

# HEAT TRANSFER IN NANOCOMPOSITES BASED ON TEXTURED POLYMER MATRIX

Razvan Florin BARZIC<sup>1</sup>, Iuliana STOICA<sup>2</sup>, Andreea Irina BARZIC<sup>2\*</sup>,  
Gheorghe DUMITRASCU<sup>1</sup>

<sup>1</sup>“GHEORGHE ASACHI” UNIVERSITY, FACULTY OF MECHANICS, Iasi  
<sup>2</sup>“PETRU PONI” INSTITUTE OF MACROMOLECULAR CHEMISTRY, Iași

**Abstract.** The paper deals with investigation of the heat transfer process in nanocomposites prepared from carbon nanofiller and polymer matrix. If subjected to shear forces, the latter presents the ability to organize after a specific concentration in organic solvent. The morphology of the used polymer is examined by atomic force microscopy, while that of the nanocomposite is analyzed by optical microscopy. The thermal conduction of the matrix is theoretically determined from its structural features, whereas heat transfer of the samples is assessed from different mathematical models.

**Keywords:** thermal conductivity, carbon nanotubes, nanocomposites.

**Rezumat.** Lucrarea investigheaza procesul de transfer termic in nanocompozite preparate din nanotuburi si matrice polimera. Cand aceasta este supusa forfecarii ea posedea abilitatea de a se organiza la o anumita concentratie in solvent organic. Morfologia polimerului este studiata prin microscopie de forta atomica, iar cea a nanocompozitelor prin microscopie optica in lumina polarizata. Datele morfologice confirma orientarea buna a agentului de ranforsare in matricea lichid cristalina supusa forfecarii. Conductivitatea termica este teoretic evaluata prin diferite modele, care au aratat o imbunatatire considerabila a acestei proprietati prin ranforsare cu nanotuburi de carbon.

**Cuvinte cheie:** conductivitate termică, nanotuburi de carbon, nanocompozite.

## 1. INTRODUCTION

The<sup>4</sup>problem of thermally conductive materials still raises the interest of researchers that have directed their efforts to design new systems with higher performance (Han & Fina, 2011). Previous reported investigations reveal that introduction of carbon-derived nanofillers in polymers represents a viable solution (Barzic *et al.*, 2012). When the reinforcement particles display anisotropic shape (such as nanotubes, nanofibers) it is possible to obtain an enhanced thermal conductivity along the particle long axis if the nanofillers are oriented. Among the factors employed for the alignment of carbon nanotubes (CNTs) in polymers one can mention: electric fields, magnetic fields, uniaxial pressure and mechanical deformation (Iakoubovskii, 2009). Literature (Dierking *et al.*, 2005) reported a study concerning the orientation of CNTs starting from the self-aligning nature of the polymer matrix. The advantage of wrapping CNTs with liquid crystal (LC) molecules is that electric fields of lower orders of magnitude are ensuring the alignment as compared to CNT alignment without the liquid crystal molecules. Moreover, there are liquid crystal polymers that are able to achieve a special texture after the deformation relaxation of their

semi-rigid chains. For instance, cellulose ethers solutions present lyotropic phase in many of organic solvents.

This paper investigates the heat transfer in nanocomposites prepared from a LC matrix and CNTs. The polymer solution is subjected to shear deformation in order to gain an ordered texture that is useful in orientation of the nanofiller. The morphology and thermal properties of the samples are analyzed.

## 2. EXPERIMENTAL

### 2.1. Sample preparation

The cellulose ether was purchased from Sigma Aldrich and used as received along with dimethylacetamide solvent. The solutions of 60 wt% polymer were casted on glass substrates and subsequently sheared. The CNTs dispersion was mixed with matrix solution and then sheared. The samples were left to dry at room temperature under saturated solvent atmosphere.

### 2.2. Characterization methods

Polarized light microscopy images (PLM) were taken on Olympus BH-2 instrument.

Atomic force microscopy (AFM) measurements were performed on SPM SOLVER Pro-M plat-

\* Corresponding author: [irina\\_cosutchi@yahoo.com](mailto:irina_cosutchi@yahoo.com)

form, having a NSG10 cantilever with a 10 nm tip radius.

