Microscopic Insight into the Nanodiamond Polymer Composites: The Reinforcement, Structural, and Interaction Properties

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SI Force Field Introduction

The interatomic interactions were described by the OPLS (Optimized Potentials for Liquid Simulations) all-atom force field.[1,2] The OPLS includes the pairwise and the bonding interaction. The pairwise interaction is composed two part of the short-range van der Waals (vdW) and the long-range electrostatic interaction. The vdW interaction is represented by 12-6 Lennard-Jones potential and the electrostatic interaction is represented by Coulombic potential. For the bonding interaction, it includes three components of bond stretching, angle bending and dihedral torsion. The OPLS force field is expressed as:

$$E_{total} = E_{bonds} + E_{angles} + E_{dihedrals} + E_{nonbonded} \quad (1)$$

$$E_{bonds} = \sum_{bonds} K_r(r - r_0)^2 \quad (2)$$

$$E_{angles} = \sum_{angles} K_\theta(\theta - \theta_0)^2 \quad (3)$$

$$E_{dihedrals} = \sum_{dihedrals} \left(\frac{V_1}{2}[1 + cos(\varphi - \varphi_1)] + \frac{V_2}{2}[1 - cos(2\varphi - \varphi_2)] + \frac{V_3}{2}[1 + cos(3\varphi - \varphi_3)] + \frac{V_4}{2}[1 - cos(4\varphi - \varphi_4)] \right) \quad (4)$$

$$E_{nonbonded} = \sum_{i>j} \left[\varepsilon_{ij} \left(\frac{\sigma^{12}}{r_{ij}^{12}} - \frac{\sigma^6}{r_{ij}^6} \right) + \frac{q_i q_j e^2}{4\pi\varepsilon_0 r_{ij}} \right] \quad (5)$$

Where E_{total} is the total energy in the system which is equal to the energy of bond stretching (E_{bonds}) plus angles shake (E_{angles}) plus dihedrals shake ($E_{dihedrals}$) plus pairwise ($E_{nonbonded}$).

The parameters are supplied by TINKER software with open source. At the link: https://dasher.wustl.edu/tinker/distribution/params/oplsaa.prm in the TINKER web site.

SII The Stress-Strain Curve of Three Dimensions

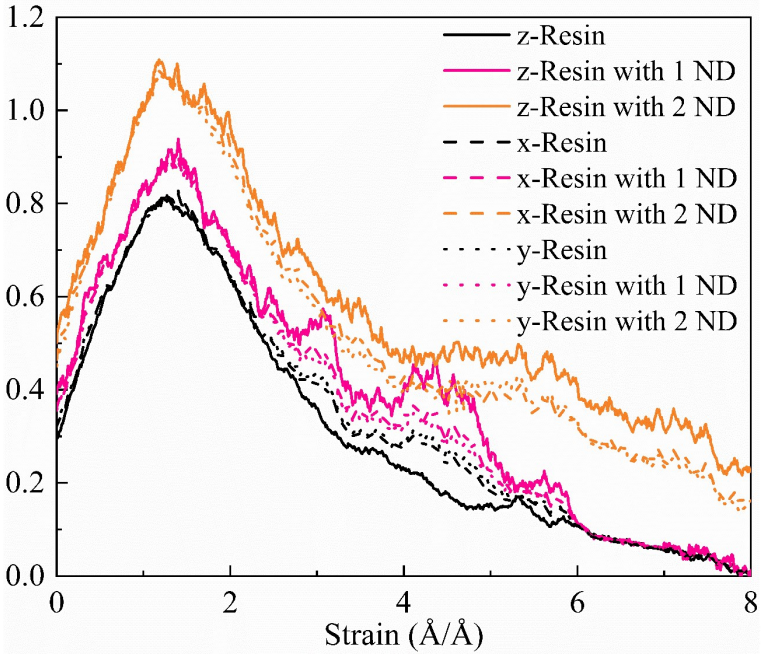

Fig. SII. Stress-strain relations of pure resin, resin composite with 1 ND, and resin composite with 2 ND in the x, y, z direction.

SIII Time Evolution of Box Size

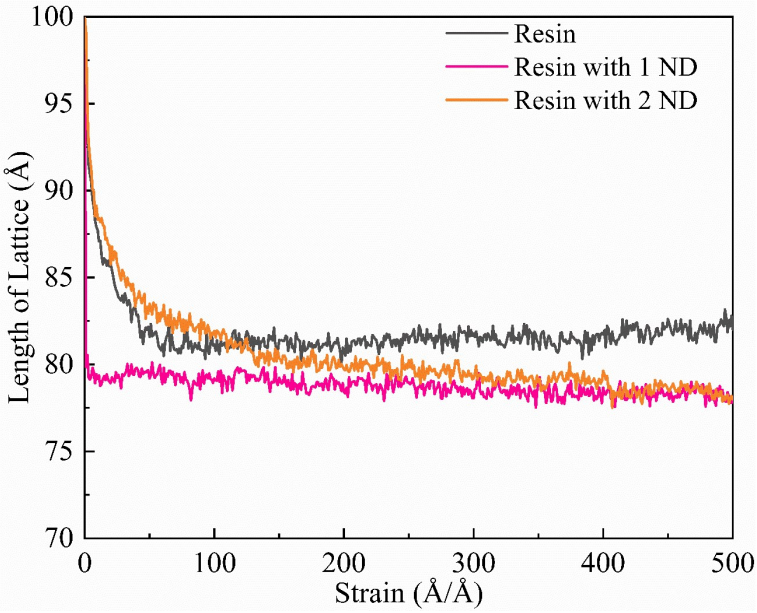

Fig. SIII. Box size evolution of pure resin, resin composite with 1 ND, and resin composite with 2 ND.

(1) Ponder, J. W.; others. TINKER: Software Tools for Molecular Design. Version 2004.

(2) Jorgensen, W. L.; Maxwell, D. S.; Tirado-Rives, J. Development and Testing of the OPLS All-Atom Force Field on Conformational Energetics and Properties of Organic Liquids. *J. Am. Chem. Soc.* **1996**, *118* (45), 11225–11236.