Elucidating the Hydration Structure of Nylon-6 using Molecular Dynamics Simulation and Anharmonic Vibrational Calculations

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The interactions between water and nylon-6 are important in understanding how hydration affects the physical properties of the polymer. In this study a weight averaged method for calculating the infrared (IR) difference spectra is used to relate the theoretical model of hydrated nylon-6 and the experimental system. The weight averaged method uses statistics from molecular dynamics (MD) simulation and vibrational frequencies and intensities from anharmonic vibrational calculation. The statistics of MD simulations reveal the water cluster sizes and the hydration shells of the amide groups of nylon-6 and water molecules in the polymer. The anharmonic calculations accurately predict the vibrational frequencies and intensities of the hydrogen stretch and bend motions of amide and water. The calculated IR difference spectra are in the amide A/hydrogen stretch region in good agreement with experiment, while the amide I-II regions require a correction for the semi-crystalline nature of nylon-6. The spectrum is assigned using the hydration shell structure of amide and water, thereby giving atomistic resolution of the hydration from the experimental IR difference spectrum. The method is trivially extendable to other hydrated polymer systems, and is currently being extended to biological protein systems.