GRADUATE STUDENT RESEARCH SEMINAR SERIES (2018)

MOLECULAR DYNAMICS SIMULATION AND UNDERSTANDING OF INTERFACE INTERACTION IN CELLULOSE NANOCRYSTAL AND HIGHLY OXIDIZED GRAPHENE OXIDE NANO-COMPOSITES

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In nature, cellulose is a unique lightweight biopolymer with outstanding mechanical and optical properties that is readily available. Rigorous investigations have been conducted to use cellulose as an ingredient in the advanced functional composites design. In this work, a hybrid film composed of homogeneous cellulose nanocrystals (CNC) and highly oxidized graphene oxide (GO) is obtained by sufficient blending and vacuum filtration. For the first time through the X-ray diffraction (XRD) spectrum, the suppression of the originally ordered hydrophobic (200) facet of CNC is observed with increasing concentrations of GO. Further, the originally ordered hydrophilic (110)/(1-10) facets of CNC remain intact. Through systematic molecular dynamics simulations (MD) of a set of simplified CNC-GO sandwich structures, the mechanism behind this hydrophilic/hydrophobic facets manipulation is revealed. The strain induced by the hydrogen bonding between the CNC hydroxyl groups and the oxidation types on GO is the dominant reason that causes the suppression of the hydrophobic facet of CNC in CNC-GO hybrid film. The interaction between cellulose (200) facet and GO is observed to weaken the (200) peak in the XRD spectrum, and the interaction between cellulose (110) facet with GO is observed to alter the positions of (110)/(1-10) peaks, regardless of the cellulose concentration. This strain induced mechanism provides an understanding for intrinsically manipulating cellulose-matrix interface and potentially engineering the cellulose based nanocomposite material properties for future advanced materials development.

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