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Author(s): H. Frauenfelder, Z#: 068832, T-10/T-Division
G. Chen, Z#: 214446, T-10/T-Division
P. W. Fenimore, Z#: 181031, T-10/T-Division

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Proteins, Fluctuations, and Complexity

G. Chen[a], P. W. Fenimore[a], H. Frauenfelder[a], R. D. Young[b]

[a] Los Alamos National Laboratory, Los Alamos, NM 8745 USA
[b] Department of Physics and Astronomy, Northern Arizona State University, Flagstaff AZ 86011-6010 USA

Abstract

Glasses, supercooled liquids, and proteins share common properties, in particular the existence of two different types of fluctuations, α and β. While the effect of the α fluctuations on proteins has been known for a few years, the effect of β fluctuations has not been understood. By comparing neutron scattering data on the protein myoglobin with the β fluctuations in the hydration shell measured by dielectric spectroscopy we show that the internal protein motions are slaved to these fluctuations. We also show that there is no "dynamic transition" in proteins near 200 K. The rapid increase in the mean square displacement with temperature in many neutron scattering experiments is quantitatively predicted by the β fluctuations in the hydration shell.

1. Introduction

Complex systems are a significant field of scientific research with full understanding far in the future. Complex systems span a broad range of fields, from supercooled liquids and glasses to biomolecules, cells, and ecosytems, and on to economic and social networks. Some fundamental questions are obvious: Are complex systems governed by universal concepts and laws? What are the crucial concepts? Proteins are good choices for studying some aspects of the complexity. They are more complicated than supercooled liquids and glasses, but less so than economic or social networks. Hence we can expect that concepts studied in detail in supercooled liquids and glasses provide some guidance for exploring biomolecules. In turn, results obtained with biomolecules may suggest new aspects of

Corresponding author XXXX