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Investigation of hygroscopic and mechanical properties of nanoclay/epoxy system: Molecular dynamics simulations and experiments

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ABSTRACT

In this study, the moisture related hygroscopic characteristics and mechanical properties of polymer–clay nanocomposites (PCNs) were investigated using molecular dynamics (MD) simulations and experiments as a function of the weight fraction of nanoclay. The hygroscopic and mechanical properties including the moisture saturation amount, moisture diffusivity, work of adhesion, and elastic modulus of the PCNs were studied using MD simulations and compared to experimental results as a function of the nanoclay content. It was demonstrated that the proposed MD simulation technique can be successfully used for the prediction of the effects of the nanoclay on the moisture diffusion characteristics as well as mechanical improvements of PCNs. It is expected that the simulation technique applied in this work can be widely used to evaluate the performances of nanocomposite materials.

1. Introduction

Epoxy resins are increasingly used in engineering applications due to their excellent properties. In particular, epoxy resins are used in epoxy-based composites (carbon/glass fiber reinforced plastic), microelectronic packaging applications (printed circuit boards, die-attach, molding compounds, and underfill), and structural adhesively bonded joints [1–3]. However, most epoxy materials are very sensitive to their use environment because the properties of epoxy materials are easily influenced by temperature and humidity. When moisture is absorbed into epoxy material, it can reduce its glass transition temperature and generate residual stress in epoxy layers due to hygroscopic swelling of the polymer structure. For these reasons, the physical reliability of epoxy-based structures can be significantly degraded in moist environments. Because the epoxy-based components of most applications have the potential of being exposed to moisture or a humid environment, many researchers have investigated the influence of moisture in polymer structures and developed moisture absorption prevention methods [3,4].

To solve these problems, in recent years, polymer–clay nanocomposites (PCNs) have drawn much attention from researchers. Many advantages of PCNs have been reported including their mechanical properties, thermal properties, permeability, and biomedical applications [5]. The most notable advantages are improvements of the elastic modulus [6], tensile strength [7], and moisture/gas barrier properties [8] in comparison to polymers without nanoclay. Because of these characteristics, PCNs have enormous potential for application in the automobile, airplane, satellite, biomedical, and other polymer industries where the enhancement of the mechanical, permeability, or thermal properties of polymers is important. However, the mechanism of the property enhancement of PCNs is still not well understood although significant experimental work has been conducted in various research fields. In particular, mechanical improvement and the moisture diffusion characterizations of PCN systems must still be investigated in depth to provide understanding of the microstructure system. The understanding of the mechanisms of the enhanced properties of PCNs would provide the ability to design PCNs with desired properties.

Recently, molecular simulation techniques have played an important role in understanding and predicting the behavior and dynamics of amorphous structures of polymer materials [9–11]. Molecular dynamics is a numerical simulation method for a general *n*-body system of atoms in which the interaction physics among neighboring atoms are approximated using a pre-defined

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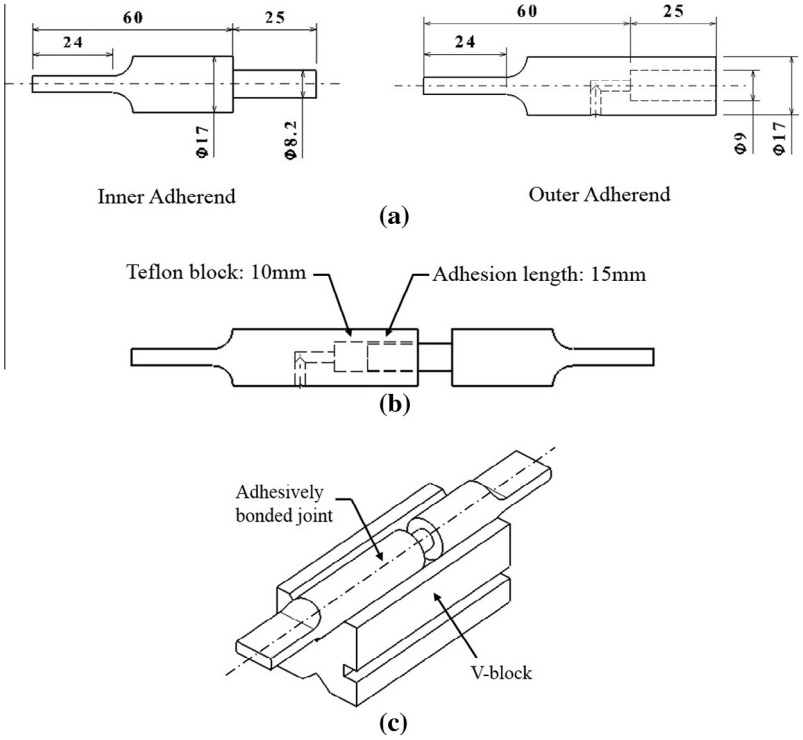

