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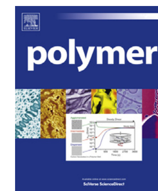

Interfacial adhesion behavior of polyimides on silica glass: A molecular dynamics study

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ABSTRACT

We investigate the adhesion behavior between polyimide and silica glass using molecular dynamics simulations, which is important for improving the manufacturing process of flexible displays. Various polyimides are simulated to understand the complex adhesion mechanisms that occur at the interface with inorganic glass. Through the pulling process implemented within the framework of steered molecular dynamics using reactive force-field, we calculate properties such as potential of mean force, pulling distance, and pulling force, which govern the adhesion behavior at the polymer-glass interface. It is found that a polyimide with a lower coefficient of thermal expansion requires a greater force but a shorter pulling distance to completely detach it from the silica surface. The change in the chain conformation during the pulling process reveals that polyimide chains near the interface dominate the molecular response due to their stronger adhesion to the glass surface. The decomposed energy terms from the interatomic potential indicate that the contribution from bonds and coulombic energy play the most significant role in the deformation of the system. Finally, failure mode analysis demonstrates that adhesive failure is the dominant mechanism regardless of the type of polyimide.

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1. Introduction

Polyimide (PI) materials have generated significant technical interest due to their thermal stability, mechanical properties, and electrically insulating nature [1–4]. These excellent material properties have made PI beneficial for a wide range of engineering applications, including laminated automobile windshields, polymer-coated optical communication fibers, and pharmaceutical glass labware with anti-frictive polymer coatings [4–6]. In particular, PI is one of the most favorable substrate materials used in the production of flexible displays as they largely determine performance and reliability of the display. [5] [7], Although conventional plastic materials are shock-resistive, lightweight, chemically stable, easy to form in various shapes, suitable for continuous process, insulating, and optically transparent, their poor thermal stability has limited their use as flexible substrates for display applications. [8] [9], Specifically, during flexible display manufacturing, the processing temperature can rise above 300 °C, over which most plastic materials decompose [9]. In this regard, the outstanding thermal properties of PIs with low thermal expansion as well as their superior glass transition temperature make them suitable as a promising candidate for the substrate of flexible displays. Outstanding thermal properties in PIs are possible due to strong electrostatic interaction between electron donor-acceptor in PI, known as charge transfer (CT) complex. [6] [10–12].

However, during the process of flexible display manufacturing, PIs tend to delaminate from the supporting glassy material, which potentially increases the risk of structural failure at the organic-glass interface. (The schematic view of detaching process is presented in Fig. S1, Supplementary Material) Therefore, developing an in-depth understanding of the interfacial adhesion behavior is of great importance for improving the structural reliability for these

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types of devices.

Adhesion is the key interfacial phenomenon observed in the assembly and packaging process for electronic devices. This interfacial adhesion is complex and is driven by a number of different factors such as physical (*e.g.*, roughness) and chemical nature of the glass surface, types of polymers, rigidity, thermal behavior, humidity, chemistry of the coupling layer between the glass and the polymer [13–15]. For a functional flexible display substrate, efficient control of the adhesion between the PI substrate and the carrier glass is particularly important. This is because the adhesive interaction must be strong enough to maintain structural integrity while also being weak enough to allow for separation of the PI from the glass; thus, the adhesion energy should be neither too strong nor too weak. If it is too strong, the detachment process causes unrecoverable damage at the interfacial region, resulting in structural failure. If it is too weak, then the glass carrier cannot perform its function of holding PI and the other components placed on its surface during assembly. Hence, developing an understanding of the adhesion mechanism and determining the governing parameters at the interface of PI and glass is critical for improving the manufacturing process.

Great efforts have been made to research heterogeneous interfaces to understand the fundamental aspects of the adhesion at the organic-inorganic interfaces such as polymeric materials placed on Si-based substrates. For example, an experimental study for aromatic PI films on SiO_2 suggests that no chemical bond is observed at the interface and the non-bonded interaction between the materials would play a key role in determining the adhesion strength [16]. In addition, a surface structure of PI modified by longer curing time and UV-exposure can increase the adhesion strength between PI and Si-based substrates [17]. A simulation study for the interfacial properties within a glassy polymer reveals that the adhesion is governed by the relation between the strength of adhesive (attraction between different materials) and cohesive (attraction within the same materials) interactions [18]. This study suggests that the cohesive interaction can be affected by incorporation of adhesion agents or altering the degree of the side chain functionalization. For the adhesive interaction, its strength depends on the interface coupling and relaxation of chains at the adherent layer. In addition, Tam et al. suggest moisture as another adhesion-determining factor, which can deteriorate the adhesion strength of the epoxy-silica interface [19]. However, despite several investigations from both experiments and simulations, comprehensive understanding of adhesion determining factors is still lacking.

