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ROLE OF MOLECULAR INTERACTIONS ON THE MECHANICS OF NANOCOMPOSITES

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Nanocomposite materials are well characterized using a variety of advanced microscopy and spectroscopy techniques. In particular, the interfaces in the nanocomposites are often tailored (in engineered composites) and evolved (in biological nanocomposites) to unique molecular characteristics that provide optimized and superior properties to the nanocomposites. In this presentation, we will describe a multiscale mechanics perspective on role of molecular interactions as well as the nano and microstructures on the mechanics of nanocomposites. Specific examples including biological and synthetic nanocomposites will be presented. We have demonstrated a quantitative correlation of energies of molecular interactions albeit nonbonded in the nanocomposites to the overall mechanics and deformation behavior of the nanocomposites. Modeling strategies spanning from ab initio, molecular dynamics to discrete element and finite element methods will be presented in the context of four nanocomposite systems: (1) seashell (nacre), (2) bone, (3) polymer clay nanocomposites and (4) scaffolds for bone tissue engineering. In addition we will illustrate the importance of molecular interactions in behaviors of swelling clays used in polymer clay nanocomposites (Figure 1).

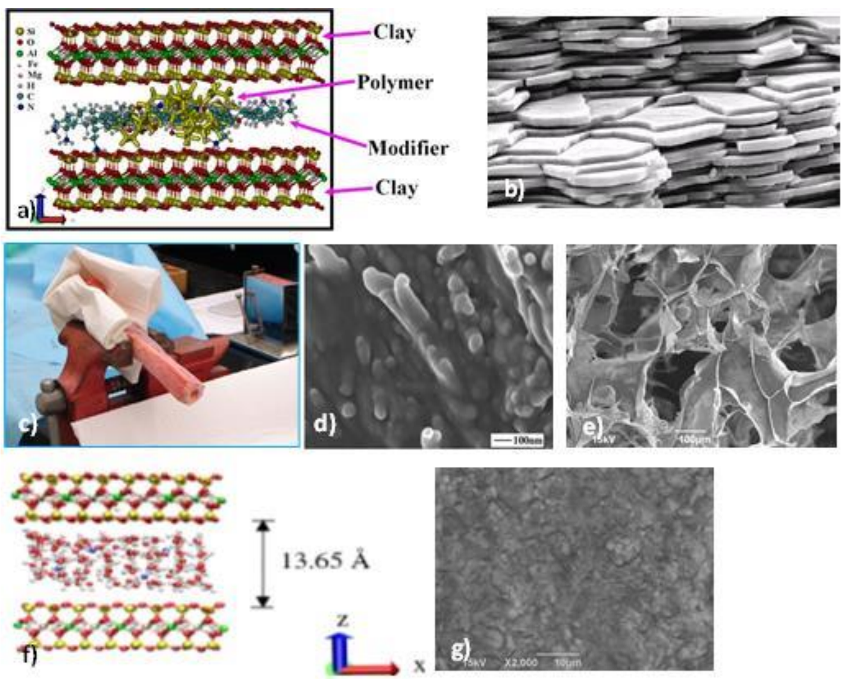

Figure 1 Molecular mechanics and multiscale modeling in nanocomposites (a) polymer clay nanocomposite (b)nacre(c and (d) bone (e)nanocomposite scaffolds for tissue engineering a(f) and (g) swelling clays used in nanocomposites.

The modeling and experimental techniques presented here bridge a significant range of length scales from nano/micro to macroscale using ab-initio, molecular dynamics, discrete element and finite element for modeling; and FTIR and photoacoustic spectroscopy, electron microscopy and nanomechanical testing for experimental investigation. The robust multiscale models presented can be used for a simulation based design of these nanocomposite systems. We report in each of these examples the significant role of proximity of mineral and organic phases on mechanics. The weak nonbonded interactions between organics and minerals; collagen and hydroxyapatite in bone, proteins and aragonite in nacre, nanoclay and polymers in polymer clay nanocomposites, and interactions in various constituents of nanocomposites that make tissue engineering scaffolds are shown to largely impact the overall mechanical behavior of the nanocomposite. These weak interactions, a hallmark of biology, but also useful in synthetic nanocomposites control mechanical behavior of nanocomposites. In the biological examples we evaluate the differences in role of weak non bonded interactions on structural stability vs. mechanics of the structure. For instance, the hydrogen bonding in collagen is important for structural stability of the molecule in bone microstructures but contributes marginally to mechanics. We will provide a summary of results for each of the material systems elucidating the impact of a large number of low energy molecular interactions on the elastic response of the nanocomposites.