

# Photo-induced deformations in optically active polymers by molecular dynamics simulations

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Photo-active polymers are of much interest from both theoretical and technological points of view [1]. The applications include artificial muscles [1], optical storage media and all-optical process for manufacturing the surface relief gratings [2]. The latter phenomenon is especially challenging for the theoretical explanation, as none of the existing theories [3] seem to suggest a satisfactory microscopic mechanism behind the photo-driven mass transport.

Most of photo-active polymers utilise azobenzene chromophores, which can exist either in prolate *trans* or bended *cis* isomeric form. The former are capable of forming the liquid crystalline (LC) phases. Under the illumination with suitable wavelength, both types of isomers coexist and constantly interchange, as the result a majority of the *trans* isomers are found to be perpendicular to the polarization of the light. This, in turn, induces the deformation of the polymer matrix. Experimental studies indicate that the sign of this deformation depends on the details of molecular architecture and typically is opposite for the polymers in LC and amorphous state.

Both effects, the presence of *cis* isomers and reorientation of *trans* ones may contribute to the photo-induced deformations. In our study we demonstrate that the second effect alone can be responsible for the opposite sign of the photo-induced deformation depending on molecular architecture. We performed the molecular dynamics simulations of two force field based molecular architectures [4], one with weak and another with strong coupling between the azobenzene and polymeric subsystems. Following the reorientation of *trans* isomers, the deformations of opposite sign are observed depending on the model. Two different microscopic mechanisms are found in each case. In weakly coupled model (LC polymers) the main microscopic effect is the phase transition in the *trans* isomers subsystem [5]. On contrary, in the strongly coupled model (amorphous systems) the microscopic mechanism found is the redistribution of polymer backbones mass [6].

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