Molecular Dynamics Simulation of Sensor-Enabled Geosynthetics

H. Yazdani[*], K. Hatami [**], T. Hawa[***], B. P. Grady[****]

[*] School of Civil Engineering and Environmental Science, University of Oklahoma, yazdani@ou.edu
[**](corresponding Author) School of Civil Engineering and Environmental Science,
University of Oklahoma, 202 W. Boyd St., Room 334, Norman, OK, USA, kianoosh@ou.edu
[***]School of Aerospace and Mechanical Engineering, University of Oklahoma, hawa@ou.edu
[****]School of Chemical, Biological and Materials Engineering, University of Oklahoma,
bpgrady@ou.edu

ABSTRACT

Geosynthetics are polymeric materials which are used in a wide range of civil engineering applications. Recently, a novel technique has been developed at the University of Oklahoma which is based on the piezoresistivity of carbon black-filled polymers which eliminates the need for conventional instrumentation to measure tensile strain in modified geosynthetics. In this technique, a polymeric material (e.g. polyethylene, PE) and an electrically conductive filler (e.g. carbon black, CB), are blended to fabricate Sensor-Enabled Geosynthetics (SEG) with piezoelectric characteristics. In this study, Molecular Dynamics (MD) simulations are used to examine the effect of the filler on the stress-strain behavior of SEG samples. Dreiding and OPLS force fields are adopted for the simulations which are carried out in the LAMMPS© environment. Results of the study indicate that adding small quantities of CB to otherwise pure PE samples may not adversely affect their tensile strength properties.

Keywords: sensor-enabled geosynthetics, molecular dynamics, carbon black, polymeric materials

1 INTRODUCTION

In less than three decades, geosynthetics have revolutionized many aspects of civil engineering practice, and in some applications they have entirely replaced traditional construction materials. There are few developments that have had such a rapid growth and strong influence on civil engineering practice as the multi-billion dollar geosynthetics technology [1].

As the number of structures and facilities involving geosynthetics increases worldwide, their safety and serviceability assessment becomes a matter of great concern. Today, health monitoring and timely measurements are used to prevent catastrophic failures and costly repairs due to inadequate structural performance resulting from uncertainties in site conditions, material properties and behavior, construction practice, environmental effects and loading conditions.

Current technology for the instrumentation of geosynthetics primarily entails the attachment of strain gauges and extensometers to a geosynthetic material. The existing technology currently employed to measure strains in geosynthetics requires fairly complex and expensive data acquisition systems. Some of the criteria that are applied when selecting a strain gauge include accuracy, long-term stability, cyclic endurance, range of operational temperature, ease of installation, tolerable amounts of elongation, and stability in a harsh environment. Strain gauges are usually calibrated against average strains from crosshead displacement in in-isolation tests. However, these calibration factors are not truly applicable to a geosynthetic layer embedded in soil due to at least three important reasons:

1- Different in-soil mechanical properties (e.g. tensile modulus) of geosynthetics compared to their in-isolation values due to confining pressure and interlocking effects,

2- Complications such as soil arching due to the mechanical interference and interaction of strain gauges and their bonding assembly (e.g. adhesive and protective sleeve) with the local soil, and

3- Unknown local stiffening effect of the bonding assembly.

These factors can introduce significant errors in measured strains in geosynthetics in field applications. Applying in-isolation calibration factors to in-soil readout data could lead to significant underestimation of reinforcement strain and axial load with potential consequences with respect to the stability and performance of the geosynthetic structures.

During the last few years, a novel technique has been developed at the University of Oklahhoma which is based on the piezoresistivity of electrically filled polymers to measure the tensile strain in modified geosynthetics without the need for conventional instrumentation [2-5]. In this technique, the polymeric material and electrically conductive filler are combined to provide Sensor-Enabled Geosynthetics (SEG). The SEG having a predetermined concentration of the electrically conductive filler provides a geosynthetic with an electrical conductivity and a strain sensitivity within the percolation region or slightly above it. The electrically conductive filler is selected from a group

consisting of metal powders, conductive carbon black, graphite fiber, carbon nanotubes, or combinations thereof. The polymer type and also the filler type, shape, arrangement and orientation can alter the mechanical and electrical properties of the blend.

