Fluctuations of Conformational States in Biological Molecules: Theory for Anomalous Kinetics of Hole Burning

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The hole burning technique enables the investigation of the dynamics of the medium degrees of freedom affecting the optical transition. It is significant that the medium modes are probed in the unexcited media despite of the optical excitation is used to create a hole[1,2]. The experiments can be performed in the wide time window from milliseconds to days. The excitations with the relaxation times in that wide range are studied. In particular two level systems (TLS) in amorphous solids can be probed very efficiently since the relaxation times of many of them fall into the experimental range. *The t*ime dependence of the hole width w that is the quantity measured, is sensitive to all possible relaxation rates. In particular, a logarithmically uniform distribution of TLS relaxation rates results in a logarithmic increase of w with time due to the interaction of the dye probe with TLS. This logarithmic dependence has been measured in various glassy materials. However the investigation of complex biological molecules shows *a* qualitatively different behavior, namely w∝ t^a, i.e. a power law in time. The exponent a ranges between ¼ and ½ (data analysis based on Gaussian broadening yields a≈1/4) [1,2].

In this contribution we argue that the anomalous power law behavior of the hole width is caused by the internal degrees of freedom of the molecule itself rather than the glassy host. To interpret the observed time dependence we use the conformational space model for the low energy states of a protein[3,4]. The equilibrium dynamics of that molecule can then be interpreted as a diffusion in conformation space. At low temperature the diffusion trajectory can be defined by percolation and the effective dimensionality of the percolation trajectory is close to one.

If each diffusion step changes the energy of the electronic transition by the random value about δ then N steps from the origin would change the energy by $\delta N^{1/2}$. Since it takes time t~N^2 for the system to pass through N steps in a one-dimensional space the energy shift scales in fact as $t^{1/4}$. Thus the time evolution of the burned hole width can be understood within the simple model of conformational dynamics.

The suggested mechanism of conformational dynamics implies low temperature properties different from those of amorphous solids, where the low energy excitations can be represented as weakly interacting TLS. This difference can be due to the effect of the finite size of the protein molecule. In particular *a* finite size affects the elastic interaction and can make it almost distant independent. Then the protein would behave similarly to the standard spin glass, where the above picture of the conformational dynamics is relevant[3].

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