Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Describing protein folding through the evolution of spatial density XIANGHONG QI, JOHN J. PORTMAN, Kent State University — The capillarity-like structure of folding nuclei is directly characterized for a wide range of two state folding proteins within a variational model that includes "neutral" cooperativity. We find that on average the volume of the folded core depends on the number of monomers as $V_{\rm f} \sim N_{\rm f}^{0.3}$. The precise relation agrees with the packing of rigid objects that are typically twice the size of a monomer in the native state. Focusing on the growth of the folded core and the interface region, we identify three different growth modes: core and interface consolidation, core dominated consolidation, and balanced growth. We also show in detail how the density of the core and interface of critical nuclei determine the common qualitative characterization as either diffuse or polarized. Such analysis will aid interpretation of ϕ-value distributions in terms of the spatial density or compactness of the critical nucleus which is much more difficult to probe experimentally than the degree of similarity to the native state.

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Date submitted: 27 Nov 2007 Electronic form version 1.4