Investigating antiplasticization of linear chain aliphatic high performance polymers

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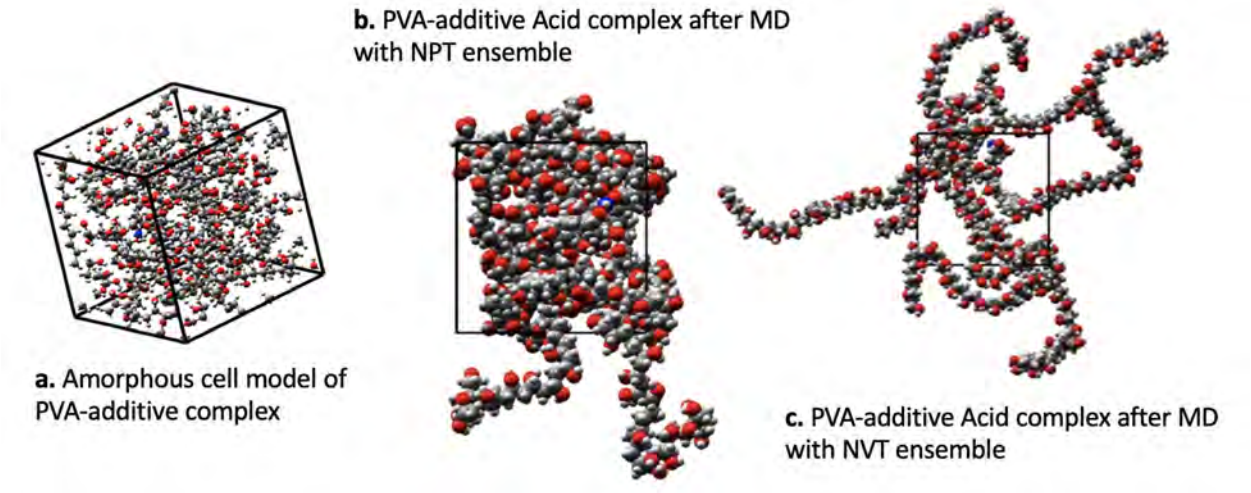
Good mechanical properties and high thermal stability of poly(acrylonitrile) (PAN) makes it a popular polymer for producing a large variety of textile products, namely high-performance fibers. However, the unique structure and high polarity of PAN's chemistry prevents it from being melt processed, with a melting temperature above its degradation temperature. To create fiber, PAN is solution spun at increased cost with the addition of stabilizers, a trade secret of industry. To create a cost effective fiber and to answer industry's call for sustainable carbon fiber precursor, this work elucidates the effect of biomass additives, antiplasticizers, on gel spun vinyl polymers. Most interesting among these were diacid isomers, glucaric acid (cis) and mucic acid (trans). Molecular Dynamics (MD) simulations were used to assess the strength of antiplasticization and experimental spinning trials were carried out to form fiber. The trans conformation of mucic acid revealed stronger antiplasticizing behavior both computationally and experimentally compared to cis conformation of glucaric acid. The family of additives investigated were found to contribute to improved spinning processability, improved Young's modulus and strength, higher structural order and increase in crystalline relaxation temperature in the formed fibers.



Computational annealing of amorphous poly(vinyl alcohol) and additive complex.