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EFFECT OF INTERFACE INTERACTION ON THE MECHANICAL PROPERTIES OF THE GRAPHENE REINFORCED NANOCOMPOSITES

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Molecular dynamic (MD) model involving a graphene platelet in polymer nanocomposite (GP) was developed in order to investigate the effect of the interface interaction on the mechanical properties of the nanocomposites when subjected to the uniaxial loading. All simulations were done using JOCTA software under COGNAC solver with full atomistic model. Nanocomposites are constructed by embedding graphene platelet into acrylate based polymer under the periodic boundary condition with different interface interaction. Nanocomposites systems underwent NPT (constant number of atoms, pressure and temperature) and NVT (constant number of atoms, volume and temperature) ensemble with applied uniform strain during the MD simulations. In terms of studying the effect of interfacial effect, the van der Waals interaction energy potential between the acrylate polymer and the graphene was changed and the tensile strength and the ultimate stress were investigated. It can be concluded that, increasing the interfacial interaction caused a significant enhancement in mechanical properties of the simulated nanocomposites as a result of the better load transfer between matrix and the filler. It's noteworthy to mention that tensile strength and the ultimate stress also followed similar tendencies. The simulation results demonstrated that the graphene platelet caused an increase in the stiffness relative to the polymer which implied the reinforcement effect of the filler.

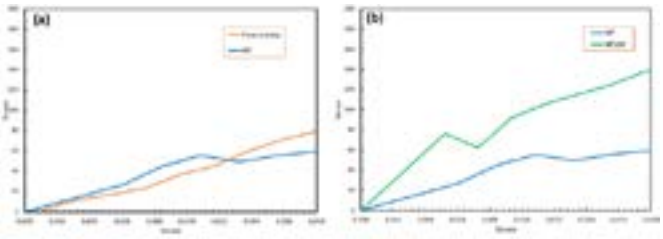

Figure 1: Stress-strain curves comparison of (a) pure matrix and GP, (b) GP and GP100.

Recent Publications

1. Ommeaymen S et al. (2018) Molecular dynamic simulation of carbon nanotube reinforced nanocomposites: the effect of interface interaction on mechanical properties. MOJ Poly. Sci.2(1):00038.
2. Gaoming D and Leon M (2014) Graphene reinforced nanocomposites: 3D simulation of damage and fracture. 95:684-692.
3. Atsushi A, Toshio N and Mitsuhiro S (2012) Atomistic molecular dynamics study of cross-linked phenolic resins. Soft Matter. 8(19):5283-5292.
4. Kaihei T et al. (2014) A computer simulation of the networked structure of a hydrogel prepared from a tetra-armed star prepolymer. Soft Matter.10(20):3553-3559.
5. Sheikh F et al. (2013) Role of nanoparticle dispersion and filler-matrix interface on the matrix dominated failure of rigid C60-PE nanocomposites: a molecular dynamics simulation study. Polymer. 54(10):2565-2576.

Biography

Ommeaymen Sheikhnejad obtained her PhD in the field of Chemical Engineering from Harbin Institute of Technology, China and holds BS and MS degrees in Pure Chemistry and Physical Chemistry respectively. She has experience in both experimental and numerical parts. In her current capacity, she works as a Researcher at the Institute of Polymer Product Engineering (IPPE) at Johannes Kepler University, Austria where she is working on the EU-funded project. She held this position from 2015 until now. At present she is actively participating in both national and international projects. Her main activities include the molecular dynamic simulation and micromechanics simulation of the composites. She is also supporting Bachelor's and Master's student in mechanical testing and simulation of crosslinked hydrogels.

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