



Depth sensing-induced inelastic deformation at heterogeneous polymer surface



L. Dai, V. Sorkin, Y.W. Zhang*

Institute of High Performance Computing, Singapore

ARTICLE INFO

Article history:

Received 6 February 2015

Received in revised form

7 April 2015

Accepted 3 May 2015

Available online 12 May 2015

Keywords:

Polymer

Depth-sensing

Interface

ABSTRACT

Depth-sensing devices such as atomic force microscope have been widely used to characterize the morphology, nanostructure, surface composition and local materials properties of heterogeneous polymers. Such measurements are based upon a fundamental hypothesis that the deformation of polymer is elastic, that is, there is no tip-induced surface inelastic alteration or damage. Using molecular dynamics simulations, we show that the inelastic alteration at heterogeneous polymer surfaces induced by the sensing tip is intrinsic and unavoidable. Such tip-induced alteration arises from the differences in Van Der Waals interactions between different atomic species in the polymer and in the sensing tip, leading to atomic shuffling and re-shuffling, which cause inelastic alteration in both molecular structures and mechanical properties at and near the polymer surface. The present work highlights the need to reinterpret the data obtained from depth-sensing testing by considering this intrinsic inelastic deformation occurring at and near heterogeneous polymer surfaces.

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1. Introduction

Heterogeneous polymers have been widely used in various engineering applications, such as electronics, biotechnology, medical devices, etc [1]. For heterogeneous polymers at the nanoscale, due to the large surface-to-bulk ratio, the composition, morphology, nanostructure, and materials properties at and near the surface region (ANSR) become crucially important for their functional performance [2]. To probe their surface structures and properties, depth-sensing devices, such as atomic force microscope (AFM), have been widely used [3–5]. However, recent studies have shown that the measurement results have poor reproducibility and large uncertainties [6,7]. The underlying reasons for this remain controversial and highly debated [3,8]. For example, it is believed that polymers are so soft that their mechanical response cannot be measured accurately due to the low system compliances of those depth-sensing devices [4]. In addition, polymers generally undergo time-dependent deformation; therefore, the effect of viscoelasticity can play an important role [7,9,10]. Furthermore, lack of accurate

information regarding the polymer surface morphology at the atomic scale (like roughness, crystallinity, etc.) can cause difficulties in interpreting measurement data [11,12]. Therefore, it is still a significant challenge to accurately probe the composition, morphology, nanostructure, and mechanical properties of heterogeneous polymers at ANSR [13].

Currently, depth-sensing devices, such as AFM [14], employ shallow-depth probing to avoid surface inelastic alteration or damage [4]. During surface sensing, polymer surface is usually chemically saturated. Thus its interaction with the sensing tip, which is normally made of silicon or carbon-based ceramics, is dominated by non-bonding Van Der Waals (VDW) interactions between the sensing tip and the atoms at ANSR of the polymer, and is generally effective within a distance of around 1 nm, which is in the same range as the probing depth of these sensing devices. It is well-known that VDW interactions are relatively weak and thus it is tacitly believed that the weak interactions between the sensing tip and polymer surface do not cause any inelastic alteration or damage to the polymer surface [12].

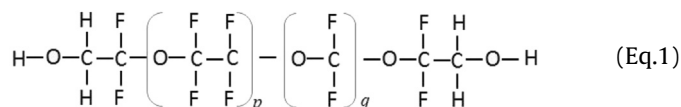
Here, we would like to show that the shallow-depth probing, which has been commonly used in depth-sensing devices, may be questionable in characterizing the surface properties of heterogeneous polymers. The basis for our argument is that, for heterogeneous polymers, VDW interactions are atom species-dependent, i.e., a different pair of atomic species will have a

* Corresponding author. Institute of High Performance Computing, 1 Fusionopolis Way, 16-16 Connexis, 138632 Singapore, Singapore. Tel.: +65 64191478.

E-mail addresses: dail@ihpc.a-star.edu.sg (L. Dai), sorkinv@ihpc.a-star.edu.sg (V. Sorkin), zhangyw@ihpc.a-star.edu.sg (Y.W. Zhang).

different equilibrium distance and also a different interacting strength. Therefore, atoms with different chemical species at ANSR of a heterogeneous polymer will interact differently with atoms in the sensing tip. It should be emphasized that for a heterogeneous polymer, this effect is intrinsic and unavoidable. Then, an important question arises: Can these VDW interaction differences cause inelastic alteration of surface structures, which in turn changes the mechanical properties of heterogeneous polymer? Unfortunately, so far, there is no answer to this question, and thus fundamental understandings on this issue are still lacking. Clearly, revealing the fundamentals of this effect and its implication on the measurement of depth-sensing devices is not only of great scientific interest, but also of direct technological impact on currently widely used depth-sensing devices. Therefore, demonstrating the existence and also revealing the fundamentals and implications of this effect is the subject of the present study.

