

References

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1 Structure and elasticity of model disordered, polydisperse, and defect-free polymer networks Colombo and Del Gado [1]

They generate a polydisperse network via the method described in Gnan et al. [2]. This method was originally develop for Molecular Dynamics simulations of microgels but it can be generalized to the case of bulk systems. This method allows for an efficient generation of fully bonded networks by using a bottom-up self-assembly approach based on bond-swapping potential.

2 In Silico Syntehsis of Microgel ParticlesGnan et al. [2]

The purpose of the parper is to build up a felxible numerical protocl able to design individual microgel particles *in silico* with properties comparable to the experimental ones. In this work they build the microgel particle and compare their swelling behavior with experimental results. they focus in the case of very small microgels, or nanogels, whose diameter in the swollen regime us approximately 50 nm, because it is possible to reproduce the network in a monomer-resolved way by using the classic bead-spring model for polymer.

Two body interaction potential between particles i and j :

$$V(\vec{r}_{i,j}, \{\vec{p}_i\}, \{\vec{p}_j\}) = V_{WCA}(r_{ij}) + \sum_{\mu \in \{p_i\}} \sum_{v \in \{p_j\}} V_{patchy}(r_{\mu v}), \quad (1)$$

$$V_{WCA}(r) = \begin{cases} 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right] + \epsilon, & r \leq 2^{1/6}\sigma \\ 0, & r > 2^{1/6}\sigma \end{cases} \quad (2)$$

$$V_{patchy}(r_{\mu v}) = \begin{cases} 2\epsilon_{\mu v} \left(\frac{\sigma_p^4}{2r_{\mu v}^4} \exp \left[\frac{\sigma_p}{r_{\mu v} - r_c} + 2 \right] \right), & r_{\mu v} \leq r_c \\ 0 & r_{\mu v} > r_c \end{cases} \quad (3)$$

- $\vec{r}_{i,j}$ is the vector connecting i and j

- r_{ij} is its length
- $\{p_k\}$ is the set of patches of particle k
- $r_{\mu v}$ is the distance between patch μ on particle i and patch v on particle j .
- σ is the particle diameter
- ε is energy
- σ_p is the sets of position of the attractive well
- $\varepsilon_{\mu v}$ is the depth of the well
- r_c is chosen by imposing $V_{\text{patchy}}(r_c) = 0$

Interaction between polymers

$$V_{\text{FENE}} = \begin{cases} -\varepsilon k_F R_0^2 \ln \left[1 - \left(\frac{r}{R_0 \sigma} \right)^2 \right], & r < R_0 \sigma \\ 0, & r \leq R_0 \sigma \end{cases} \quad (4)$$

- k_F is the spring constant
- R_0 is the maximum extension of the bond

Introduce temperature in the swelling,

$$V_\alpha = \begin{cases} -\varepsilon \alpha & r \leq 2^{1/6} \sigma \\ \frac{1}{2} \alpha \varepsilon \left[\cos \left(\gamma \left(\frac{r}{\sigma} \right)^2 + \beta \right) - 1 \right] & r \in \left(2^{1/6} \sigma, R_0 \sigma \right] \\ 0 & r > R_0 \sigma \end{cases} \quad (5)$$

- α controls the solvophobicity of the monomers and plays the role of a temperature.

3 Three-body potential for simulating bond swaps in molecular dynamics

Bibliography

- [1] J. Colombo and E. Del Gado. Stress localization, stiffening, and yielding in a model colloidal gel. *Journal of Rheology*, 58(5):1089–1116, Sept. 2014. ISSN 0148-6055, 1520-8516. doi: 10.1122/1.4882021.
- [2] N. Gnan, L. Rovigatti, M. Bergman, and E. Zaccarelli. *In Silico* Synthesis of Microgel Particles. *Macromolecules*, 50(21):8777–8786, Nov. 2017. ISSN 0024-9297, 1520-5835. doi: 10.1021/acs.macromol.7b01600.