Thermal conductivity of the nanocomposites samples was determined using the parallel, series, Lichtenecker and Maxwell-Eucken models, defined by Eqs. (1)-(4), respectively:

$$k_c = k_m \phi_m + k_p \phi_p \quad (1)$$

$$k_c = 1 / [(\phi_m / k_m) + (\phi_p / k_p)] \quad (2)$$

$$k_c = k_m^{\phi_m} + k_p^{\phi_p} \quad (3)$$

$$k_c = k_m \frac{2k_m + k_p + 2\phi_p(k_p - k_m)}{2k_m + k_p - 2\phi_p(k_p - k_m)} \quad (4)$$

where  $k$  is thermal conductivity,  $\phi$  is the volume fraction of the nanofiller, the index “c” is for composite, “m” is for matrix and “p” is for nanoparticles.

The calculations require the knowledge of the polymer thermal conductivity, which in this case was assessed from the theory of Bicerano (Bicerano, 1996):

$$k = 0.135614 + 0.126611 \cdot {}^1\chi^{BB} / N + 0.108563(N_N + N_O - 0.125N_H) / N \quad (5)$$

where  ${}^1\chi^{BB}$  is the fraction of first order connectivity index that contributes to the bonding among the backbone atoms;  $N_N$ ,  $N_O$ ,  $N_H$  are the number of nitrogen, oxygen, and hydrogen atoms in the structural unit, and  $N$  is the number of non-hydrogen atoms.

### 3. RESULTS AND DISCUSSION

The morphology of the LC polymer was investigated by microscopy methods in order to examine the changes of the matrix surface features induced by the shearing process. It is well known that cellulose derivatives LC solutions subjected to shearing are able to develop a peculiar texture observed under the form of bands. This phenomenon is favoured by the semi-rigid character of the macromolecular chains, which after cessation of the shear force develop a typical texture consisting in two types of periodicities. The main pattern is viewed as fine, long, parallel, equidistant lines running perpendicular to the shear direction. At low shear rates (under  $100 \text{ s}^{-1}$ ) main bands appear as a result of the sinusoidal variation in the fibrillar (oriented macromolecules) trajectory. The secondary bands are smoother and slightly tilted from the shear direction. They are formed parallel to shear direction and are produced due to some competitive processes, like orthogonal deformation to bulk orientation and hydrodynamics of the solvent evaporation. Figure 1 reveals all these aspects, including the morphology of the LC matrix prior to shearing (right image) and the main band texture (left image) produced after removing the deformation force. The resulted morphology of the LC polymer is maintained even after solvent evaporation, leading to films with textured surface. The data presented in Figs. 1 and 2 regard the analysis of the matrix topography under solid form.

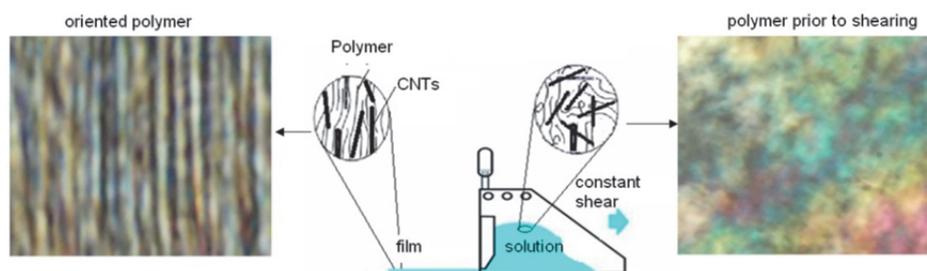


Fig. 1. Polarized light microscopy images of the studied polymer before and after shear orientation.

In order to examine more closely the two types of bands, AFM imaging was employed. This method highlights formation of both periodical structures along and perpendicular to the shear direction (Fig. 2). The 3D image shows that on the top of the main bands of few microns width there are noticed smaller bands of nanometric dimensions, which are thought to be essential for CNTs alignment. Figure 3 presents the morphology of the reinforced matrix with CNTs. The PLM image reflects the good orientation of the nanofiller inside the matrix along the shear direction.

The thermal conductivity variation with nanofiller amount is theoretically determined and the results are depicted in Figure 4.

