MODELING OF NANOFIBERS INTERACTION WITH THE ENVIRONMENT

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Abstract

Nanomaterials change our life. Every day they find applications in new branches of technology. At the same time, some branches of technology, like civil engineering, are rather conservative and do not accept new approaches lightly. Nanotextiles exhibit a number of qualities that make them a promising material for civil engineering applications. They can potentially play a role of filters, protective layers, armature and others. Properties of the nanotextiles can be significantly influenced by parameters of technological process. Pure experimental search of the optimal technological parameters to achieve the desired properties of the final material can be very tedious. Thus, a theoretical dependence of the properties of the nanotextile on parameters of the technological process must be established. Two independent tasks must be solved for this: the dependence of nanotextile structure on technological parameters, and determination of physical, chemical or biological properties of a nanotextile of a given structure. In this paper we discuss steps necessary for the solution of the second task.

Nanotextile is a material with extremely large porosity, which makes standard macroscopic models for the description of its properties inappropriate. Thus, any successful model must be based on the specific structure of the nanotextile. After the structure is known the next step is to understand all important interactions between nanofibers and the environment. The set of such interactions depend on the problem under consideration. Finally, the properties of the material should be determined as a numerical solution of the corresponding 3D model.

Keywords: Van der Waals, DLVO potential, Monte Carlo simulations

1. INTRODUCTION

Nowadays there exist a lot of theories allowing a successful modeling of physical properties of macroscopic materials, e.g. [1]. However, when applied to modeling of micro- and nano- materials, these theories predict the results quite different from the observed in the experiments. This fact is explained by structure of such materials, and new types of their interactions with the environment. Good example of such interaction is provided by van der Waals forces. In macroscopic sample the volume, where van der Waals forces are important, is limited by very thin layer close to the surface of the sample. The volume of this layer is negligible in comparison with the total volume of the sample. This is the reason why normally van der Waals force is not taken into account when modeling physical properties of macroscopic substances. On the other hand, consider a nanotextile composed of nanofibers with diameter small than 1 μm. The diameter of such fibers is comparable with the characteristic range of van der Waals interaction. Consequently, the effective volume of space influenced by this force is comparable with the volume of the fiber, and, thus, with the volume of the sample itself. In other words, unique structure of nanotextiles ensures their much stronger interaction with the environment in comparison with standard macroscopic materials. Even relatively thin layer of nanotextile can potentially provide a level of protection of a substrate, comparable with much thicker layer of standard protective material [2].

Every successful simulation of physical properties of a nanomaterial must take into account its structure. There are different methods to determine this structure. Sambaer et al. analyze SEM photos of nanotextiles in order to determine size distribution of fibers and pores [3, 4]. Other method is based on analysis of a structure of a

cross-section of textiles [5, 6]. Both mentioned methods allow to create a 2D model of one layer of nanotextile. The three-dimensional model is obtained by creation of a sandwich-like structure.

However, determination of the microscopic structure of the material is not enough to perform the simulation. The correct set of physical interaction has to be chosen, and the choice depends on the specific problem which has to be solved.

2. INTERACTIONS WITH NANOFIBERS

As mentioned above, the understanding of interactions between the nanofibers and the environment is very important for the successful description of their properties. In macroscopic world we usually neglect some interactions (van der Waals forces, dipole interactions etc.). However, at micro- and nano-scales this is not possible anymore, because such forces can have a substantial influence on the resulting properties.

The specific set of interactions which should be taken into account depends on the problem under consideration. For example, Sambaer et al. study filtering properties of nanotextiles [7]. Small particles flowing with the air through the filter interact with nanofibers and can be caught by several types of attractive forces. In this case, the most important interactions between nanofibers and the particles are hydrodynamic forces of different kind: drag force, lift force, adhesion force, and friction force.

On the other hand, civil engineering applications assume different modes of interaction of nanotextiles with the environment, and, thus, require different set of basic forces. One of the most promising applications of nanotextiles in civil engineering is protection of a surface of construction material from the aggressive influence of the surrounding. In this situation the nanotextile is attached to the surface of the protected material. For example, a well-known problem with plasters is a washout of small stones by rains. Even a relatively thin layer of hydrophobic nanotextile applied to the surface of the plaster can protect it from this danger.

The physics of protective layers is somewhat different from the physics of filters. In filters the main mechanism of transport of air, particles or humidity is convection, while in protective layers the main role is played by diffusion. Also, the time scale of the corresponding processes is larger, so that weaker interactions like van der Waals forces can exhibit themselves.

