

## APS Meeting 2020

Title: Molecular Dynamics Investigation of the Structural and Mechanical Properties of Off-Stoichiometric Epoxy Resins

Abstract: We carried out molecular dynamics (MD) simulations to measure the mechanical properties of various off-stoichiometric polymers regarding amine to epoxy ratios ( $r$ ) and to understand the stiffness of the polymers in terms of their structures. The aerospace-grade API-60 epoxy resin is used as an adhesive bond for assembling large-scale composite structures via the co-curing-ply bonding method. This method will produce a reliable and certifiable composite joint without additional fasteners. Calculated Young's modulus was measured from the uniaxial tension simulation with several high strain rates, and the experimental modulus was estimated by extrapolating the simulation results. We found that the stiffness was associated with molecular packing caused by chemical cross-linking. We also found that the number of network clusters gradually decreased as the ratio approached  $r = 1.0$ , which made the tighter cluster and the system much stiffer with an increase in the molecular weight and the degree of cross-linking. Structural properties such as  $R_g$ , MSD were measured to figure out the degree of stiffness with respect to the  $r$ .