高分子電解質水溶液のナノレオロジー特性

Nano-rheological Properties of Aqueous Polyelectrolyte Solutions

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Materials enabling impact-energy absorption of high-velocity projectiles are of great interest for applications like aerospace. In such a frame, shear-thickening fluids were found very useful. Here, we studied nano-rheological properties of aqueous solutions of low-molecular-weight polyelectrolytes containing poly-([2-(methacryloyloxy) ethyl] trimethyl ammonium) as polycations (PC) and poly-(acrylamide-co-acrylic acid) as polyanions (PA). Those poly-ion complex mixtures exhibited experimental evidences of shear dilatancy.[1] We investigated the related underlying molecular mechanisms by employing Non-equilibrium Molecular Dynamics (NEMD) with the SLLOD algorithm[2] as provided in LAMMPS.[3] We compute the shear viscosity and found dilatancy for systems containing poly-ions at high shear rates (Fig. 1). The higher the amount of PA and PC molecules, the greater the shear thickening effect. We analyzed further molecular structures with tools like pair distribution functions, cluster size analysis, and energy profiles. Our method and findings underscore the importance of accounting for the molecular scale in the design of materials to make them absorb the impact energy efficiently.

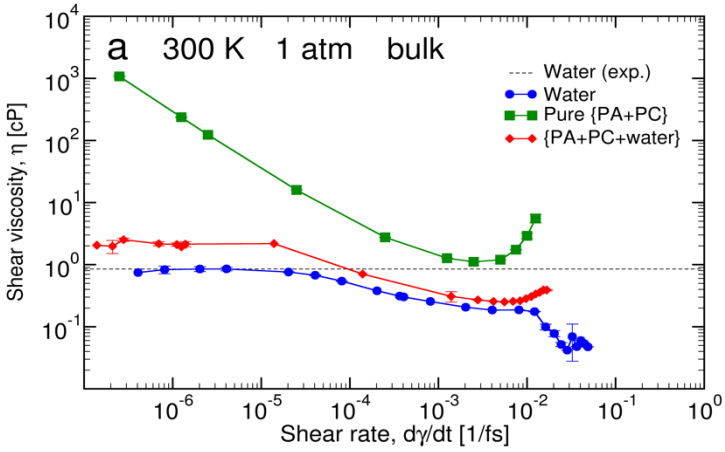

Figure 1: Shear viscosity as a function of the shear rate for water (blue lines and filled circles), pure polycations (PC) and polyanions (PA) (green lines and filled squares), and a mixture of PC, PA, and water (red lines and filled diamonds).

References:

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