2.1. Van der Waals force

Van der Waals force is the weakest type of interaction between neutral atoms and molecules. In this type of interaction such neutral atoms are attracted to each other due to spontaneous origination of dipoles because of chaotic motion of electrons around the atomic nuclei. There exist several possibilities for the formation of such dipoles, which lead to different sub-types of van der Waals forces: London dispersion force, interaction of permanent and induced dipoles [8].

Peridynamics is a method of analysis of influence of van der Waals forces on mechanical behavior of nanofibers. In this methods all interactions are treated as long-range interactions. The analysis shows that existence of van der Waals forces may increase the strength and stiffness of nanofiber net [9]. Bobaru used polyethylene fibers with molecules aligned along the axis of the fiber. Atoms along the fibers are connected by covalent bonds, while neighbor polymer chains are attracted by van der Waals forces (**Fig. 1**). Eyring kinetic theory of fracture was applied and the analysis was performed with the help of Monte Carlo method [10]. The rate of bond breakage is given by

$$\dot{p} = \tau \exp\left\{\frac{-U + \beta\sigma}{kT}\right\} \tag{1}$$

where U is activation energy of the bond, β is the activation volume for the bond, σ is the external stress responsible for bond fracture, τ is thermal vibration frequency of the bond, k and T stand for Boltzmann constant and absolute temperature respectively [11].

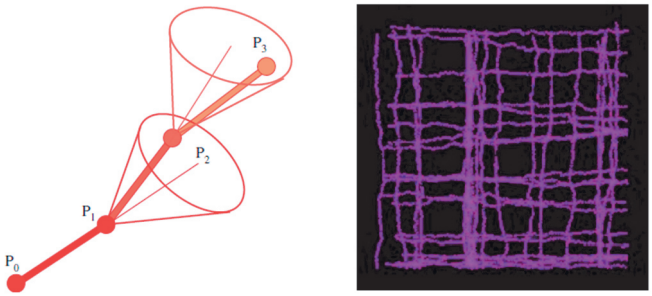

Fig. 1 Peridynamics method: generating a new node in a direction that remains inside the con (left], the resulting optical network (right) [9]

With the help of this model Bobaru estimates influence of molecular mass, rate of deformation and temperature on strength of polyethylene fibers.

2.2. DLVO potential

Recently, Derjaguin, Landau, Verwey, Overbeek (DLVO) model has found wide application in simulation of interactions between electrically charged particles in dielectric liquid. This theory can be applied to interactions of non-organic nanoparticles with nanofibers, but also to description of motion of microorganisms. Below is the main equation used to calculate a potential U between two balls with radius a and charge Z separated by distance r. The influence of the environment is described by permeability ε, concentration of ions n, and temperature T. These basic equation can be modified in many ways [12].

$$\beta U(r) = Z^2 \lambda_B \left(\frac{\exp(\kappa a)}{1+\kappa a} \right)^2 \frac{\exp(-\kappa r)}{r} \tag{2}$$

$$\lambda_B = \frac{e^2}{4\pi\varepsilon_0 \varepsilon k_B T} \tag{3}$$

$$\kappa^2 = 4\pi\lambda_B n \tag{4}$$

$$\beta^{-1} = k_B T \tag{5}$$

Kaledin et al. studied glass microfibers covered with nanofibers of aluminium oxide and hydroxide. The fibers had length of 250 nm and diameter of 2 nm. The whole system looks like a cylinder with very rough surface. It was found, that such connection creates a strong electrical field, which can attract nano- and micro-particles from distance of 0.3 mm in several seconds. However, the electrical field in this experiment is by order of several magnitudes stronger than predictions of DLVO model. The resulting field can attract different particles, such as viruses, bacteriophages, bacteria or latex spheres. These unwoven materials absorb submicron particles using their natural electrical charge from much larger distances than their geometrical size [13].

3. CONCLUSION

In order to simulate physical properties of nanotextiles three general steps must be performed. The first step is analysis of the problem and determination of the basic physical interactions important for the studied phenomena. The second step is to choose a corresponding mathematical model of the physical force. This step is very important and many researches are working on improvement and modifications of existing models to make them applicable to wide variety of situations. Finally, an appropriate numerical scheme has to be chosen, such as Monte Carlo method. The results also depend on the geometrical structure of the material. To estimate the influence of the structure on the properties of nanotextiles one can perform simulations using

same numerical method and expressions for the potential, but assuming different geometrical structures of the material. Example structures for such calculations include chaotic network of straight lines, solid volume with large number of spherical holes of different sizes, sandwich structures etc.

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