

An Interface Phenomenon in Polymer Matrix Composites Induced by Influence of Constant Magnetic Fields

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The goal of this work is to find out mechanism of constant magnetic field influence on formation of polymer surface layers in a Polyvinyl chloride composite filled with ferrite microparticles. Calculations of a magnetic field in a polymer surface layer of the microcomposite were performed by Fourier's method assuming three different sets of simplifying assumptions. Results of these calculations are presented for different values of concentration of ferrite particles in the polymer matrix composite. They and data of a known experimental investigation indicate that polymer surface layer friability structures in the polymer matrix composites of this type significantly depend on the concentrations of the filler.

Keywords: Composite, Magnetic Field, Polymer Surface Layer, Friability, Mathematical Modeling, Artificial Intelligence Problem.

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1. INTRODUCTION

Creation of new construction materials stimulates the technical progress. Specifically, viability of new electric devices largely depends on characteristics of magnetic materials they are partially made of [1, 2]. Since traditional magnetic substances are fragile, require significant processing efforts, and have high densities; devices containing these materials become cost drivers and bring highly undesirable excessive weight in a bunch of important applications [3]. Synthesis of new organic magnets [4-8] can partially satisfy the need in light magnetic materials. However, their industrial mastering requires significant expenditures [9]. A material with needed magnetic properties can be obtained through filling a polymer with magnetic microparticles [3], [10, 11]. Hence, it is much more beneficial to satisfy the above mentioned need with composites containing industrially mastered polymers.

To reach desired magnetic properties of the composite, one often has to increase the filler concentration significantly [12-22]. Unfortunately, it can cause notable deterioration of mechanical properties of the material [10, 11], [23]. However, these properties of the microcomposite can be improved through influencing its formation by a constant magnetic field (CMF) if the filler concentration is higher than the one at which the phase transition occurs [24]. Since properties of polymer matrix composites (PMCs) with fine powder fillers are determined to the great extent by physical and chemical changes of the polymers situated in their polymer surface layers [9], it can be explained by the following. Polymer macromolecules are oriented in a CMF. The greater the value of H^2 is, the more oriented the macromolecules are. Besides, if the CMF is non-uniform, then they are pushed out of the regions of high values of H^2 with the force that is proportional to the value of $H \cdot |\nabla H|$. Thermal motion of these macromolecules opposes both these effects. For macromole-

cules a polymer matrix composed of, both these effects can be neglected at the temperature of the polymer melting and values of the magnetic field that can be achieved under laboratory conditions [25]. However, in a polymer surface layer of the composite the interaction of a macromolecule with the magnetic field is influenced not only by the temperature field but also by the aggregative absorption mechanism [9]. It gives the opportunity to regulate properties of a PMC through influencing the formation of its surface layer structure by a CMF. To figure out which one of two above mentioned interface phenomena causes the improvement of mechanical properties of the polymer matrix microcomposite with sufficiently high concentration of magnetic particles and synthesized under influence of a CMF, one has to know how to calculate the magnetic field in a polymer surface layer of such the PMC near the phase transition. Although the mathematical model of calculation of a magnetic field in the PMC of this type that is valid near the phase transition is presented in the recent research [24], it was not determined in the paper [24] whether the improvement of mechanical properties of the polyvinyl chloride (PVC) composite with sufficiently high concentration of the Fe_3O_4 fine powder and formed under the influence of the external CMF was caused by the orientation of polymer macromolecules of the surface layers or by their pushing out of regions of high values of H^2 . The goal of this work is to show that the improvement of mechanical properties of the PMCs with sufficiently high magnetic filler concentrations reached through influencing their formation by CMFs [24] can be explained by the second effect.

