International Journal of Engineering Science 69 (2013) 69–76

Contents lists available at SciVerse ScienceDirect

International Journal of Engineering Science

journal homepage: www.elsevier.com/locate/ijengsci

Micromechanical analysis of nanoparticle-reinforced dental composites

Yi Hua [a], Linxia Gu [a,b,*], Hidehiko Watanabe [c]

[a] Department of Mechanical and Materials Engineering, University of Nebraska-Lincoln, Lincoln, NE 68588-0656, United States
[b] Nebraska Center for Materials and Nanoscience, Lincoln, NE 68588-0656, United States
[c] Department of Adult Restorative Dentistry, University of Nebraska Medical Center, College of Dentistry, Lincoln, NE 68583-0750, United States

ARTICLE INFO

Article history:
Received 13 March 2013
Received in revised form 28 March 2013
Accepted 1 April 2013
Available online 25 April 2013

Keywords:
Dental nanocomposites
Representative volume element
Sensitivity
Interphase

ABSTRACT

The mechanical behavior of TiO_2 nanoparticle-reinforced resin-based dental composites was characterized in this work using a three-dimensional nanoscale representative volume element. The impacts of nanoparticle volume fraction, aspect ratio, stiffness and interphase zone between the resin matrix and nanoparticle on the bulk properties of the composite were characterized. Results clearly demonstrated the mechanical advantage of nanocomposites in comparison to microfiber reinforced composites. The bulk response of the nanocomposite could be further enhanced with the increased nanoparticle volume fraction, or aspect ratio, while the influence of nanoparticle stiffness was minimal. The effective Young's modulus and yield strength of the composite was also significantly affected by the interphase stiffness. Results obtained in this work could provide insights for the optimization of nanoparticle-reinforced dental composites.

1. Introduction

Resin-based composites (RBCs) are currently among the most popular dental restorative materials due to their good aesthetic properties (Xia, Zhang, Xie, & Gu, 2008). Compared to dental alloys and ceramics, the application of RBCs to posterior teeth is still restricted to some extent due to their inferiority in wear resistance, fracture toughness and shrinkage behavior as well as bond longevity of dentin bonding agents. Recently various nanoparticles are used to improve the performance of RBCs and the results show that desired property enhancements can be achieved in these composites with small amounts of nanoparticles (Turssi, Ferracane, & Ferracane, 2006; Wetzel, Rosso, Haupert, & Friedrich, 2006; Yu, Ahn, Lim, & Lee, 2009). The mechanical behavior of nanocomposite is regulated by its microstructures such as nanoparticle volume fraction, aspect ratio and stiffness. In addition, the interphase zone at the nanoparticle/matrix interface raised increased attention. The interphase is the region formed between nanoparticle and matrix, due to altered molecular structure of the resin matrix at the interface with nanoparticles (Eitan, Fisher, Andrews, Brinson, & Schadler, 2006; Zhang, Zhang, Friedrich, & Eger, 2006). The role of interphase is not fully understood due to controversial results in the literature. Yu et al. reported that an interphase zone within a Al_2O_3 nanoparticle-reinforced epoxy was stiffer than the matrix (Yu, Yang, & Cho, 2009). On the contrast, Odegard et al. stated that the interphase within a silica nanoparticle/polyimide composite was softer than the matrix (Odegard, Clancy, & Gates, 2005). Another challenge is to quantify the interfacial bonding strength between resin matrix and nanoparticles. Due to complicated properties of the interphase zone, weak bonding areas are quite likely to exist and

* Corresponding author at: Department of Mechanical and Materials Engineering, University of Nebraska-Lincoln, Lincoln, NE 68588-0656, United States. Tel.: +1 402 4727680; fax: +1 402 4721465.
E-mail address: lgu@unl.edu (L. Gu).

0020-7225/$ - see front matter
http://dx.doi.org/10.1016/j.ijengsci.2013.04.001

composite damage may occur at a lower loading. A systematic study on the role of interphase including its damage behavior on the bulk behavior of the composite is needed, especially for nanoparticle-reinforced dental composites (Barbero, Abdelal, & Caceres, 2005; Lee, Chiang, Lin, Huang, & Dong, 2000).

