Possible Mechanism of Chemical Depolymerization of Nylon-6 by Ionic Liquids

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The chemical depolymerization using ionic liquids was investigated by molecular simulation methods, which are molecular dynamics (MD) and density functional theory (DFT). Nylon-6, which is categorized into thermoplastics, is chosen for that matter. It is depolymerized by [PP13+][TFSI-]. All bonding energies in the repeat unit of the polymer were estimated by DFT. An overextension beyond the equilibrium bond-length was treated as the onset of the bond breakage from a physics perspective, thus the distribution of bond lengths was analyzed in the presence of ionic liquids to decide the bond breakage criteria. From MD results, the identities and numbers of broken bonds were obtained. In addition, the bond length distributions of three different types of IL ([PP13+][TFSI-], [TMPA+][TFSI-] and [TMPA+][Br-]) were analyzed to compare effects of different cations and anions. From this study, two important mechanisms involved in the chemical depolymerization, which might be used for checking depolymerization capability of ionic liquids were determined; 1) disentanglement of polymer and 2) breakage of unstable bonds. With an appropriate thermal input, ionic liquids surely make the depolymerization process more energy-efficient.