4Pp105 A simple simulation of an ion movement in solution in presence of a magnetic field

OL. R. Dunin-Barkovskiy, Y. Tanimoto Institute for Molecular Science, Myodaiji, Okazaki 444-8585, Japan

Preface. Recent experimental results on magnetic field dependent growth of silicate membrane ("chemical gardens") [1] promise one the possibility of control over shape of objects growing from an ionic solution (gel membranes, dendrites and possibly crystals) by means of strong magnetic fields. In particular, growth of chiral silicate membranes was observed [1]. The mechanism of such effect of magnetic field was principally explained, but its details are still objects of discussion. We made an attempt to illustrate the mechanism of appearance of chirality in shape of growing objects by means of a simple computer simulation of movement of an ion in a filled vessel under strong magnetic field.

Model. In the present model, motion of an ion is treated by the random walk model coupled with circular motion due to a Lorentz force. The ion is considered as a point moving with thermal velocity along a circle trajectory, the radius of which is determined by the velocity and the applied magnetic field. In some time ("free pass time"), randomly distributed within some interval, it undergoes scattering and changes direction of its movement. If the ion reaches the vessel wall, it is being scattered inside the vessel. Direction of the movement at the start and after each scattering is random, in the case of collision with a wall the direction is limited within the semi sphere opposite to the wall plane. The value of velocity of the ion movement is being calculated on the base of temperature and mass of the ions in the gas-like approximation.

Results of simulation. In spite of the simplicity, the model gives an acceptable illustration to theoretical explanation of the experimentally observed chilarity in silicate membrane growth [1]. Several pictures for the cases of two values of applied magnetic fields, both at the center of the vessel and near its wall, are presented in Figure 1. The trajectories are shown in projection on the plane normal to the field. In the presented case the parameters were:

the vessel radius	3mm
temperature	300K
the magnetic field	0 or 5T
the ion charge and mass	-4 and 92 (correspond to SiO_4^{4-} ion)
free pass time	0.2mks
duration of "observation"	0.1ms

References

1. I. Uechi, A. Katsuki, L. Dunin-Barkovskiy and Y. Tanimoto, J. Phys. Chem. Submitted.

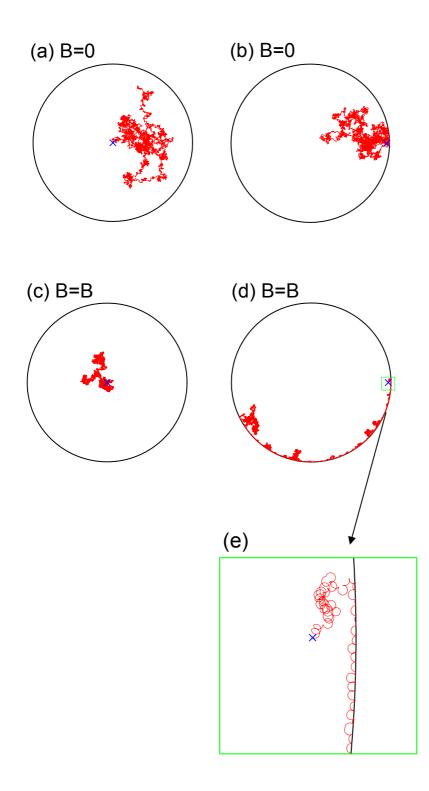


Figure 1. Results of simulation of thermal movement of an ion in magnetic field. (a) and (b) present zero magnetic field, (c) and (d) correspond to B=5 T. The trajectories are presented in projection on the plane normal to the magnetic field.