§27. Condensation and Crystallization of Strongly Coupled Coulomb Polymers

Tanaka, M., Grosberg, A. Yu (MIT), Tanaka, T. (MIT, USA)

As the research of fundamental plasma science, the structure formation of connected charged particles at very low temperatures and that due to addition of Debye-screening ions (salt) were studied by means of molecular dynamics (MD) simulations [1]. The physics of *polyampholytes* that comprise of both positively and negatively charged monomers (molecules) is quite complicated and has remained as unresolved problem until now because of strong *electrostatic correlations* of charged monomers and their ability of self-neutralization [2,3]. The coupling parameter, $\Gamma = e^2/\epsilon a k_B T$, is a good measure of such objects, which becomes larger than unity when charge correlations are playing their roles.

As temperature T is lowered, the volume of polyampholytes decreases monotonically, as shown in Fig.1, if global charge neutrality is as good as $|\delta Q| \leq \sqrt{N}$, where δQ is charge deviation and N the number of charged monomers in the system. In Fig.1, T_0 is the base temperature at which the Coulomb energy equals thermal energy $e^2/\epsilon a = k_B T_0$, and filled and open circles correspond to cooling and heating stages, respectively. This attractive nature of strongly correlated particles should be quite remarkable compared to high-temperature *gas plasmas* which tend to expand as much as possible due to thermal motions.

Fig.2 is the bird's-eye view of (six) strings, corresponding monomers for a condensed globule, and the monomers in the central cross section, respectively, from left to right. The white and dark spheres represent positive and negative monomers, respectively. Even though connecting strings in the left panel are well entangled, we see clear ordering of charged monomers in the middle and right panels. Precise measurement of this Coulomb crystal reveals that it has the characteristics of the body-centered crystal (bcc), which is one of the compact forms of highly condensed matters.

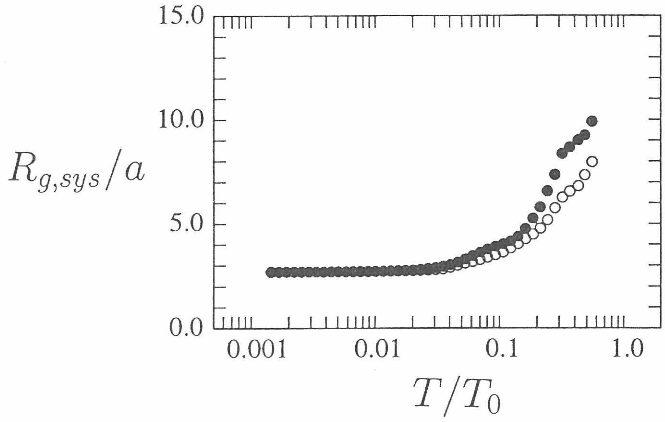

Fig.1: Temperature dependence of gyration radius of (neutral) charged polymers.

References

[1] M. Tanaka and T. Tanaka, *Phys.Rev., E59*, in press (2000).
[2] M. Tanaka, A.Yu Grosberg, V.S. Pande, and T. Tanaka, *Phys.Review, E56*, 5798 (1997).
[3] M. Tanaka, A.Yu Grosberg, and T. Tanaka, *J. Chemical Phys.*, 110, 8176 (1999).

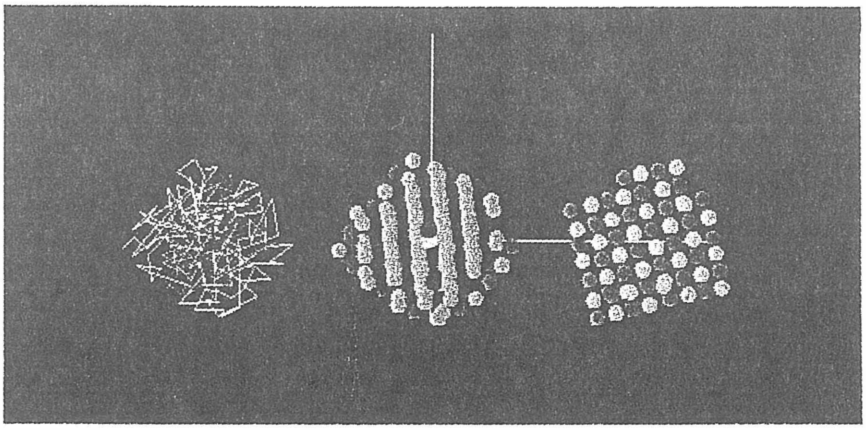

Fig.2: Bird's-eye view plots of crystallized polyampholyte.