

Relaxation in jammed monolayers of elongated particles

Tatochenko M.O.¹, Bulavin L.A.², Kovalchuk V.I.², Lebovka, N.I.¹, Vygornitskii N.V.¹

¹Department of Physical Chemistry of Disperse Minerals, F. D. Ovcharenko Institute of Biocolloidal Chemistry, NAS of Ukraine, Kyiv 03142, Ukraine.

²Department of Physics, Taras Shevchenko Kiev National University, Kyiv 01033, Ukraine.

The relaxation in systems of elongated particles (discorectangles) adsorbed on a plane was studied numerically. The initial jamming state was formed using the random sequential adsorption (RSA) model. The off-lattice model was used. The aspect ratio of particles (length-to-width ratio) was varied within the range $\varepsilon=1\div 13$. After formation of jamming state it was relaxed via translational and rotational Brownian motions.

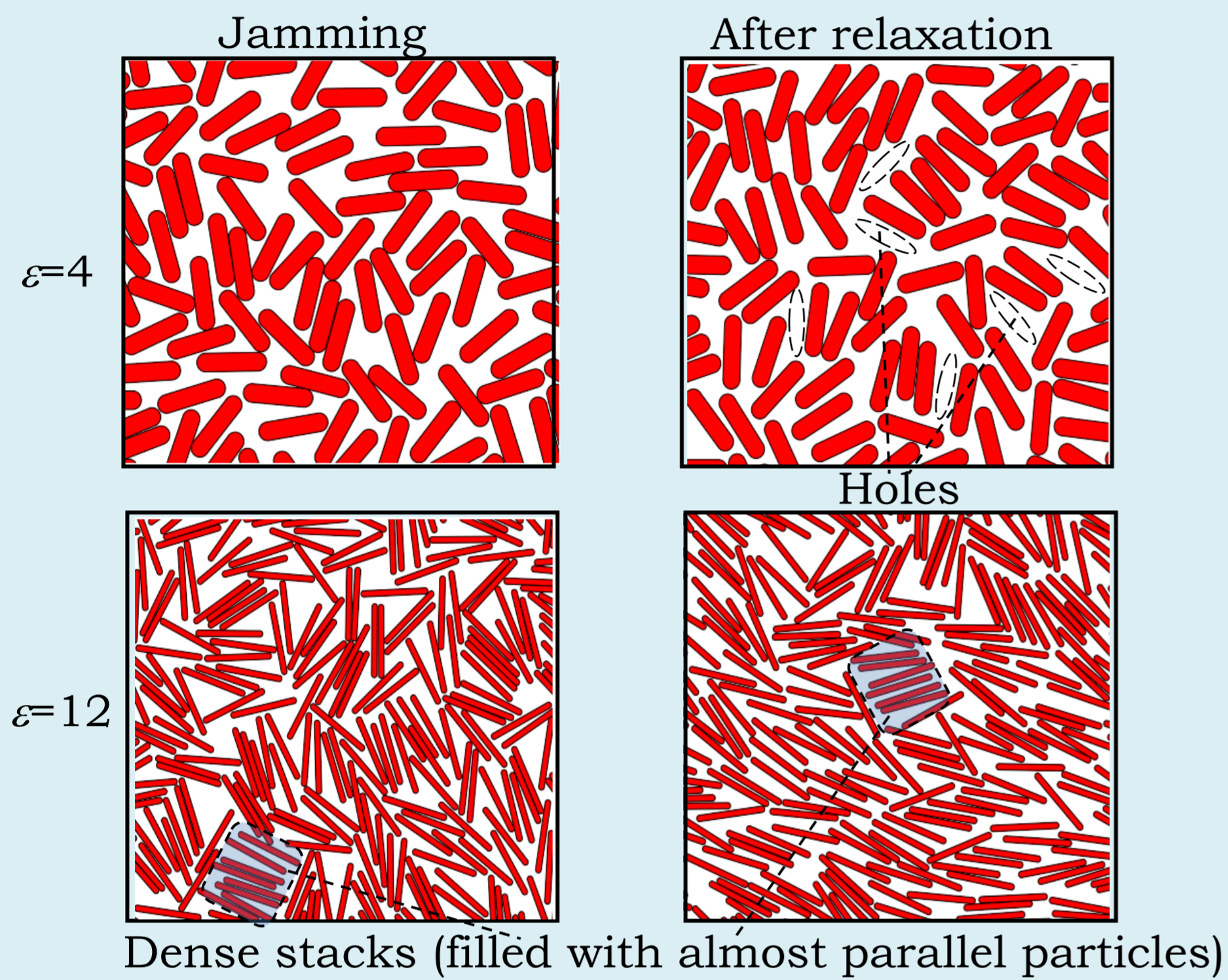


Figure 1: Patterns in a jamming state and after complete relaxation for particles with aspect ratio $\varepsilon=4$ and $\varepsilon=12$.