2. THE CHOICE OF MODELS OF THE CALCULATION OF THE MAGNETIC FIELD IN A POLYMER SURFACE LAYER OF THE PMC

In the recent research [24], to prepare PMCs, PVC was mixed with Fe_3O_4 fine powder. The mixture was

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exposed to pressure and temperature as high as respectively 10 MPa and 420 K and to the external magnetic field so strong that all powder particles were in the state of the magnetic saturation. Taylor's theorem allows us to suppose that calculating the magnetic field in the vicinity of the filler particle situated in the PMC we can neglect the influence of the other Fe₃O₄ particles. Therefore, in the model # 1 the calculation is performed for a single spherical Fe₃O₄ particle with the uniform magnetization density \vec{M} placed in the external CMF \vec{H}_0 (see Fig. 1). However, the size of the surface layer can turn out to be large enough for the other filler particles to influence the magnetic field inside of it significantly. In this case, this problem can not be solved precisely due to randomness of filler particle disposition in a PMC. Therefore, it can be referred to the class of artificial intelligence problems and should be solved using simplifying assumptions. In the recent research [24], PMC samples were prepared in the form of cylinders with their diameters equal to $2.5 \cdot 10^{-2}$ m and their heights equal to $5 \cdot 10^{-2}$ m. Since the sample height is 5 times smaller than its diameter, in the model # 2 the boundary effects are neglected and it is assumed that the Fe₃O₄ particles create the quasi lattice in the 3-dimensional space as shown on Fig. 2. Calculations according to the model # 3 are performed to estimate the error of magnetic field calculation according to the model # 2 that arises due to the substitution of the disposition of filler particles shown on Fig. 2 for the chaotic disposition of filler particles in the PMC in the framework of the model # 2. Therefore, the filler particle disposition in the model # 3 is the quasi lattice that can be obtained from the quasi lattice of the model # 2 through shifting filler particle layers denoted on Fig. 2 by numbers $4 \cdot p - 1$ where $p = 1, \tilde{p}$, $\tilde{p} = q/2$ if q is even and $\tilde{p} = (q-1)/2$ if q is odd (here and below q is the number of horizontal filler particle layers in the quasi lattice of the model # 2) at the distance equal to the half of the lattice period in the direction of the x-axis with subsequent shifting them at the same distance in the direction of the y-axis. Such the assumptions about dispositions of filler particles allow applying Fourier's method to the calculation of the magnetic field in the frameworks of the models # 2 and # 3. Since the quasi lattices in these models are different, their periods can be different too if the total mass of the filler in the sample is fixed. Therefore, in what follows D and \tilde{D} denote periods of the quasi lattices in the models # 2 and # 3 respectively. If all filler particles have a cubical shape, h is the height of the sample and l is the length of the edge of the filler particle; then from Fig. 2 it follows that the numbers of horizontal filler particle layers in the quasi lattices of the models # 2 and # 3 are equal to $(h-l)/D+1$ and $(h-l)/\tilde{D}+1$ respectively. The quasi lattices of the models # 2 and # 3 can be viewed as sets of cells that are periodically situated in the part of a space bounded by two planes that contain respectively the top base and the bottom one of the sample with the same

periods in the directions of the x-, y- and z-axes that are equal to D and \tilde{D} respectively. From Fig. 2, it follows that the volumes of the smallest cells of this type in these quasi lattices are equal to D^3 and $2 \cdot \tilde{D}^3$ respectively. In the case of the quasi lattice of the model # 2 and in the case of the quasi lattice of the model # 3, positioning all such the cells along one line does not change the volume of the part of the space they occupy. Therefore, if V_0 is the volume of the sample and N_0 is the number of magnetic particles in the microcomposite, the periods of these quasi lattices are given by such the expressions: $D = \sqrt[3]{4 \cdot V_0 / N_0}$, $\tilde{D} = \sqrt[3]{5 \cdot V_0 / 2 / N_0}$. To be able to compare results of calculations in the frameworks of the models # 2 and # 3 with respective results of calculations in the framework of the model # 1, we assume that the volume of the filler particle in the model # 1 is equal to the volume of the filler particle in each one of the models # 2 and # 3. Thus, $R = \sqrt[3]{3/4 \cdot \pi} \cdot l$ (see Figs. 1 and 2).

