ANOMALOUS DIFFUSION IN TWO DIMENSIONAL CROWDED MEDIA. A MONTE CARLO STUDY

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SUMMARY

We perform a computational Monte Carlo study of small particles diffusion in two dimensional media with obstacles in different concentrations. For small times diffusion is anomalous, but for long times it is normal. The diffusion is much anomalous in more crowded media and the crossover time from one regime to another is also higher for increasing macromolecular crowding.
Keywords: crowded media, anomalous diffusion, time dependent diffusion coefficient

INTRODUCTION

Molecular diffusion in complex media has close association with a wide range of phenomena in biological systems being of crucial importance in sustaining life. For example, the diffusive behavior of signaling ions plays a very important role for cell activity.

The very high concentration of cellular macromolecules strongly affects diffusion processes inside cells. Cellular macromolecules occur in various shapes and sizes and in order to understand cell dynamics it is important to better understand diffusion process in such a complex and crowded media. Under crowded conditions, short range interactions dominate and a rigorous solution of diffusion equation is difficult to found [1].

There are some published data, both experimental and computational, describing diffusion processes in crowded media. Experimental evidences regard smaller diffusion coefficients for tracers in crowded media than in quasi-ideal solutions [2-9]. Computational studies show anomalous diffusion for small times and normal one for long time, the process
being strongly dependent on the macromolecular crowding conditions [10-16].

The aim of this paper is to study small particle diffusion process in two
dimensional (2D) crowded media with different concentrations for obstacles and to analyze
the dependence of the parameters that quantitatively describe this process on the crowding
conditions.

**Materials and Methods**

Cells are full of obstacles which obstruct diffusion: membranes, organelles and
other proteins. To properly understand what is happening inside a cell, the possibility of
anomalous diffusion in crowded media must be taken into account. In normal diffusion the
mean-square displacement of diffusing specie is proportional to time,

\[ \langle r^2 \rangle = (2d)Dt \]  (1)

where \( D \) is diffusion coefficient and \( d \) is the topological dimension of the media where
diffusion occurs [17]. In the case of anomalous diffusion the mean-square displacement is
proportional to a non-integer and subunit power of time

\[ \langle r^2 \rangle \sim t^\alpha \]  (2)

where \( \alpha \) is called anomalous diffusion exponent [17].

In the case of anomalous diffusion there is a time dependence of diffusion
coefficient which is dictated by the physical structure of the medium in which solutes
diffuse. We may define an effective diffusion coefficient as

\[ D_{eff} = D_{0} f(t) = \frac{1}{2d} \frac{\langle r^2 \rangle}{t} \]  (3)

with \( D_{0} \) diffusion coefficient for infinitely diluted solutions and we notice that

\[ D_{eff} \propto \frac{\langle r^2 \rangle}{t} \sim t^{\alpha - 1} \]  (4)

These equations illustrate that plotting the \( \log(\langle r^2 \rangle) \) versus \( \log(t) \) we obtain
anomalous diffusion exponent, from the slope of the curve and respectively \( \log(\langle r^2 \rangle/t) \)
versus \( \log(t) \) we may emphasis diffusion coefficient time dependence.

In this paper we focus on diffusion of small particles in crowded media and we
perform Monte Carlo simulations of diffusion in square two-dimensional (2D) obstructed
lattices. We are interested in anomalous diffusion exponent dependence on the concentration
of the obstacles.

The simulations are carried out on 300x300 square lattices with cyclic boundary
conditions and containing randomly distributed tracers and obstacles. Both tracers and
obstacle particles occupy 1 single site in the lattice. We consider tracers in concentration

22
[T]=0.01 and the following concentrations for obstacles: [O]=0, [O]=0.15, [O]=0.25, [O]=0.35 and [O]=0.405 respectively. All these concentrations are under the percolation threshold.

At every time step a random number is used to decide which tracer to move. It moves to a randomly chosen unoccupied nearest-neighbor site. For each Monte Carlo time step the sequence is repeated N_{tot} times (N_{tot} is the total number of mobile particles within the lattice) in order to assure that statistically each molecule moves once in the time step. We use 10000 time steps and we perform 20 runs, the values of mean-square displacement being averaged for all the particles and for these runs.

**Results**

The root-mean displacements for tracers within 2D lattices with different concentrations of obstacles are presented in the Figure 1.

![Figure 1. Time dependence of the root mean square displacement for tracers in 2D lattices with different concentrations of obstacles: [O]=0 for solid line, [O]=0.15 for dashed line, [O]=0.25 for dotted line, [O]=0.35 for dash dotted line and [O]=0.45 for dash dot - dotted line.](image)

If we take the ratio $\langle r^2 \rangle / t$ versus time in double logarithmical scale we reveal the time dependence of diffusion coefficient for small times (anomalous diffusion) and the fact that it becomes constant for long times (normal diffusion) but having smaller value than that corresponding to ideal solutions (see the Figure 2). Using this plot we may
determine the anomalous diffusion coefficient from the slope of decreasing region and the crossover time from anomalous diffusion to normal one as the intersection of the fittings lines corresponding to the decreasing respective constant regions, as it is illustrated in the Figure 2.

The values of the anomalous diffusion exponents and those of the crossover times are presented in the Table I.

**Table I. The values of the anomalous diffusion exponents and those of the crossover times.**

<table>
<thead>
<tr>
<th>Obstacles concentration</th>
<th>α</th>
<th>log(τ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>[O]=0</td>
<td>1.0003 ± 0.0001</td>
<td>-</td>
</tr>
<tr>
<td>[O]=0.15</td>
<td>0.9934 ± 0.0008</td>
<td>2.74</td>
</tr>
<tr>
<td>[O]=0.25</td>
<td>0.9836 ± 0.0001</td>
<td>3.0</td>
</tr>
<tr>
<td>[O]=0.35</td>
<td>0.9378 ± 0.0002</td>
<td>3.1</td>
</tr>
<tr>
<td>[O]=0.405</td>
<td>0.8600 ± 0.0003</td>
<td>3.2</td>
</tr>
</tbody>
</table>

We notice that for an unobstructed 2D lattice the value of anomalous diffusion exponent corresponds to classical diffusion and there is not a crossover time because the regime of anomalous diffusion is missing. This is a strong argument for the validity of the simulation algorithm.

24
Discussions and conclusions

The results presented here totally agree to theoretical predictions and with simulation results for other cases. They show that in a 2D crowded media diffusion is anomalous for small times and it becomes normal for longer times. The degree of abnormality of diffusion is quantitatively expressed by the anomalous diffusion exponent. This quantity increases with increasing obstacles concentration. Also, the crossover time from the two regimes of diffusion increases with increasing obstacles concentration. For the normal diffusion regimes at long times, the values of diffusion coefficient decrease with increasing of macromolecular crowding, being strongly different from the value corresponding to the normal diffusion in 2D unobstructed media.

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References