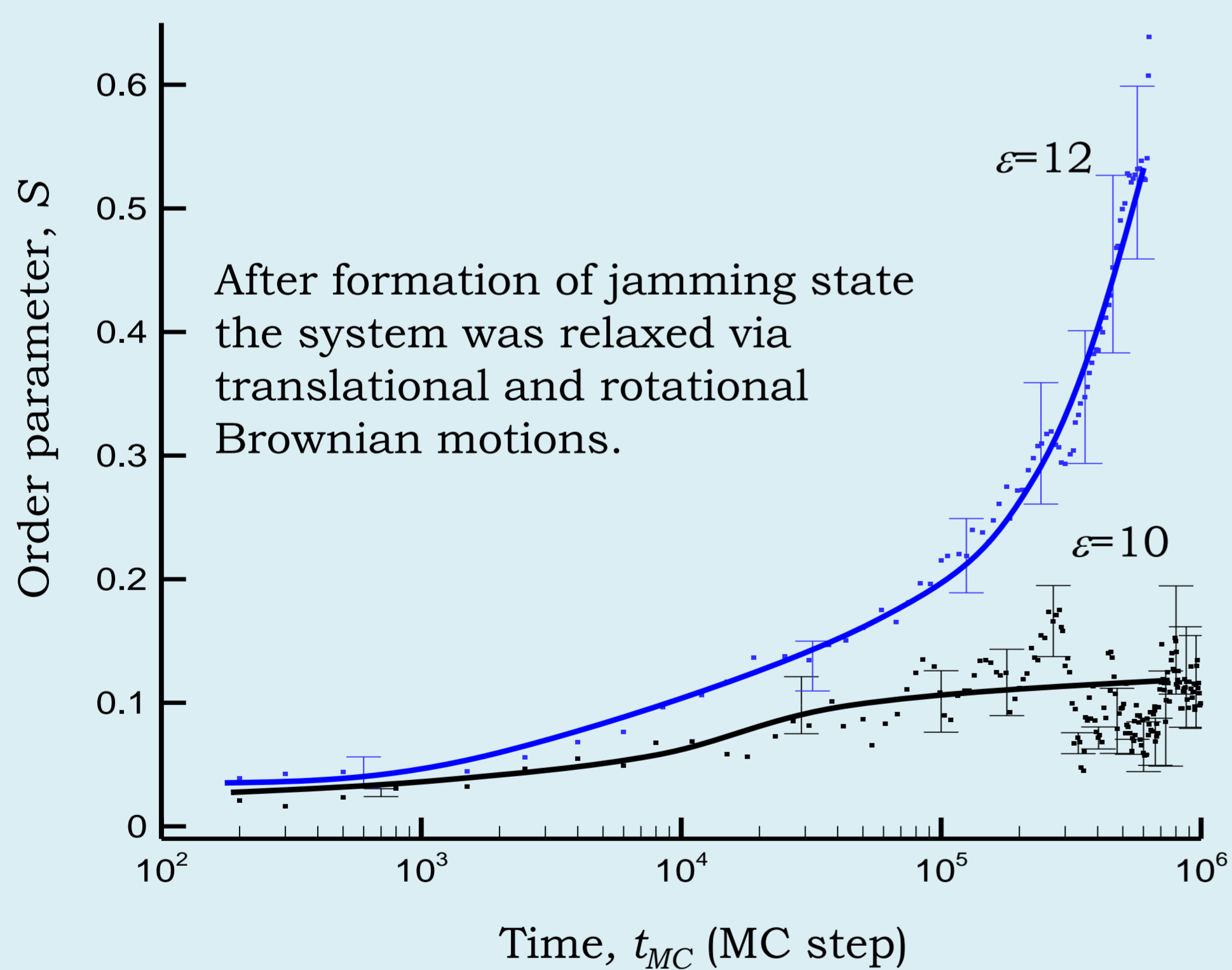


Figure 2: Order parameter, S , versus the time, t_{MC} , during the relaxation for particles with aspect ratio $\varepsilon=4$ and $\varepsilon=12$.