In the present work, we aim to understand fundamental aspects of the interfacial adhesion phenomena for various types of PIs placed on SiO_2 glass. Among several methodologies for measurement of adhesion properties, *e.g.*, peeling [14] [20], pulling [21], blister testing [22], and a laser spallation method [23] [24], the pulling test is chosen for mimicking the experimental detaching process of PI from the carrier glass during manufacturing of display. The pulling method is applied within the framework of the Steered Molecular Dynamics (SMD) method, which has been successfully implemented in simulations by employing the same physical protocols of pulling in experiments. [19] [25–28], During a pulling test, adhesion determining properties such as potential of mean force (PMF), pulling distance, and detaching force are calculated with reactive force-field (ReaxFF). Furthermore, characteristic responses depending on the thermal properties of polymer chains are obtained, using both coefficient of thermal expansion (CTE) values from experiments and supplemented qualitatively through simulation of variations in the chain conformation. The change in chain conformation during detachment is also examined in detail, particularly at the interfacial region. In addition, each energy term in the potential is decomposed to clearly determine which term contributes significantly to deformation during the pulling process. Finally, an investigation of the failure mechanism is performed to determine whether adhesive or cohesive failure occurs at the interface.

2. Materials and methodology

2.1. Materials

In this study, three different types of PI structures are investigated. The molecular structures of all PIs are depicted in Fig. 1. We employ the same diamine- 3,3′-dihydroxy benzidine (DHBZ) with different kinds of dianhydride- 3,3′,4,4′-biphenyl tetracarboxylic dianhydride (BPDA), Bicyclo[2.2.2]oct-7-ene-2,3,5,6-tetracarboxylic dianhydride (BTDA), and 4-(2,5-dioxotetrahydrofuran-3-yl)-1,2,3,4-tetranaphthalene-1,2-dicarboxylic anhydride (DTDA); *i.e.*, DHBZ-BPDA, DHBZ-BTDA, and DHBZ-DTDA. For simplicity, all PI structures are only denoted with the type of the dianhydride for rest of the paper; *e.g.*, DHBZ-BPDA

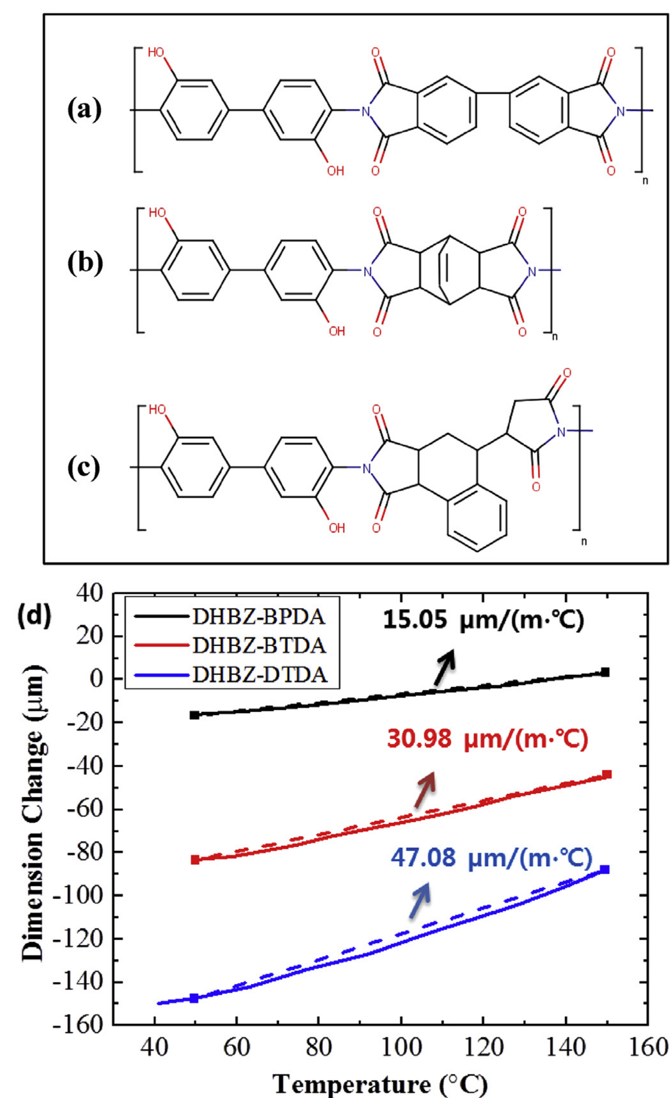

Fig. 1. The molecular structure of (a) DHBZ + BPDA, (b) DHBZ + BTDA, and (c) DHBZ + DTDA. (d) The coefficient of thermal expansion (CTE) for polyimide structures from experiment. The solid line is the experimental data and the dashedline is the fitted data to obtain CTE values between 50 °C and 150 °C.

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