MONTE CARLO STUDY OF VESICLES

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ABSTRACT

Model of self-avoiding polymerized vesicles are investigated by Monte Carlo simulations. Flaccid polymerized vesicles are *not* crumpled, while deflated polymerized vesicles exhibit fully collapsed configuration.

1. FLACCID POLYMERIZED VESICLES

Details of the simulation technique have been already reported in the previous papers.[1,2]

The mean squared radius of gyration, $\langle R^2 \rangle$, and the mean volume, $\langle V \rangle$, of vesicles are expected to scale with the exponents ν_R and ν_V as

$$\langle R^2 \rangle \sim N^{\nu_R}, \qquad \langle V \rangle \sim N^{3\nu_V/2}, \tag{1}$$

respectively, where N is the number of monomers constituting the vesicle. Our Monte Carlo results for $\langle R^2 \rangle$ and $\langle V \rangle$ are $\nu_R = 0.95 \pm 0.05$ and $3\nu_V/2 = 1.48 \pm 0.04$. The fact that the exponents exhibit their upper limiting value ($\nu \leq 1$) implies that flaccid polymerized vesicles are not crumpled. The absence of the crumpled phase can be explained by the large bending rigidity which is induced due to the short range repulsive interactions between adjacent hard spheres representing monomers.

2. DEFLATED POLYMERIZED VESICLES

Polymerized vesicles under negative pressure difference $\Delta p = p_{\rm in} - p_{\rm out}$ between inside and outside have been also investigated by using the "stress ensemble." The shapes of vesicles are expected to deviate from flaccid configurations in accordance with the cross-over scaling forms,

$$\langle R^2 \rangle \approx N^{\nu} X(x), \qquad \langle V \rangle \approx N^{3\nu/2} Y(x), \tag{2}$$

where $\nu \approx 1.0$ and $x = \bar{p}N^{\varphi\nu/2}$ is the scaled pressure variable with $\bar{p} \equiv \Delta p a^3/k_BT$ (a is the radius of a sphere). The crossover exponent $\varphi = 4.40 \pm 0.20$ is determined from several attempts to obtain optimal overlap of the curves for all values of N. In Fig.1, $X = \langle R^2\rangle/N^{\nu_R}$ and $Y = \langle V\rangle/N^{3\nu_V/2}$ are plotted as a function of $x = \bar{p}N^{\varphi\nu/2}$. One observes power-law behavior of the scaling functions for $|x| > 10^4$, namely,

$$X(x) \approx \frac{X_-}{|x|^{\rho}}, \qquad Y(x) \approx \frac{Y_-}{|x|^{\tau}}, \tag{3}$$

with $\rho = 0.140 \pm 0.007$ and $\tau = 0.185 \pm 0.008$. These results imply that $\langle R^2\rangle \sim N^{\nu_R^-}$ and $\langle V\rangle \sim N^{3\nu_V^-/2}$ with $\nu_R^- = \nu_R(1 - \varphi\rho/2) = 0.66 \pm 0.08$ and $3\nu_V^-/2 = (3\nu_V/2)(1 - \varphi\tau/3) = 1.08 \pm 0.08$.

Our result for ν_R^- is very close to the lower limiting value for the exponent $\nu = 2/3$, corresponding to the "fully collapsed" configuration. This compact structure is also observed by the exponent for the volume, $3\nu_V^-/2$, since $\langle V\rangle \sim Na^3$ is expected for this configuration.

Results for inflated vesicles ($\bar{p} > 0$) will be published elsewhere.[2]

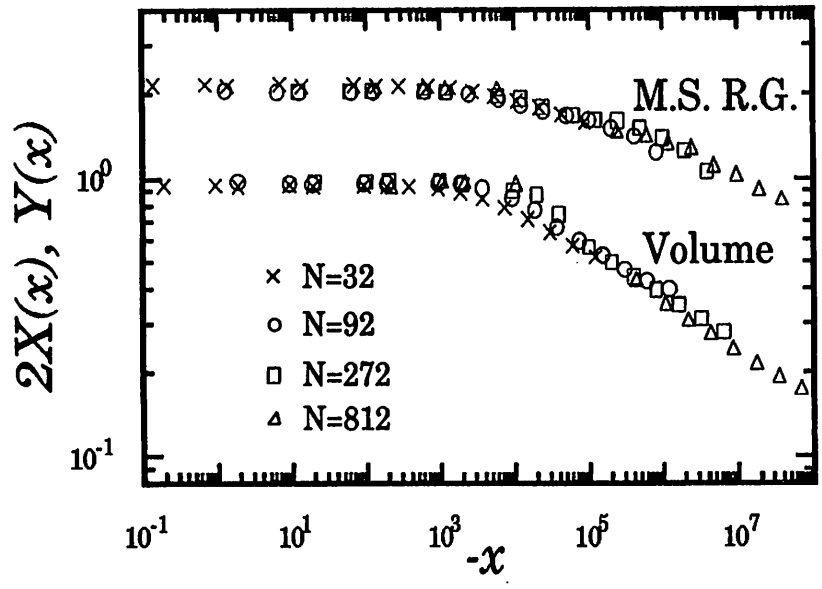

Fig.1 : Scaling plots of the mean square radius of gyration and the volume for the deflated ($\bar{p} < 0$) polymerized vesicles. Here $x = \bar{p}N^{\varphi\nu/2}$, $X = \langle R^2\rangle/N^{\nu_R}$ and $Y = \langle V\rangle/N^{3\nu_V/2}$ with $\varphi = 4.40$, $\nu_R = 0.95$ and $\nu_V = 0.99$ are used. $X(x)$ is shifted to avoid the overlap of two curves.

References

1. A. Baumgärtner and J. -S. Ho, *Phys. Rev. A.* 41 5747 1990.
2. S. Komura and A. Baumgärtner, *Phys. Rev. A.* 44 3511 1991.