Contribution ID: **183** Type: **poster**

Complex dynamics of guest molecules in all-optical poling: kinetic Monte Carlo modelling

We study theoretically the kinetics of non-interacting photo-switchable guest molecules (model azo-dye) dispersed in host (model polymer matrix) in the all-optical poling process close to the glass transition temperature Tg. The polymer matrix is simulated using the bond-fluctuation model. The kinetics of multiple trans-cis-trans cycles is formulated in terms of transition probabilities which depend on local free volume in the matrix and its dynamics. Close to Tg complex dynamics of guest molecules is observed, what implies the presence of dynamic heterogeneities of the matrix in space and time which influences guest molecules. A qualitative physical picture of mosaic-like states - intertwined areas of free- and hindered angular motion of guest molecules - is proposed and the role of related short and longer scales in space for the promotion of complex dynamics of guest molecules is discussed.

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