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Atomistic study of interfacial creep behavior in epoxy-silica bilayer system

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A B S T R A C T

Epoxy-bonded bilayer material systems are commonly used in various engineering applications. The mechanical durability of these material systems are generally related to the interfacial properties between the bonded materials, which have aroused great concern for ensuring the long-term performance. In this paper, the interfacial creep behavior in bilayer system consisting of SU-8 monomer and silica substrate is investigated using molecular dynamics simulations. The threshold stress is found for the onset of interfacial creep in bilayer material system. The relationship between creep displacement and applied constant force is quantified by an analytical model. The microstructural changes during creep process are captured to demonstrate creep deformation process, including extension and sliding movement of epoxy, which unravels the mechanism of creep behavior at atomistic level. This study provides a new approach to understand the creep deformation at the nanoscale, and the corresponding molecular dynamics simulations show the promising results to obtain the information of the interfacial creep behavior in the bilayer material system.

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1. Introduction

Creep is a time-dependent phenomenon which reflects the long-term behavior of materials. The deformation of materials caused by creep has led to many unexpected accidences in industry and infrastructure. For example, solder materials, which are widely applied in electronic packing and micro-electromechanical systems, suffer from creep failure and fatigue under different temperature conditions [1,2]. Creep fatigue was also included in the common weakening in reactor systems of nuclear power plants [3] and gas turbine engines for aircrafts [4]. Accordingly, the improvement of creep resistance in materials becomes significant and urgent to avoid destructions and tragedies in real life. Existing literature present a lot of experimental and theoretical work from macroscale to nanoscale for understanding the creep behavior in different material systems, such as metals [5–7], alloys [8–10] and composites [11–14]. The mechanism of creep in different systems is associated with the hierarchy of material internal structures. In the past decades, the development of layered-structure composite materials for higher strength and better properties has raised a significant issue of creep at the interface for application. Specifically, the ceiling collapse of Interstate 90 connector tunnel in Boston, Massachusetts, in 2006 was related to creep failure in epoxy adhesive [15]. However, the ongoing research in creep behavior focuses on each component separately in composite materials, while overlooking the creep deformation at the interface which need to be further clarified and studied.

Epoxy is widely used as joining adhesives for wide industrial applications ranging from building constructions, such as FRP-reinforced concrete and FRP-wood composites, to microelectronic device and electronic packing, such as metal-ceramic composites and epoxy molding compounds. The sustainability and durability of these adhesive-bonded material systems under external load, temperature, humidity or cyclic actions of these ambient variations during service lifetime have been undergone extensive investigations for serviceability and safety concern [16–19]. The performance of these bonded structures significantly depends on the interfacial property as the interface usually creates the weak link for the whole material systems. The bonding quality between two dissimilar materials is mainly influenced by the interfacial

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imperfection characteristics, external loading and environmental conditions. As to bonded composites for engineering application, the overall responses of the material systems under creep deformation have been investigated in recent years [20–25]. Experiments combined with analytical models based on viscoelasticity and finite element analysis have been conducted to reveal the creep behavior of epoxy-bonded systems [20,22], but the existing theories are not yet fully explained the mechanism of interfacial creep at this stage. Although the response of interface plays an important role in creep deformation process, the interfacial creep behavior remains unclear. This is partly due to the indiscernible interfacial deformation progress from the experiments, which is a normal situation for macroscopic approach.

To get in-depth knowledge of the interfacial creep behavior in bonded material systems, the computational simulation from nanoscale perspective is taken. Molecular dynamics (MD) simulation is useful for exploring the dynamical processes of configuration changes and achieving the atomistic information in materials [26–28]. With the aid of MD simulations, the deformation of materials and the effect of environmental factors on the interfacial performance have been captured and revealed in bonded material systems. A series of thorough studies on epoxy-bonded materials have shown the detrimental effect of humidity and high temperature on the interfacial properties [29–31]. Some recent research on creep behavior in different nano-crystalline and nano-twinned metals shows that MD simulations are capable in giving both the change of internal microstructures and direct results of mechanical properties during creep deformation process, which is limited in empirical models [7,32]. The creep-fatigue relationship in amorphous polymer are revealed by capturing the changes of the van der Waals and dihedral energies and the structural changes through MD simulations, which indicates the chain sliding movement during creep [33]. These important findings on interfacial properties and creep behavior achieved using MD simulations have proved the large potential to investigate the interfacial creep at atomistic scale.