In this study, a nanoscale representative volume element (RVE) was used to predict the mechanical behavior of TiO_2 nanoparticle-reinforced resin-based dental composites and the results were validated against that obtained by the non-interaction approximation (NIA). The mechanical advantage of this nanoparticle-reinforced composites compared with that reinforced by glass fibers was illustrated. The influences of nanoparticle volume fraction, aspect ratio and stiffness were examined in terms of effective Young's modulus and yield strength of the composite. In addition, the interphase zone created by alternated dynamics of resin matrix molecules in the vicinity of the nanoparticles was considered. The effect of interphase stiffness on the bulk properties of the composite was evaluated. Cohesive material was used to the interphase and the damage at interphase was investigated. The results of the investigation are expected to provide some design parameters for the microstructural optimization of nanoparticle-reinforced dental composites.

2. Finite element modeling

The microstructure of the TiO_2 nanoparticle-reinforced resin-based dental composites is represented by a three-dimensional RVE (100 nm each side), as shown in Fig. 1(a). Total 30 of identical TiO_2 nanoparticles are assumed as spheres and randomly dispersed. The nanoparticle centers are generated using the random sequential adsorption algorithm (Widom, 1966), in which the probability of finding a nanoparticle at a given position is the same in all directions. The nanoparticle diameter depends on the nanoparticle volume fraction and aspect ratio. In the baseline model, the nanoparticle volume fraction (V_p) is set as 5%, and aspect ratio (A_r) is chosen as 1. Then the nanoparticle diameter is calculated as 14.7 nm. Lower volume fraction and larger aspect ratio result in a smaller nanoparticle diameter. The material properties of TiO_2 nanoparticles are adopted with Young's modulus $E_p = 282.76$ GPa and Poisson's ratio $\nu_p = 0.3$ (Sivasankaran, Sivaprasad, Narayanasamy, & Iyer, 2010). The resin matrix of urethane dimethacrylate (UDMA) monomer is taken from the published experimental test as $E_m = 3.9$ GPa, $\nu_m = 0.3$ and yield strength, defined as the stress at which material would experience plastic flow, $\sigma_y = 60$ MPa (Lassila, Nohrstrom, & Vallittu, 2002). The two phases are meshed with 4-node tetrahedral linear element (C3D4), as shown in Fig. 1(b). A mesh convergence study is conducted and the minimum mesh size of 0.5 nm is chosen. Periodic boundary conditions are imposed to the RVE faces. A uniform 3% strain is applied to the model along the x-direction.

3. Cohesive zone material model

A cohesive zone material model (ABAQUS) is adopted to simulate the damage behavior in the interphase region. This model is implemented via cohesive elements, including a linear traction-separation law, which relates the stress vector to the strain vector across the cohesive zone. Both stress and strain vectors have three components in three directions, one component normal to the surface and two shear components. Before damage initiation, the traction-separation relationship is given by

$$t = \begin{Bmatrix} t_n \\ t_s \\ t_t \end{Bmatrix} = \begin{bmatrix} K_{nn} & K_{ns} & K_{nt} \\ K_{ns} & K_{ss} & K_{st} \\ K_{nt} & K_{st} & K_{tt} \end{bmatrix} \begin{Bmatrix} \varepsilon_n \\ \varepsilon_s \\ \varepsilon_t \end{Bmatrix} = K\varepsilon \quad (1)$$

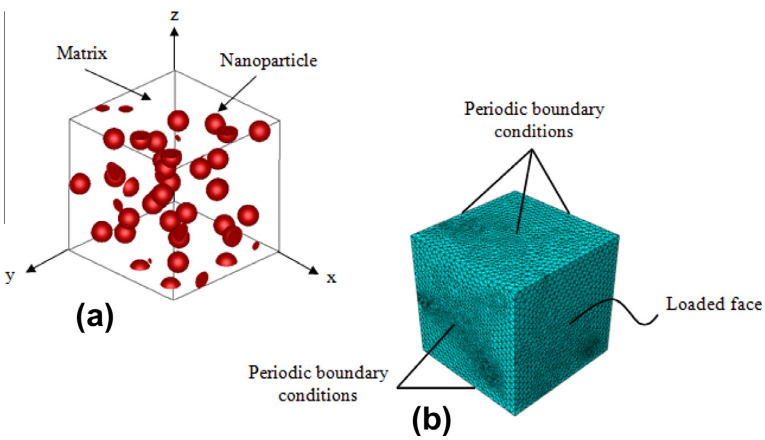

Fig. 1. Typical (a) geometry and (b) mesh of a three-dimensional RVE with random distributed sphere-shaped nanoparticles.