The surface morphologies and mechanical properties of heterogeneous polymer films play an important role in many nanoelectromechanical-systems (NEMs) [15–17], such as in mechanical sensors, actuators, head-disk drives. Here, we select a diamond-like-carbon (DLC) [18] tip and a heterogeneous polymer film, that is, perfluoropolyether (PFPE, or named ZDOL [19]) film overlying on a DLC substrate as a model system for our study. It is noted that this system has been widely used in hard-disk drives [12]. It is well-known that DLCs are hard, hydrophobic, chemical inert, and thermally stable, and have been widely used as coat in NEMs [20]. The chemical formula of ZDOL [21] is,



where, $p = q = 10$. ZDOL is an amorphous polymer with a linear backbone chain mainly consisting of C- and O-atoms, and side-chain F-atoms bonded to C-atoms in the backbone. This polymer

has been widely used as a lubricant, which can effectively reduce the interfacial adhesion and friction for DLC-coated components [22,23]. Therefore, this model system is not only useful for revealing new physical insights into the surface and sub-surface atomic deformation in heterogeneous polymers under depth-sensing, but also for providing practical understandings on the interactions between these important materials, that is, a DLC sensing tip and a ZDOL film.

Given the daunting challenge associated with the experimental access to the interfacial structures and atomic activities in the extremely small contact zone confined and buried in between ZDOL film and the DLC-tip, molecular dynamics (MD) simulations provide a powerful tool that enables us to conveniently define the VDW interaction between different chemical species, track individual atomic movements, and extract the contact information, such as contact force, atomic morphology and atomic deformations, thus effectively filling the gap in our understanding of contact profiles, mechanical properties and also buried activities at the contact interface during depth-sensing [24–26]. Hence, in the present work, we perform MD simulations on the depth-sensing of a DLC-tip on the ZDOL film overlying a DLC substrate. Our goal is to demonstrate the presence of tip-induced inelastic surface alteration and reveal the fundamental understandings and implications of this tip-induced change in polymer surface structure and also its modifications of mechanical properties.

2. Model

Fig.1a shows the full atomic model, including a DLC tip, a 4 nm-thick ZDOL film and a 5 nm-thick DLC substrate. Periodic boundary conditions were applied along the lateral (X, Y) directions. The DLC structure was obtained by a heating-cooling process from the crystalline diamond to an equilibrated amorphous state as described before [27]. Concerning the ZDOL film, individual ZDOL chain was firstly built up with a molecular weight of 1888 Da (unified atomic mass unit). Then, multiple ZDOL chains were mixed into an amorphous cell with desired size and density of 1.83 g/cm³ as described before [28]. The atomic interactions of DLC were

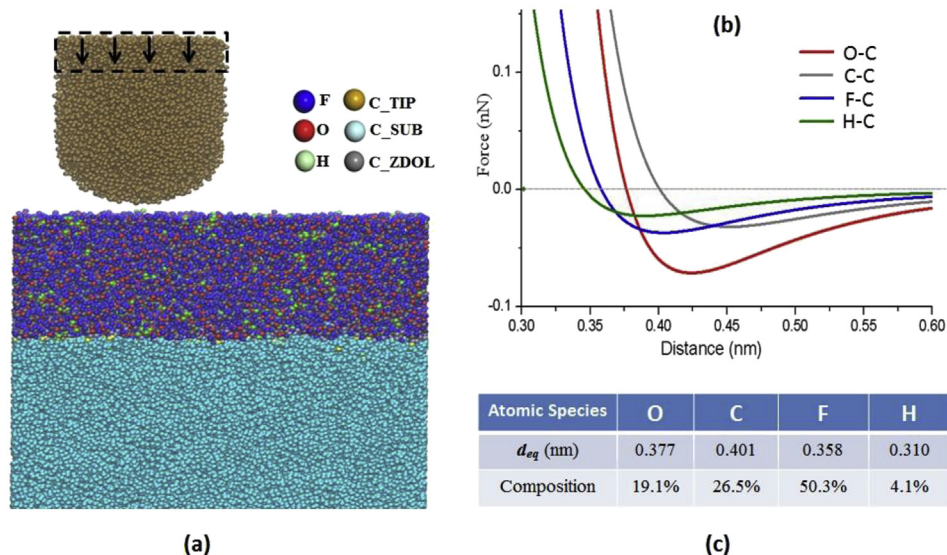


Fig. 1. (a) Front view of the atomic model for DLC-tip/ZDOL/DLC-substrate: F-atoms (blue), O-atoms (red), H-atoms (green), and C-atoms (grey) of the ZDOL film and C-TIP (brown), C-SUB (cyan, in substrate) atoms are shown. (b) VDW force-distance curves between different ZDOL atom species and C atom. (c) VDW equilibrium distance (d_{eq}) and constituent composition (atom species fraction) for ZDOL polymers. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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