

Seeded nucleation of protein crystals

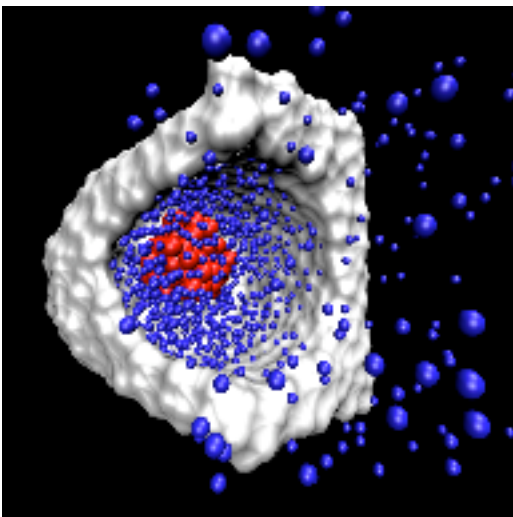
J.A. van Meel
FOM Institute for Atomic and Molecular Physics
Science Park 104, 1098 XG Amsterdam, NL

R.P. Sear
Dept of Physics, U. Surrey
Surrey GU2 7XH, UK

D. Frenkel*
Department of Chemistry, U. Cambridge
Lensfield Road, Cambridge CB2 1EW, UK

In the 1880's, when Kamerlingh Onnes started his program to liquify helium, he was confident that it could be done because he was guided by the principle of corresponding states. However, this principle only applies to molecules that have similar interaction potentials. Kamerlingh Onnes was lucky, because it so happens that helium is indeed "similar" to the gases that had already been liquified in the 1880's.

In protein solutions, we can observe a total breakdown of the corresponding-states principle. Such "anti-Van der Waals" behaviour has important consequence for the kinetics of protein crystal nucleation. I will discuss simulations of homogeneous protein crystallisation and report on very recent results concerning seeded nucleation. Our simulations reveal a surprising mechanism by which micro-porous materials promote protein-crystal nucleation.



Snapshot of a simulation of a crystal nucleation event. A small protein crystal (red) forms in a pore in the surface of a disordered medium.