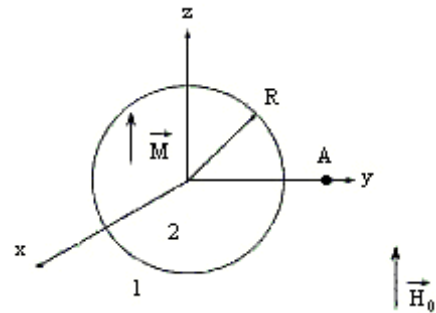


Fig. 1 – Set up of the model # 1.

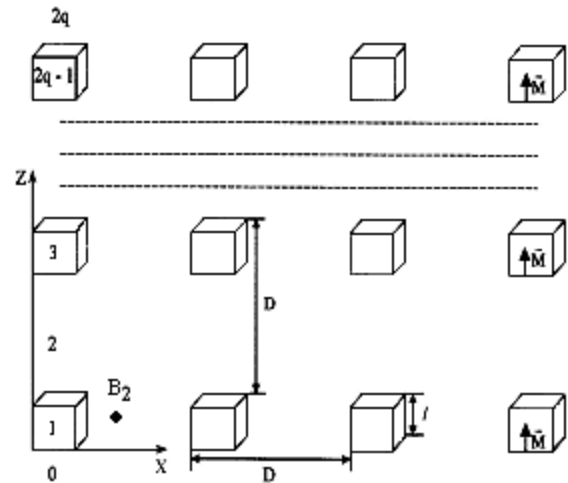


Fig. 2 – Filler particle disposition assumed in the model # 2.

3. RESULTS OF NUMERICAL CALCULATIONS

The values of $H|\vec{\nabla}H|$ and H^2 at the point A chosen at the center of the surface layer (see Fig. 1) were calculated in the framework of the model # 1. In the frameworks of the models # 2 and # 3, these values were calculated at the points respectively B_2 and B_3

that have same coordinates z and y as centers of the respective filler particle side faces have and are situated at the centers of the surface layers, and then these values are averaged over all filler particle layers of the respective quasi lattices. Calculations were performed for the samples with the volumetric concentrations of the filler equal to 0.1 %, 1 %, and 10 %. The sizes of the surface layers of these samples are respectively the following [26]: 4.1×10^{-5} m, 2.3×10^{-5} m, and 1.2×10^{-5} m. The values of $H|\bar{\nabla}H|$ calculated in the frameworks of the models # 1, # 2, and # 3 are presented in Table 1 in units $10^{14} \text{ A}^2/\text{m}^3$. As for values of H^2 calculated in the frameworks of the models # 1, # 2, and # 3, they are presented in Table 2 in units $10^{10} \text{ A}^2/\text{m}^2$. As it was explained in Section 3, the difference between the respective values of $H|\bar{\nabla}H|$ calculated in the frameworks of the models # 2 and # 3 can be interpreted as the error bars of the value $H|\bar{\nabla}H|$ calculated at the center of a surface layer and the difference between their average value and the respective value of $H|\bar{\nabla}H|$ calculated in the framework of the model # 1 can be interpreted as the contribution of the filler particles to the value of $H|\bar{\nabla}H|$ at the center of a surface layer. From the data presented in Table I, it follows that the value of $H|\bar{\nabla}H|$ at the center of the surface layer situated in the vicinity of a filler particle is significantly influenced by the other filler particles if the volumetric concentration is equal to 0.1% and that the ratio of the portion of the value of $H|\bar{\nabla}H|$ generated by these particles to the uncertainty in the value of $H|\bar{\nabla}H|$ due to chaos in filler particle disposition in a sample goes to zero as this concentration increases. Similarly, the difference between the respective values of H^2 calculated in the frameworks of the models # 2 and # 3 can be interpreted as the error bars of the value of H^2 calculated at the center of a surface layer situated in the vicinity of a filler particle, and the difference between their average value and the respective value of H^2 calculated in the framework of the model # 1 can be interpreted as the contribution of the filler particles to the value of H^2 calculated at the center of a surface layer. From the data presented in Table 2, it follows that the value of H^2 calculated at the center of the surface layer situated in the vicinity of a filler particle is influenced by the other filler particles insignificantly, and that the significance of the influence of these particles on this value increases as the filler concentration in a sample increases. Using the experimental data presented in the reference [24], we formulate the following observations:

1. Young's modules of the samples of PMCs composed of PVC mixed with a Fe_3O_4 fine powder and created in the presence of an external CMF are notably greater than Young's modules of the respective samples

created in the absence of an external CMF under exactly same the other conditions if the filler concentrations are relatively high.