In this paper, the molecular dynamics (MD) simulation of SEG materials is discussed. The long-term objective of the study is to investigate the influences of polymer and filler properties, filler concentration and the fabrication method on the electrical and mechanical properties of SEG materials using validated atomic-scale numerical models. As an initial step toward this long-term objective, this paper describes selected details of an MD simulation approach as applied to an example pure and blended polymer composite to study their mechanical behavior. Specifically, preliminary results of an MD simulation study of a pure polyethylene (PE) matrix and a carbon black (CB)-blended PE sample subjected to uniaxial tensile stress are presented and compared.

2 MOLECULAR DYNAMICS SIMULATIONS

2.1 Molecular Structure of Models

Molecular models of SEG in this study were developed by generating the position of each atom using a code written in MATLAB$^©$. The PE chains were generated on a tetrahedron lattice and the graphite structure was used for CB as there is no universally accepted structure for CB [6].

Each atom in the model was assigned an ID number and the atomic structure of the composite was visually inspected for proper connectivity of atoms before each numerical simulation (Fig. 1).
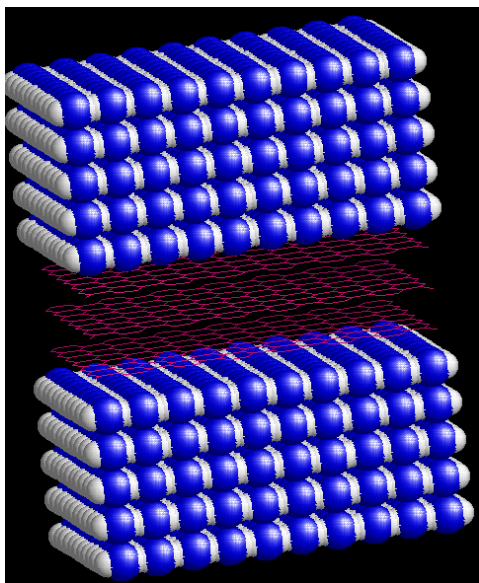

Figure 1: Atomic structural model of the PE-CB blend in this study.

Periodic boundary conditions were employed to replicate the unit cells in three dimensions. Selected data on the polymer chains are given in Table 1.

Number of CH$_2$ units	2000
Number of C atoms in graphite	118
Molecular weight of PE molecules (g/mol)	28052.7
Molecular weight of CB molecules (g/mol)	1416

Table 1: Data on the molecular system employed in this study

The molecular weight of each CH$_2$ unit was determined and multiplied by the number of the units. The lengths and molecular weights of the chains in different unit cells were kept constant to establish consistent matrix properties [7]. The same structures were used for the polymer in both the pure and composite (i.e. SEG) systems simulated in this study.

2.2 Force Field

Once the molecular structure of each composite model was developed, bond stretching, angle bending and dihedral potentials between the atoms were defined using corresponding force fields. In this study, the potential energy between the PE molecules was defined using the Dreiding force field [8] and that between the CB atoms using the OPLS force field [9].

The non-bonded van der Waals (VDW) interactions within or between all molecules were approximated using the Lennard-Jones 12-6 (LJ) potential. The functional forms of the interaction between the atoms force fields are shown in Table 2.

Interaction	Potential	Functional Form
Bond	Harmonic	$E(r) = \frac{1}{2}k_r(r-r_0)^2$
Angle	Harmonic Cosine	$E(\theta) = \frac{1}{2}k_\theta\left[\cos\theta - \cos\theta^0\right]^2$
Dihedral	Cosine	$E(\vartheta) = \frac{1}{2}k_\vartheta\left\{1 - \cos\left[n_\vartheta(\vartheta - \vartheta^0)\right]\right\}$
Non-bonded	Lennard-Jones	$E_{VDW} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right]$

Table 2: Potential energy functions used in this study

2.3 Simulation Characteristics

The MD simulations were carried out in LAMMPS$^©$ environment [10] in the Isothermal-Isobaric (NPT) Ensemble at 300 ^{o}K with 1-fs time steps. The elastic properties of the pure polymer and the SEG were evaluated in two steps. First, the molecular model was brought to an intial state of equilibrium. Then, the model was subjected to tensile strain and was solved to a new state of equilibrium. The size of the simulation box was $20 \times 20 \times 30$ Å.

