



Avoiding the global change in climate

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Abstract. Nowadays, humankind extracts most of the energy it consumes from fossil fuels. Unfortunately, it entails building up the carbon dioxide in the atmosphere. People have to cut the emissions of this gas drastically to avoid the global change in the climate in few decades. One of the options they have consists in using solar energy as a primary energy source. In this case, the main difficulty consists in the large scale energy storage needed for satisfying needs in energy at night. In this work, we give an example of energy storage in polymer surface layers of a polymer matrix composite filled with magnetic microparticles. Specifically, in the recent research V. B. Demchuk argued that improvement of mechanical properties of Polyvinyl chloride (PVC) composite materials filled with ferrite microparticles reached at sufficiently high filler concentrations through influencing the formation of these microcomposites by constant magnetic fields (CMFs) occurs thanks to the fact that PVC macromolecules situated in the polymer surface layers of these microcomposites are pushed out of regions of high magnetic field intensity. His reasoning is based on integrated analysis of laboratory measurements and numerical calculations. In this paper, we present computational abstractions that allow handling the chaotic disposition of the filler particles during calculation of magnetic fields in polymer surface layers of microcomposites near phase transition points under the constraint due to limited performance of modern computers.

Keywords. *Global change in climate; Polymer surface layer; Phase transition; Integrated analysis, Chaotic disposition.*

1 Introduction

Cutting emissions of the carbon dioxide drastically is a top priority for humankind because building up this gas in the atmosphere causes global changes in the climate. They can become irreversible if nothing will be done regarding this matter during next few decades. This problem is challenging since people extract energy mainly from fossil fuels. Unfortunately, scientists have not come up with the technology of large scale carbon capturing yet. Moreover, such the technology entails difficulties with the storage of the extracted gas. Specifically, large quantities of the carbon dioxide cannot be stored in oceans due to ecological considerations. Besides, they cannot be stored underground since the leakage of this gas puts in danger human lives. Therefore, significant effort should not be put in this direction. Solar energy is the source that is rich enough to become a new primary energy source for the humankind. Although this source is not available round the clock, potentially it can satisfy all human needs in electricity many

times over. Therefore, to switch to extracting most of the needed energy from this source, people have to come up with the technology of the large scale energy storage [1]. Each year the amount of energy that is stored in the result of photosynthesis is enough to satisfy all human needs in energy several times [2]. Hence, chemical bonds are a proper place to store energy. To avoid additional expenditures, it is important to discover examples of the energy storage in chemical bonds of the industrially mastered materials. In this work, we provide an example of such the storage in polymer surface layers of polymer matrix composites (PMCs) containing only those polymers that are mass-produced. In Section 2, we present this example and describe the research methodology that led to its discovery in the reference [3]. In Section 3, we illustrate one of the elements of this methodology. Section 4 contains a brief summary.

2 Storing energy in polymer surface layers of PMC

Mechanical properties of an industrially mastered polymer filled with magnetic microparticles can be improved through influencing the formation of the composite with a constant magnetic field if the filler concentration is higher than the one at which the phase transition occurs [4]. There are two interface phenomena that can be responsible for this improvement. Specifically, a constant magnetic field can orient macromolecules of the polymer surface layer and these molecules can be pushed out of the regions of the high magnetic field intensity [3]. In the reference [3], V. B. Demchuk argues that it is the second phenomenon that is responsible for the above mentioned effect. Although he uses classical considerations, they are relevant since the classical physics is the limiting case of the quantum one. Both these phenomena assume energy storage in chemical bonds. Traditional numerical analysis of real life problems assumes parallel computing and is hindered by various scale effects induced by a choice of boundary conditions. Unfortunately, these effects become extremely important near phase transition points [5]. Therefore, in the paper [3], to figure out which interface phenomenon is responsible for the improvement of the mechanical properties of the microcomposite, the Cyber-Physical System (CPS) methodology is used. In a CPS, computing experiences the lack of resources and is integrated with physical processes. Finding new computational abstractions is important for development of this emerging field [6]. Such the generalization of notions is essential of the framework of computational thinking. For example, the abstraction of an algorithm is not supposed to produce the desired output within a finite modern processor time frame [7]. The following section presents computational abstractions that allow calculating magnetic fields in polymer surface layers of microcomposites near phase transition points.

3 Handling chaotic dispositions of magnetic particles during calculations of the magnetic fields

In the recent research [4], to prepare PMCs, PVC was mixed with Fe_3O_4 fine powder. The mixture was 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 Fe_3O_4 particles. Therefore, in the model # 1 the calculation is performed for a single spherical Fe_3O_4 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 cannot 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 [4], PMC samples were prepared

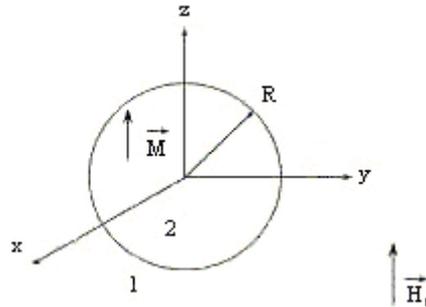


Figure 1: Set up of the model # 1.

in the form of cylinders with their diameters equal to $2.5 \cdot 10^{-2}$ m and their heights equal to $5 \cdot 10^{-3}$ 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 Fe_3O_4 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

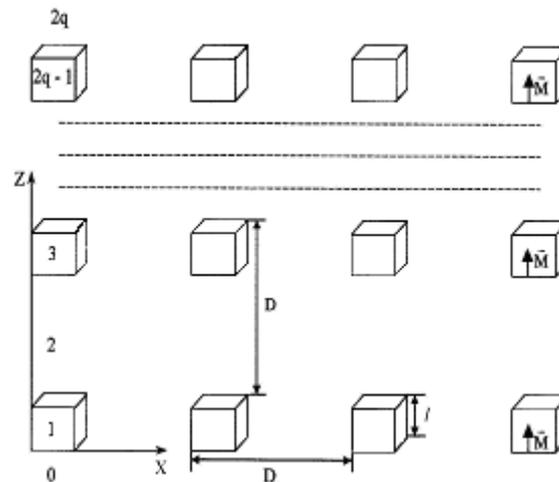


Figure 2: Filler particle disposition assumed in the model # 2.

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 one 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 $p = \overline{1, \tilde{p}}$, $\tilde{p} = q/2$ 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.

4 Conclusions

During next few decades people have to make radical changes in the way they extract energy. They cannot keep extract energy mainly from fossil fuels even if they come up with the technology of the large scale carbon capturing since the extracted gas cannot be stored in oceans and underground due to respectively ecological and safety considerations. Humankind should turn its attention to solar energy. This source is so rich that all human needs in energy are only its tiny portion. However, people cannot take advantage of this source at night. Therefore, to start using solar energy heavily people have to come up with the technology of large scale energy storage. In this work, it is pointed out that such the storage can be realized in chemical bonds of mass-produced materials. Specifically, energy can be stored in polymer surface layers of industrially mastered polymers filled with magnetic microparticles [3]. This effect was discovered thanks to integrated analysis of the results of numerical modeling and the ones of experimental measurements. In this work, we present the computational abstractions that allow handling random disposition of the magnetic microparticles inside a polymer composite filled with magnetic microparticles near a phase transition point during calculation of a CMF in a polymer surface layer of the composite.

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