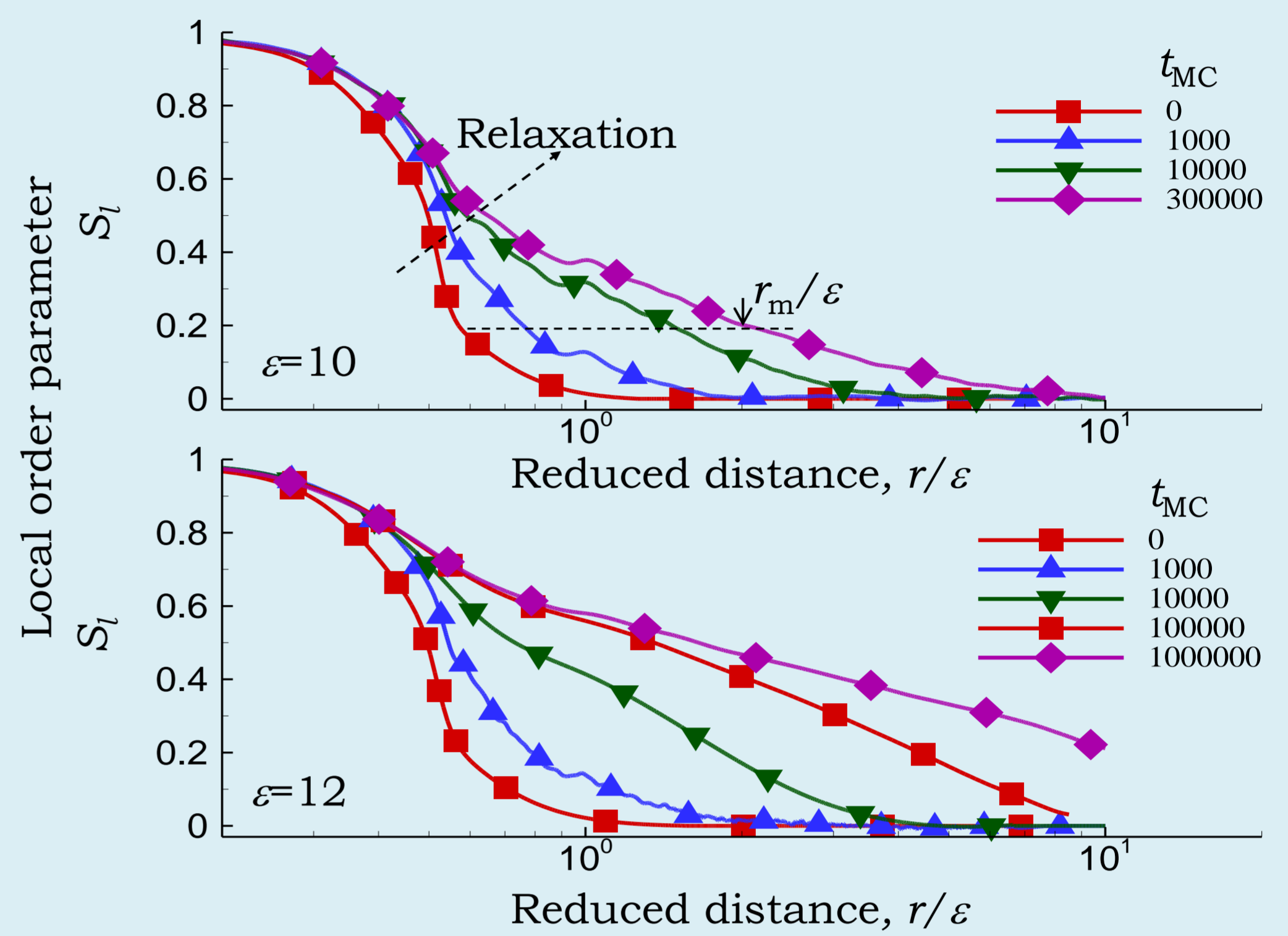


Figure 3: Local order parameter, S_l , versus the reduced distance r/ε for different values of t_{MC} .