The Lichtenecker model does not predict accurately the thermal conductivity at low CNT amounts since at 0 % nanofiller it should lead to the value matrix, namely  $0.18 \text{ W/m K}$ . the series model gives the smallest values of the samples' conductivity, being considered the lowest limit. In our opinion the real thermal behaviour is a combination between parallel and Lichtenecker

approaches. All applied models indicate that reinforcement generates a considerable increase in thermal conductivity values upto almost three

orders of magnitude if considering the parallel approach. These data make the analyzed sample suitable for heat dissipation applications.

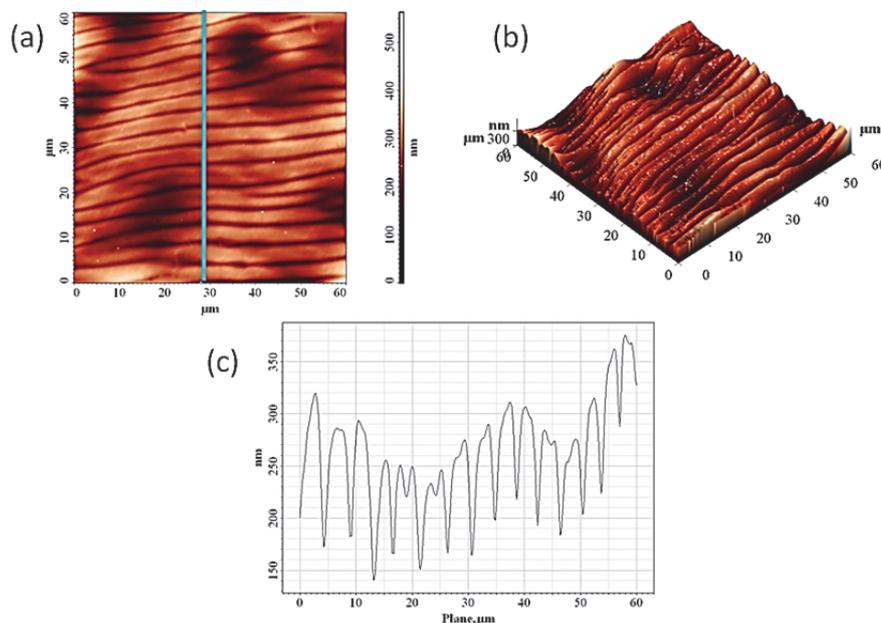


Fig. 2. AFM 2D (a) and 3D images (b) and cross-section profile (c) of the studied polymer subjected to shear orientation.

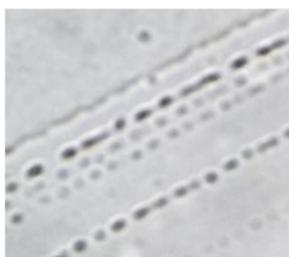


Fig. 3. Polarized light microscopy image of the studied nanocomposites.

the bands are formed perpendicular and parallel to the deformation force direction. The small bands present nanometric dimensions, being useful for alignment of CNTs in the LC polymer along the shear direction. This conclusion is supported by PLM image. The thermal conductivity is enhanced by addition of CNTs and leads to results that recommend the analyzed nanocomposites as thermo-conductive materials, particularly at high percents of nanofiller (14 %) in the LC matrix.

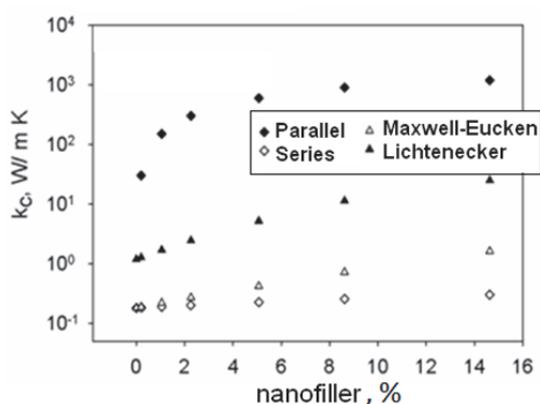


Fig. 4. Thermal conductivity dependence on the nanofiller amount for studied nanocomposites.

#### 4. CONCLUSIONS

The shear deformation leads to a specific morphology of the matrix consisting in two periodicities. According to PLM and AFM images

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