Electrostrictive Behavior of Amorphous Polytetramethylene Oxide Elastomer

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The electroactive polymers include electrostrictive and dielectric elastomers, such as polyurethane. They have been demonstrated to be potentially useful due to their large actuation strains together with a high energy density. Some of polyurethanes, known to exhibit a rather strong electroactivity, are block co-polymers with hard segments and soft segments. Soft segments consist of poly(tetramethylene oxide) (PTMO), which have ether bond, $-(CH_2)_4O-$ in their repeat units, as shown in Fig. 1. We performed the atomistic simulation of the amorphous PTMO and compare its strain as a function of the magnitude of applied electric field, aiming to reveal how the microstructure of PTMO influence the electrostriction properties when they are electrically polarized by the application of a homogeneous electric field. Fig. 1 shows the atomic configuration of amorphous PTMO and the elasticity of amorphous PTMO and its potential gradient under the applied electric field is – 1.0 V/nm (left) and 1.0 V/nm (right). Here, we assume that the 3 axes are equivalent considering the amorphous phase due to small anisotropy in amorphous condition. A periodical unit cell for an amorphous PTMO atomic structure is shown in Fig. 1, where x = 2.51 nm, y = 2.77 nm, z = 2.75 nm, and all angles equal 90°. The amorphous chemical composition is $C_{480}H_{972}O_{120}$ which consists of six $C_{80}H_{162}O_{20}$ PTMO independent single chains, which consists of repeated $-(CH_2)_4O)_4-$ chains. Obtained potential gradient shows are under the -1.0 V/nm and + 1.0 V/nm for z direction. The negative potential gradient was emerged for E= -1.0 V/nm, and positive potential gradient was emerged for E = +1.0 V/nm.

The electric force leads to the PTMO compressed in electric field direction, and expanded in normal direction to the electric field. Dark color points are oxygen atoms in the $-(CH_2)_4O-$ repeating units.

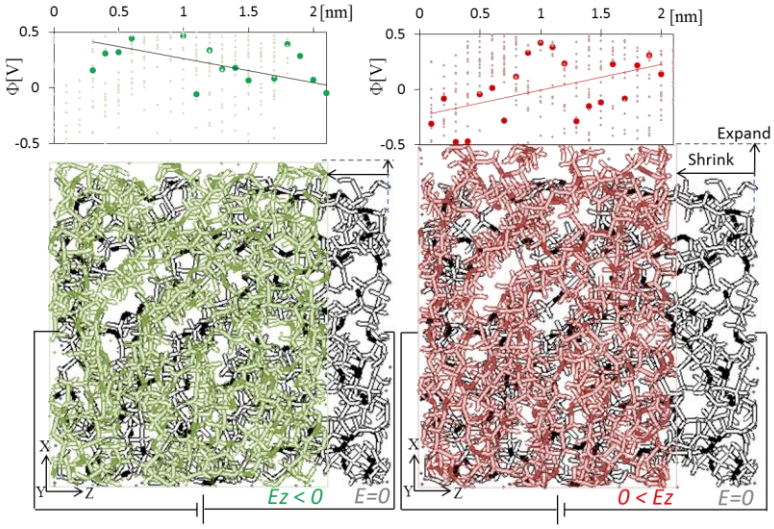

Fig. 1. The elasticity of amorphous PTMO and its potential gradient under the applied electric field is – 1.0 V/nm (left) and 1.0 V/nm (right).