Fig. 1. Specimen of the tubular single lap joint: (a) inner adherend and outer adherend; (b) assembled adhesively bonded joint; (c) adhesively bonded joint on the V-block.

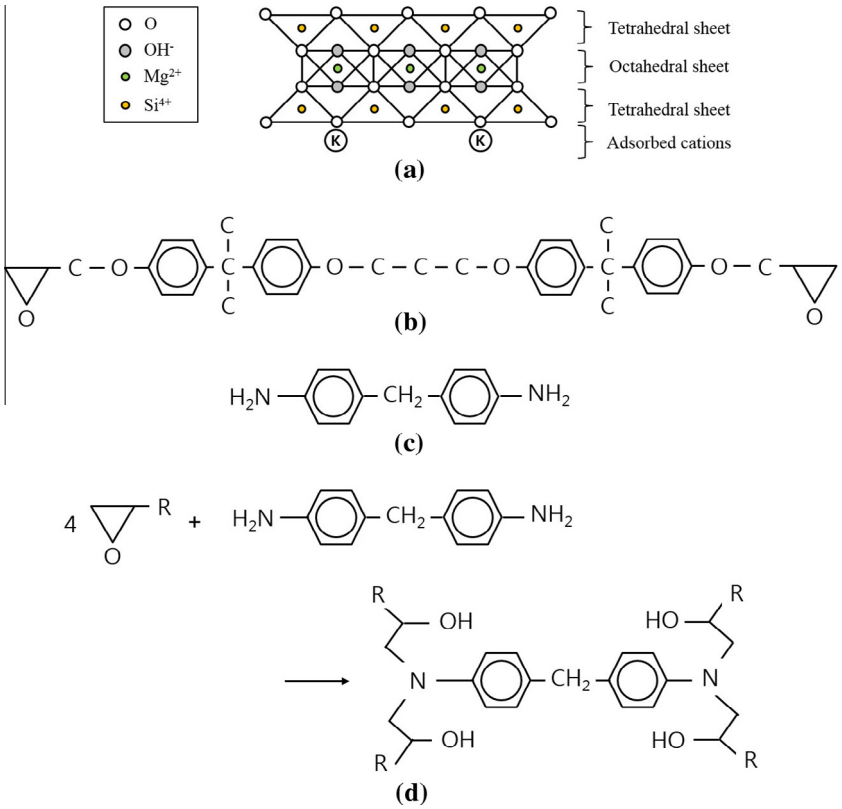

Fig. 2. Chemical structure of the PCN molecules: (a) unit structure of layered silicate nanoclay; (b) epoxy resin (DEGBA); (c) cross linking agent (MDA); (d) chemical reaction involved in the curing of a DEGBA with a MDA molecule.

force field or potential energy expression. This technique can be beneficial for polymer materials by increasing the understanding of chemical and physical processes at the molecular and atomic level. Although several researchers have studied the moisture diffusion characteristics and mechanical properties of polymer systems using molecular dynamics, this topic requires more in-depth study. In this study, the mechanical properties with respect to moisture and the hygroscopic characteristics of PCNs were