

Dynamics of chains as a tool to study thermomechanical properties of proteins

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Abstract: Polymer dynamics can be formulated on different levels of detail. One approach eliminates microscopic degrees of freedom and a polymer molecule is represented by a simplified structure - a chain. Dynamics of chain is due to thermal energy, which is a reason a transitions between polymer's states. In the simplest case a chain is an ideal chain. Monomers of ideal chain have fixed length, and their orientation is independent of the orientations and positions of neighbouring monomers. This is reason that two monomers can co-exist at the same place, so ideal chain model doesn't describe correctly the local structure of polymer, but correctly describe the property on large-scale. In reality, however monomers in a chain interact each other in space. One of such interaction is a steric effects, since monomer has a volume. Additionally there exists also electrical interactions between parts of polymer. Environment is another factor, which influence on polymer and can be source of thermodynamic forces. Polymers often operate under such non-equilibrium conditions, therefore dynamics of polymers has to fulfil laws of nonequilibrium thermodynamics. In a living systems there are a special polymers-proteins, that can operate under non-equilibrium conditions. During biochemical processes, they changes its states. I my work I will analyse influence, above mentioned, internal and external factors, which influence on proteins during changes of its states. In this context I will also present a certain formalism of non-equilibrium thermodynamic when non-Markovian processes appear.

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