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Protein Crystallization Based on the Entropy Criterion

Crystallization of proteins from solution is important in their processing and purification for bio and medical applications. It is also related to the pathology of cataract formation and other diseases. We shall model the protein interactions (such as lysozyme and cytochrome C) by a two-Yukawa potential with attractive and repulsive forces. Neutron scattering has shown that prior to crystallization, proteins form a "cluster phase". Interestingly, the peculiar structure factors S(q) of the clusters can be captured by the simple 2-Yukawa potentials. We show that this 2-Yukawa potential is closely related to the Derjaguin-Landau-Verwey-Overbeek (DLVO) interaction in colloidal chemistry. We use the Ornstein-Zernike integral equation based on an accurate "ZSEP" closure to obtain the structure factors S(q). We also apply the Giaquinta-Giunta rule (1992) based on the residual entropy ΔS_n to establish the threshold of fluid-solid transition given by the 2-Yukawa potential with different parameters (K_1, Z_1, and Z_2), i.e., the parameters of interaction strength and interaction ranges, respectively. We found that the single-phase crystallization rule of Giaquinta and Giunta is useful in determining the protein crystallization limits.

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