

# A Monte Carlo simulation of protein nucleation on porous membranes

Efrem Curcio<sup>1,2</sup>, Valerio Curcio<sup>3</sup>, Gianluca Di Profio<sup>2</sup>, Enrico Drioli<sup>1,2</sup>

1. Department of Chemical Engineering and Materials, University of Calabria

Via P. Bucci CUBO 44A, 87030 Rende (CS) Italy

2. Institute on Membrane Technology ITM-CNR, c/o University of Calabria

Via P. Bucci CUBO 17C, 87030 Rende (CS) Italy

3. I.S.A. "Michele Fanoli", Viale dello Sport 28, 35013 Cittadella (PD) Italy

Two-dimensional Ising model has been used to study the heterogeneous nucleation of protein crystals on porous polymeric hydrophobic membranes.

2D Ising model has been successfully applied to study heterogeneous nucleation on square lattice with nearest-neighbor interactions and free boundary conditions[1]. Sear (2006) used the same approach to determine the heterogeneous nucleation rate on microscopic impurities, and it was found more than four orders of magnitude faster than homogeneous nucleation[2].

It is here considered a 2D Ising model on a finite square lattice  $\Lambda=\{1\dots N\}^2$  with spin  $\sigma$  in the configuration  $\sigma\in\Omega$ , with  $\Omega=\{-1,+1\}$ .

The energy function of the system for spin-spin and spin-field interactions is:

$$E(\sigma) = J \sum_{ij} \sigma_i \sigma_j - h \sum_i \sigma_i + J_s \sum_{ij} \sigma_i \sigma_j \quad (1)$$

where  $\sigma_{ij}=\pm 1$  is the state of spin,  $J$  is the coupling constant between free neighbouring spins,  $h$  the external magnetic field, and  $J_s$  is the strength of the coupling between a free spin and a fixed spin of the wall. It is assumed  $J_s=0$ , that is the polymeric surface does not preferentially attract either phase; justification arises when considering free energies of surface/spin-up and of surface/spin-down phases identical for a contact angle of  $90^\circ$ , a value close to those experimentally measured for polymeric PVDF surfaces.

All the simulation described use a lattice of size  $N = 40$  and a coupling constant  $J=0.7kT$ , where  $k$  is the Boltzmann' constant, larger than the critical point of the 2D Ising model at  $J=0.44kT$ .

Simulation makes use of the standard Metropolis Monte Carlo method for spin flipping: flip is always accepted if it lowers the energy or, otherwise, accepted with probability of  $\exp(-\Delta E/kT)$ , where  $\Delta E$  is the energy difference due to spin flip, and  $k$  is the Boltzmann constant.

The theoretical findings are compared to those obtained from classical nucleation theory (CNT), and to experimental data from protein model hen egg white lysozyme (HEWL) crystallized on polyvinilidene fluoride (PVDF) membranes.

## Bibliography

[1] E.N.M. Cirillo, J.L. Lebowitz, "Metastability in the two-dimensional Ising model with free boundary conditions," J. Stat. Phys. 90 (1998) 211–226

[2] R.P.Sear, Heterogeneous and Homogeneous Nucleation Compared: Rapid Nucleation on Microscopic Impurities, J. Phys. Chem. B 110 (2006) 4985–4989