

Mechanical properties of nanocomposite systems

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The interaction zone and the bridge formation hypotheses are often used to explain the changes in mechanical properties and glass transition temperature that accompany by the addition of nanoparticles to a polymer matrix. We employ a formalism that relies on local stress fluctuations to calculate the local mechanical properties of nanocomposites in order to examine the validity of these theories. Advanced Monte Carlo techniques involving chain connectivity algorithms are used to create statistically independent configurations and aid in the efficient sampling of the stress. Three types of polymer particle interaction are considered. An increase of the mechanical properties is found for attractive and neutral particles, while for repulsive ones a decrease is observed. For the attractive case, the formation of a stiff glassy layer is apparent in the vicinity of the nanoparticle. The distribution of local moduli for the nanocomposite is narrower than that of the unfilled polymer, suggesting that nanoparticles reinforce glassy polymers by reducing the degree of mechanical inhomogeneity. Results are presented for the effect of particle size, polymer chain length, volume fraction and surface area of the particles on mechanical properties. Oscillatory deformations are also considered in order to address the effects of frequency on the mechanical properties of nanocomposites.

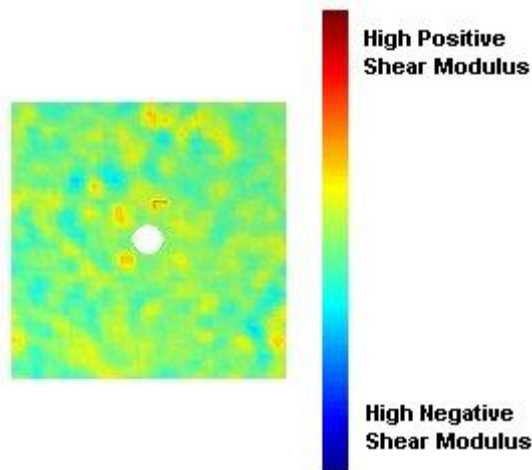


Figure 1: Color map of the local shear modulus around an attractive nanoparticle

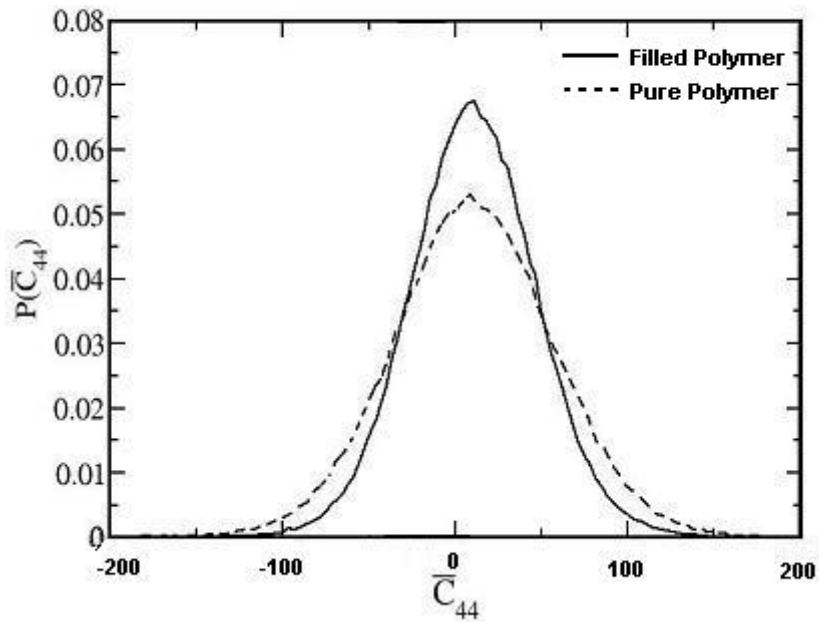


Figure 2: Distribution of the local Shear Modulus, C_{44} , for pure and filled polymer. The particle in the filled polymer is attractive.

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