

Structure and Dynamics of Hybrid Polymer/Gold Nanoparticle Systems through Atomistic Molecular Dynamics Simulations.

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Abstract

Hybrid polymer/nanoparticle systems are a relatively new class of materials that has attracted growing scientific and technological interest [1-4]. In this work, the properties of polyethylene chains around of a gold nanoparticle at a temperature of 450 K are investigated using classical atomistic molecular dynamics simulations.

A classical Morse-type potential, which was parameterized based on the results of density functional calculations [1], used in order to describe the interaction between the polymer and the gold nanoparticle. Several gold nanoparticles with Wulff construction were studied, with diameter ranging from around 2.5–5 nm [2] and polyethylene chains consist of 22 monomers [3]. A typical snapshot of the model system is shown in Figure 1.

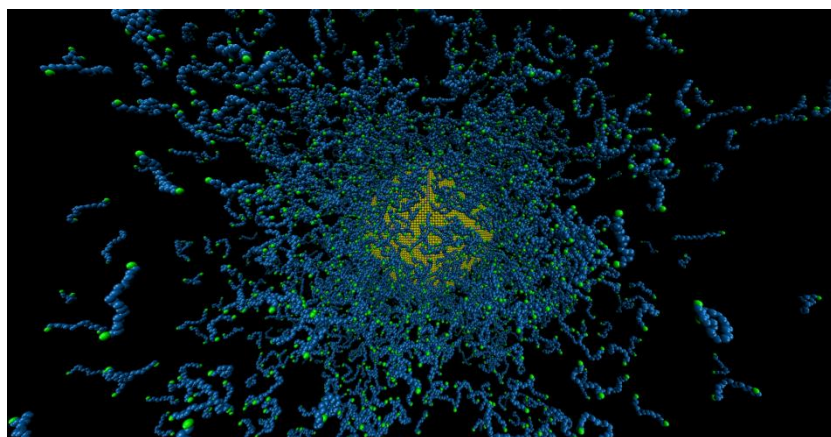


Fig. 1: Snapshot from MD simulation of hybrid polyethylene/gold nanocomposite at 450K. Au nanoparticle (3101 atoms, diameter of 5.02 nm) and polyethylene (5040 chains, 22-mers per chain) are shown. With yellow is the Au and with grey are the edges of Au nanoparticle. With blue are the CH₂ and with green the CH₃ monomers.

The structural, conformational, and dynamical properties of the chains were analyzed and compared to the behavior of the bulk polyethylene system. In more

detail, we report data concerning polymer density profiles, bond order parameter, segmental and terminal dynamics (Figures 2 and 3). All properties are examined as a function of distance from the Au NP.

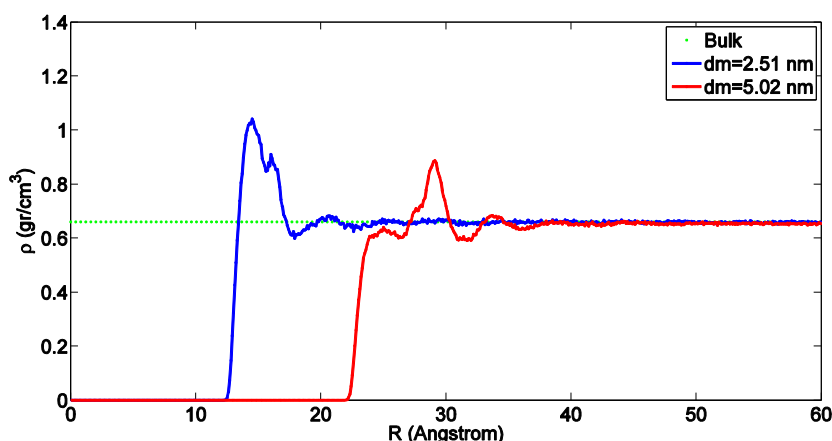


Fig. 2: Monomer density profiles of polyethylene as a function of R (distance from the center of mass of the gold nanoparticle) for the two hybrid systems.

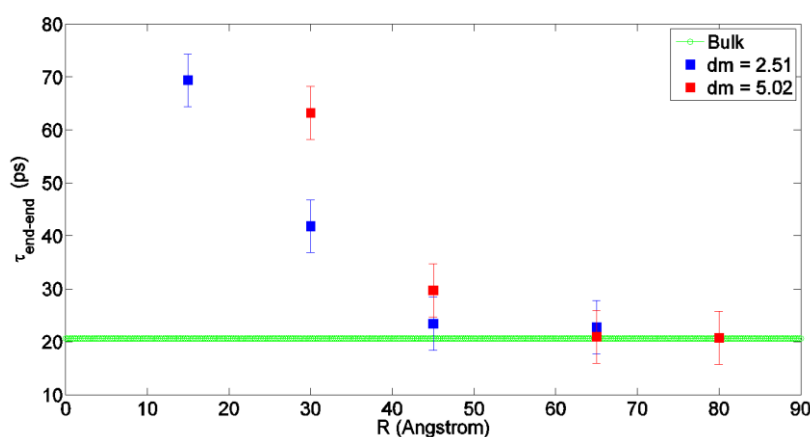


Fig. 3: Relaxation time of polyethylene segment v_{1-3} along R (distance from the center of mass of the gold nanoparticle) for the two hybrid systems.

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