The objective of this study is to grasp the onset and the evolution of creep response at the interface through MD simulations (*i.e.* investigating interfacial creep using the atomistic approach). In this study, the bilayer structure including SU-8 and silica is chosen as a representative model in consideration that silica is widely used as substrate for many engineering applications, and SU-8 has an extensive application as epoxy-based adhesives. Steered molecular dynamics (SMD) simulation is employed to mimic the creep test at the interface under constant force condition. Our work can give new insights for the predictions of creep behavior in bonded material systems and lay the foundation for future study upon temperature and moisture effects on the interfacial creep behavior. The fundamental understanding of creep behavior at the interface can provide suggestions to improve the creep resistance for bonded material system in various applications.

2. Model and simulation

2.1. Atomistic models

The material system used in this study comprises one epoxy monomer bonded with the crystalline silica (SiO_2) substrate. SU-8 has been commonly used as photosensitive epoxy-based adhesive in MEMS applications. In practice, SU-8 adhesive is a crosslinked network. As the creep response of adhesive layer is initiated from the movement of single polymer chain, only one SU-8 monomer by the presentation of eight epoxy groups was used in the simulation to directly obtain the interaction between the adhesive and the substrate during the creep process. Such simplification has been successfully applied to investigate the interfacial behavior in other literature [28,29,34,35]. The chemical formula and molecular structure of SU-8 monomer is shown in Fig. 1. Silica, as the common mineral or aggregate, is the significant component with large proportion in concrete, and also widely utilized as substrate for synthetic layered structures during fabrication process. The atomistic model of silica substrate was constructed from the unit cell of crystalline silica with the lattice parameters of $a = 4.913$ Å, $b = 4.913$ Å, $c = 5.405$ Å with $\alpha = 90°$, $\beta = 90°$, $\gamma = 120°$, as shown in Fig. 1. The bulk size was increased by repeating in x, y, and z direction, and then was cleaved in a way that the normal vector of the cleaved surface is at [001] direction as to create an orthogonal slab for simulation. Furthermore, hydrogen atoms were used for bond termination at the surrounding surface of silica. The entire SiO_2 substrate has the dimensions of $a = 50.849$ Å, $b = 118.328$ Å, $c = 12.707$ Å with $\alpha = 90°$, $\beta = 90°$, $\gamma = 90°$, comprising 6930 atoms as shown in Fig. 1. The corresponding fully atomistic model of bilayer structure including SU-8 and silica for this study was built in Materials Studio software [36] as shown in Fig. 1. The non-periodic boundary conditions were applied in all three directions for later simulation.

Interactions between the atoms in SU-8 epoxy monomer and silica are described by the consistent valence force field (CVFF) [37], and the application of CVFF in this bilayer system has been validated and parameterized in the previous study [30]. CVFF contains both the valence and non-bonded interactions. The valence terms are the bonded interactions including two-body bond stretching, three-body angle bending, four-body dihedral angle torsion terms, while non-bonded interactions include van der Waals and Coulombic terms. The reduced form of the CVFF potential function using the harmonic form for bond stretching term is taken in this simulation, considering its applicability for the structure consisting of organic and inorganic phases [38]. The CVFF potential function in this reduced form is expressed as:

$$E = \sum_b K_b (b - b_0)^2 + \sum_\theta K_\theta (\theta - \theta_0)^2 + \sum_\phi K_\phi (1 + s \cos n\phi) + \sum_{i,j} \varepsilon_{ij} \left[\left(\frac{r_{ij}^*}{r_{ij}} \right)^{12} - \left(\frac{r_{ij}^*}{r_{ij}} \right)^6 \right] + \sum_{i,j} \frac{q_i q_j}{\varepsilon r_{ij}} \tag{1}$$

where K_b, K_θ, K_Φ represent force constants; b_0, θ_0 and Φ represent equilibrium bond length, equilibrium bond angle and dihedral angle, respectively; b and θ are bond length and bond angle; ε_{ij} denotes the depth of the van der Waals potential well, and r_{ij}^* denotes the length when the van der Waals potential reaches its minimum state; r_{ij} is the distance between particle i and particle j with charges q_i and q_j, respectively. In the simulation, the van der Waals and Coulombic interactions are truncated at a cutoff distance of 10 Å in the simulation. Partial charges of all the atoms in this bilayer system are calculated by charge equilibration (QEq) approach [39], as it is available for different material systems and the results are in good agreement with experiments and *ab initio* calculations [39].

2.2. Simulation of creep test

The molecular dynamics simulations were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [40]. During the equilibrium process, the bilayer material system is first relaxed using an NVE (conserving number of atoms, volume and energy) ensemble for 100 ps, followed by an independent relaxation at room temperature of 300 K using an NVT

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