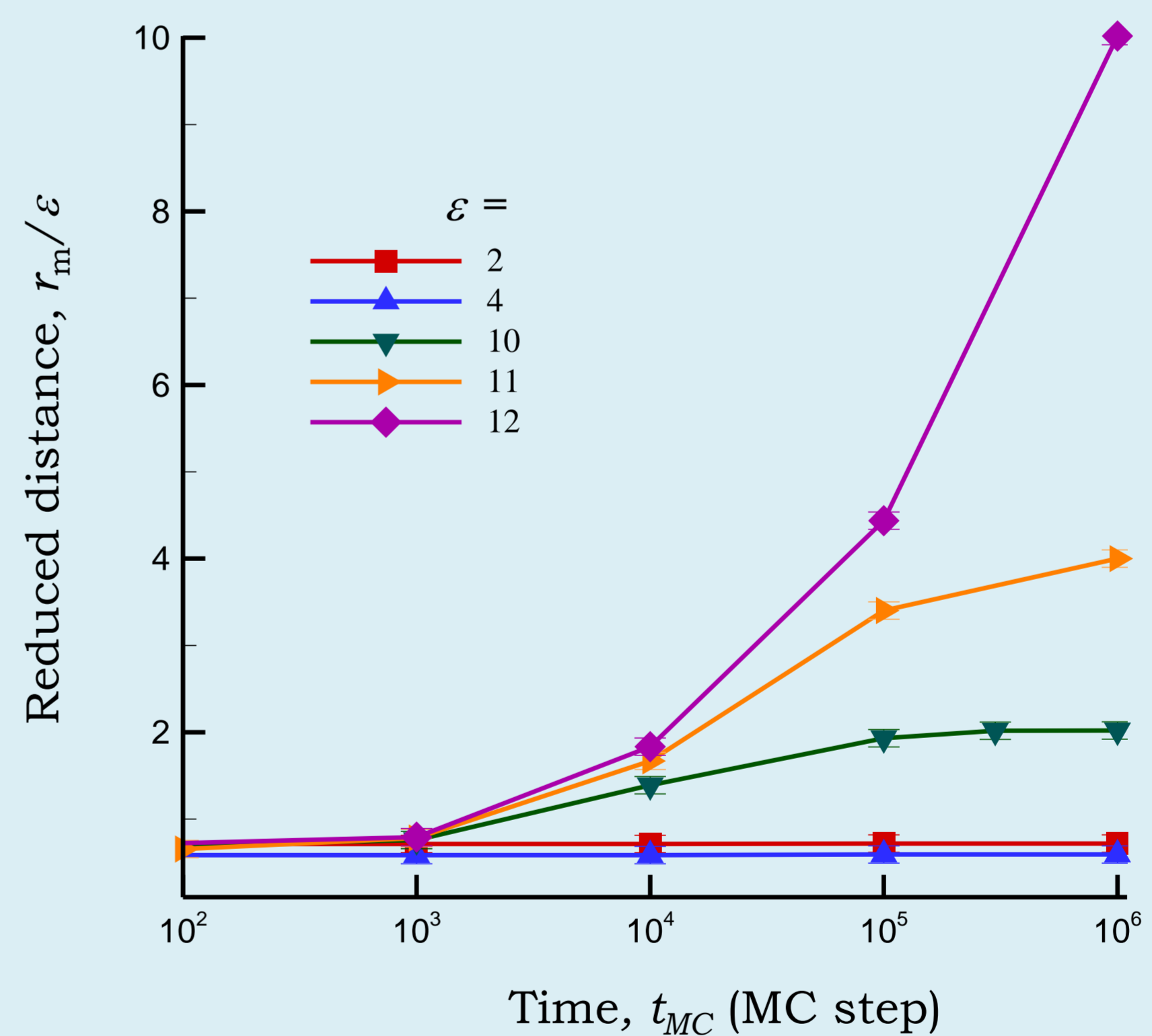


Figure 4: Reduced distance, r_m/ε , versus the time, t_{MC} , for different values of aspect ratio, ε .

Conclusions

For systems with relatively small aspect ratios ($\varepsilon \leq 9$) the relaxation into the isotropic state with $S=0$ was always observed. In the intermediate range, $9 < \varepsilon \leq 12$, the relaxation into the isotropic or nematic phase was observed. In systems with higher aspect ratio ($\varepsilon > 12$), the relaxation into the nematic phase was always observed. The transition to the nematic phase occurs due to the enlargement and consolidation of stacks of particles.

Acknowledgements: The authors acknowledge funding from the National research foundation of Ukraine, Grant No. 2020.02/0138 (M.O.T., N.V.V.), and National Academy of Sciences of Ukraine, Project Nos. 7/9/3-f-4-1230-2021 (N.I.L.)