§29. Molecular Dynamics Study of the Structure Organization in Strongly Coupled Chain of Charged Particles

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The strongly-coupled Coulomb systems are found in condensed matters, highly compressed laser-irradiated plasmas and the stellar interiors [1]. In these circumstances, the Coulomb interactions organize the structure of matters and determine their equilibrium properties. The polyampholyte studied here is the charged chain composed of a random sequence of positive and negative monomers [2].

We examine in this study the dynamical and equilibrium properties of a strongly-coupled chain of charged particles (polyampholyte) submerged in an immobile viscous medium using the molecular dynamics simulations [3]. The equations of motion for the monomers are,

$$m\frac{d\mathbf{v}_i}{dt} = \mathbf{F}_{LR}(\mathbf{r}_i) - \frac{3T}{a^2}(2\mathbf{r}_i - \mathbf{r}_{i+1} - \mathbf{r}_{i-1}) + \mathbf{F}_{th} - \nu m\mathbf{v}_i, \quad (1)$$

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i. \quad (2)$$

The electrostatic Coulomb force, which is a long-range force, is given by

$$\mathbf{F}_{LR}(\mathbf{r}_i) = \sum_j \frac{Z_i Z_j e^2}{|\mathbf{r}_i - \mathbf{r}_j|^2}\hat{\mathbf{r}}_{ij}. \quad (3)$$

The polyampholyte relaxes to an equilibrium conformation typically in $300\omega_{pe}^{-1}$ due to folding of the chain for low temperatures, and expands several times faster for high temperatures, where ω_{pe} is the plasma frequency. Three regimes with distinct conformations as stretched, oblate and spherical are observed under the Coulomb force at high, medium and low temperatures, respectively (see Fig.1). The change in the conformations minimizes the free energy through the electrostatic potential. The root-mean-squared size of the polyampholytes in these regimes is scaled, respectively, as $R_g \sim N^{1/2}$, $(NT)^{1/3}$, and $N^{0.3}T^{0.8-1.0}$, where N is the number of monomers on the chain and T the temperature. The crossover point of the regimes are characterized by the unique values of the monomer distance $2R_g/N^{1/3}$, being insensitive to the length and stiffness of the chain. The present results agree well with the Flory theory in the high and medium temperature regimes. The densely-packed state at low temperatures is first obtained here without the use of the lattice model. The transition among the different regimes under the Coulomb force is exactly reversible. However, the transition under the cooperation of the Coulomb force and the attractive short-range force exhibits a hysteresis against successive changes in temperature.

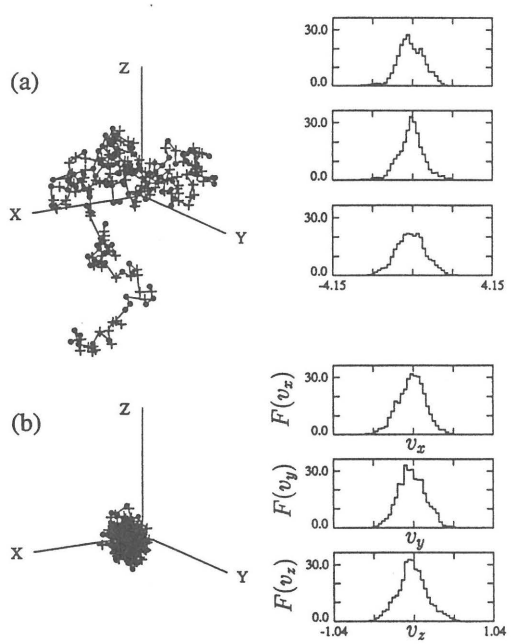

Fig.1. The equilibrium conformation of the neutral polyampholytes at the high (a) and low (b) temperature regimes.

References

[1] H.Hora, Plasmas at High Temperature and Density (Springer, Berlin, 1991).
[2] A.Y.Grosberg and A.R.Khokhlov, Statistical Physics of Macromolecules (AIP Press, New York, 1994).
[3] M.Tanaka, T.Tanaka, V.S.Pande, and A.Y.Grosberg, Bull.Amer.Phys.Soc., 41, 1522 (1996); NIFS Report No.498 (1997).