Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Mechanical Properties of Polymeric Nanocomposites with Liquid Inclusions[1] HEYI LIANG, ZHEN CAO, ANDREY DOBRYNIN, Univ of Akron —

We study mechanical properties of polymeric nanocomposites of liquid inclusions in network matrix using molecular dynamics simulations and analytical calculations. The shear modulus of nanocomposite is shown to be a non-monotonic function of the elastocapillary number $\gamma_{\mathrm{SL}}/(G_{\mathrm{N}}R)$, where $\gamma_{\mathrm{SL}}$is the interfacial energy network/liquid interface, $G_{\mathrm{N}}$is the shear modulus of network and $R$is the initial size of liquid inclusion. First, in the range of elastocapillary numbers, $\gamma_{\mathrm{SL}}/(G_{\mathrm{N}}R) <<1$, the composite shear modulus increases with increasing this parameter value. In this interval of elastocapillary numbers, a liquid inclusion softens the network such that the composite modulus $G_{\mathrm{comp}}$is smaller than G_N.This is in agreement with the classical Eshelby theory. However, for elastocapillary numbers $\gamma_{\mathrm{SL}}/(G_{\mathrm{N}}R) \approx 1$, the liquid inclusions reinforces the network, $G_{\mathrm{comp}}>G_N$. In this range of parameters the surface energy of the deformed liquid inclusions strengthens the composite. When the elastocapillary number increases further, $\gamma_{\mathrm{SL}}/(G_{\mathrm{N}}R) >>1$, the interfacial energy of network/liquid interface dominates the mechanical response of the composite resulting in composite weakening. Analysis of the elongation ratio of the liquid inclusion shows that it decreases with increasing elastocapillary number $\gamma_{\mathrm{SL}}/(G_{\mathrm{N}}R)$. The classical Eshelby's theory of inclusions fails to explain this phenomenon. We develop a new linear elasticity model of this class of nanocomposite materials capable to explain this unusual mechanical response of nanocomposite materials.

[1] NSF DMR-1409710

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Date submitted: 06 Nov 2015 Electronic form version 1.4