2. Young's modules of the samples of PMCs composed of PVC mixed with a Fe_3O_4 fine powder and created in the presence of an external CMF are slightly lower than Young's modules of the respective samples created in the absence of an external CMF under exactly same the other conditions if the filler concentrations are relatively low.

3. Poisson's ratios of samples of PMCs composed of PVC mixed with a Fe_3O_4 fine powder and created in the presence of an external CMF are notably greater than Poisson's ratios of the respective samples created in the absence of an external CMF under exactly same the other conditions if the filler concentrations are relatively high.

4. Poisson's ratios of samples of PMCs composed of PVC mixed with a Fe_3O_4 fine powder and created in the presence of an external CMF are only slightly greater than Poisson's ratios of the respective samples created in the absence of an external CMF under exactly same the other conditions if the filler concentrations are relatively low.

Table 1 – The calculated values of $H \cdot |\bar{\nabla}H|$ in units $10^{14} \text{ A}^2/\text{m}^3$.

Model Number	Volumetric Filler Concentration		
	0.1 %	1 %	10 %
1	2.059	10.65	47.09
2	2.45	13.21	52.02
3	2.43	12.69	41.22

Table 2 – The calculated values of H^2 in units $10^{10} \text{ A}^2/\text{m}^2$.

Model Number	Volumetric Filler Concentration		
	0.1 %	1 %	10 %
1	130.64	130.55	130.01
2	130.93	131.80	134.70
3	130.48	134.02	140.38

Thus, we can assert that at some value of the filler concentration the phase transition occurs in the microcomposite synthesized under the influence of a CMF. The first phase of the microcomposite corresponds to relatively low concentrations of the filler whereas the second one corresponds to relatively high concentrations of the magnetic particles. The results of numerical calculations of the value of $H \cdot |\bar{\nabla}H|$ and the value

of H^2 at the center of a surface layer in the vicinity of a filler particle in the frameworks of the models # 1, # 2, and # 3 indicate that the contributions of the other filler particles to the value of $H \cdot |\bar{\nabla}H|$ is significant at low filler concentrations and can be neglected at high filler concentrations and that such the contributions to the value of H^2 are insignificant at all the considered values of filler concentrations. Therefore, we assert

that four above mentioned experimental observations can be explained by the following two assumptions:

1. Magnetic fields that can be created under laboratory conditions can significantly alter formations of surface layer friability structures of PMCs with fine powder magnetic fillers.

2. These structures in PMCs with low magnetic filler concentrations formed under the influence of external CMFs are different from these structures in PMCs with high magnetic filler concentrations formed under the influence of external CMFs. This fact explains the above mentioned phase transition.

4. CONCLUSION

In this paper it is argued that in the laboratory experiment [24] the external CMFs significantly influence the formations of the polymer surface layer friability structures of the PMCs. These structures in the PMCs with low filler concentrations formed under the influence of the external CMFs are different from the structures in the PMCs with high filler concentrations

formed under the influence of the external CMFs.

The calculation results presented in Tables 2 indicate that although the value of H^2 calculated in the surface layer situated in the vicinity of a filler particle is influenced by other filler particles insignificantly, the significance of the influence of these particles on this value of H^2 increases as the filler concentration in a sample increases. Therefore, the mechanical properties of the PMCs with higher Fe_3O_4 fine powder concentrations should be investigated and the results of the calculations of the magnetic fields in their surface layers should be analyzed to check whether a new phase transition occurs.

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