

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Fragility of Polymer Nanocomposites with Ideal Nanoparticle Dispersion BEATRIZ PAZMINO, Physics Dept., Wesleyan University, Middletown, CT, JACK DOUGLAS, Polymer Division, NIST, Gaithersburg, MD, FRANCIS STARR, Physics Dept., Wesleyan University, Middletown, CT — We investigate the impact of the addition of nanoparticles (NP) on the fragility of a model glass forming polymer melt by molecular dynamics simulation. We first consider a fixed density path and find that the fragility changes, like the change in the glass transition temperature, follow directly from the attractive or repulsive polymer-NP interactions. We further show how the fragility can be connected with local vibrational changes, quantified by the Debye-Waller factor. We contrast these results with those we obtain along a path of fixed pressure, more experimentally relevant. For the isobaric case, we find changes in packing can have a larger effect on fragility than surface effects due only to NP interactions at fixed system density.

Beatriz Pazmino
Physics Dept., Wesleyan University, Middletown, CT

Date submitted: 14 Dec 2009

Electronic form version 1.4