The equilibrium state for both cases of pure and composite systems was first obtained to establish a presscribed stress-strain relationship. There are two general steps in MD which are required to attain an equilibrium state. First, a stable energy state needs to be attained at a prescribed temperature and secondly, a minimum initial stress state needs to be attained within the simulation box. The stable energy state was obtained by consecutively applying the canonical (NVT) and microcanonical (NVE) ensembles to the initial model. Then, the isothermal–isobaric (NPT) ensembles were applied on the molecular model to minimize the initial stresses [11].

In the MD simulations carried out in this study, two opposite sides of the simulation box were uniformly subjected to a unidirectional strain up to 20% (Fig. 2). The mechanical reponses of both the pure and composite polymeric materials were assumed as piecewise linear elastic. The energy of the simulation box in each case was measured for each strain increment and then the uniform stress in the system was calculated as:

$$\Delta\sigma = \frac{2\Delta E}{\Delta\varepsilon} \qquad (1)$$

where $\Delta\sigma$ is the change in uniform tensile stress, ΔE is change in the energy of the system, and $\Delta\varepsilon$ is the incremental strain in the ith step.
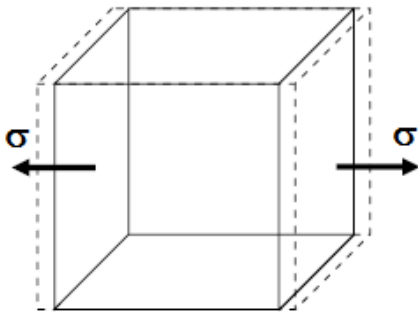

Figure 2: Uniaxial tension on the simulation box.

3   RESULTS

Fig. 3 shows the stress-strain behavior of pure and composite systems simulated in this study. The simulated mechanical responses of both the pure and blended systems appear to be somewhat undulatory, which is believed to be a numerical effect. However, these preliminary results indicate that adding small quantities of CB (e.g. 5% in this example) to otherwise pure PE samples may not adversely affect their tensile strength properties. These results need further verification. However, they have important implicatuions to the development of SEG materials. In genneral, SEG products are expected to contain increased concentrations of CB as compared to conventional geosynthetic products (which are, e.g. within the range 1-

4%). One concern related to adding significant amounts of CB to polymers is a possible reduction in their tensile strenth, ductility and other mechanical properties. The study described in this paper is part of the authors' on going study to determine suitable quantities of conductive nano-particles that can be used to fabricate SEG products without compromising the mechanical properties of their host polymers.
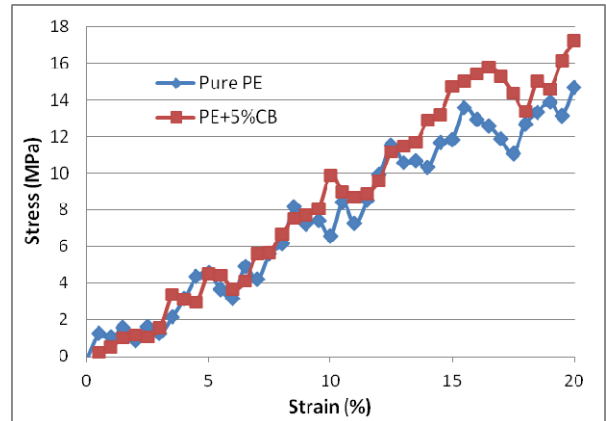

Figure 3: MD stress-strain responses of pure PE and composite PE/CB systems.

4   CONCLUSIONS

The stress-strain behavior of an example sensor-enabled geosynthetic (SEG) material was investigated using molecular dynamics simulation. The host polymer in both pure and composite systems was polyethylene (PE). Carbon black was added to polyethylene to produce a SEG material with piezoresistive properties. Prelimiary results of the study, while requiring further validation, indicate that adding small quantities of CB (e.g. 5% in this example) to otherwise pure PE samples may not adversely affect their tensile strength properties.

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