The mechanical behaviors of Polyethylene/Silver Nanoparticle Composites: an insight from Molecular Dynamics study

Chuan Chen [1*], Shin-Pon Ju [2]

[1] Department of Information Management, Meiho University, Pingtung 912, Taiwan

[2] Department of Mechanical and Electro-Mechanical Engineering, National Sun Yat-sen University, Kaohsiung 80424, Taiwan

* Chuan Chen, +88687799821Ext8678, chchen@meiho.edu.tw

Abstract—the mechanical properties of pristine polyethylene (PE) and its composites with silver nanoparticles (PE/Ag NPs) at two Ag NP weight fractions of 1.05 wt% and 3.10 wt% were studied by molecular dynamics simulation (MD). It can be seen from the stress-strain distribution of the tensile process that the embedded Ag NPs can significantly improve the Young's modulus and tensile strength of the pristine PE, which is due to the improve of the local density and strength of the PE near the Ag NP surface in the range of 12 Å. Regarding the effect of temperature on the mechanical properties of pristine PE and PE/Ag NP composites, the Young's modulus and the strength of the pristine PE and PE/Ag NP composites decreased significantly to 350 K and 450 K, consistent with predicted melting temperature of pristine PE, which lies at around 360 K. At such temperatures as these, PE material has stronger ductility and a higher mobility of Ag NPs in the PE matrix than those at 300 K. With the increase of tensile strain, Ag NPs tend to be close, and the fracture of PE leads to a similarity between both the Young's modulus and ultimate strength found for the pristine PE and those found for the PE/Ag NP composites at 350 K and 450 K.

Keywords: Silver Nanoparticle, Molecular Dynamics, Polymer/ Nanoparticle Composite, Mechanical Properties, Thermal Properties