} = 2.07, T_{extr} = 298 K.

Conclusion

1. Introduction 1 wt. of nanocarbon material "Taunit" little can increase the thermal characteristics of the ABS copolymer, but a more than 2-fold increases the value of the absorption of microwave radiation, which leads to a significant intensification of heat nano-modified ABS copolymer in a microwave field.

2. The proposed methodology of mathematical modeling of microwave heating nano-modified polymer-carbon materials can solve a number of application of scientific and engineering problems, including determine the heating modes to achieve the desired characteristics of plastic material.