

Abstract Submitted
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Dynamical Transition in polypeptides YUNFEN HE, ANDREA MARKELZ, University at Buffalo, SUNY, Buffalo, NY, USA — Two of the possible causes for the so called dynamical transition (the rapid increase in flexibility for biomolecules at ~ 200 K) are: thermally activated side chain diffusive motions with hydration dependent activation energies; or a glass transition in the biological water directly adjacent to the biomolecule. If the transition is strictly due to side chain activation, it should not depend on protein structure. Previously we demonstrated that the dynamical transition remains after tertiary structure was removed using THz time domain dielectric spectroscopy (0.2 -2.0 THz, 0.5-5ps). Here measurements on polyalanine as a function of chain length show that the dynamical transition does not occur for peptide length shorter than 5. However, the transition is observed for 5 mer and higher. Structural and simulation studies indicate that the 5 mer transiently occupies structured forms [1,2]. These results suggest that A) the dynamical transition is not due to thermally activated side chain motion and B) secondary structure is necessary for the dynamical transition. Secondary structure possibly induces sufficient ordering in the adjacent water to result in a fragile to strong glass transition resulting in increased protein flexibility [3]. [1] KAH Wildman et al. Solid State Nucl. Magn. Reson. 24 (2003) 94-109. [2] Yuguang Mu, et al. Proteins 58, (2005) 45-52. [3] S.H. Chen et al. PNAS (2006) 9012–9016.

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