Surface roughening due to patchy particles in (1+1) dimensions - A computational study

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In recent years new extraordinary material synthesis techniques have been developed, which have made possible the fabrication of so called ‘patchy’ particles - particles of nanometers to micrometers sizes, which have inhomogeneous or ‘patchy’ surfaces. They interact mutually through highly directional, short range forces, and are capable of aggregating into very novel structures. We have carried out a computational study of the ballistic deposition of model patchy particles in 2D. This study simulates the physical processes where particles are projected on to a substrate and undergo deposition to form a cluster. In our study the particles interact with each other through highly directed, strong and short range forces. This is done using the so called Kern-Frenkel model.

We found that the growth process shows a phase transition which occurs at a critical patch size of $p_c = 0.6454$. For adhesive patch sizes below a well-defined critical value the growth of cluster kinetically terminates. That is, the cluster essentially stops growing, because the growth becomes stochastically improbable and we have a ‘blocked’ phase. For patch sizes above the critical patch size the aggregation continues indefinitely, which is a ‘growing’ phase. We have studied the changes in the growth process, the surface morphology of the clusters for varying patch sizes. The surface morphology of the cluster in the growing phase well above $p_c$ is that of a typical ballistic growth, which is characterized by a surface roughness $w(t)$ that increases as $t^\beta$ for $t << t_x$, and remains constant for $t >> t_x$, where $t_x$ is known as the cross-over time and $\beta$ the growth exponent. For ballistic deposition of homogeneous particles $\beta = 0.33$ and we also obtain similar values. We obtain a dramatically different morphology for patch sizes near $p_c$, that is, in the critical region like the growth of a fractal, tree-like structure to mushroom like structures. In the critical region, the surface width values is found to be much higher than the normal ballistic deposition model and the growth exponent dramatically deviated than from the expected KPZ prediction. Recent studies on deposition of highly anisotropic particles near at air-water interface appear to belong to KPZ class with quenched disorder. Our study also appears to be similar to the growth of the interface due to pinning effects.

Our study gives an insight for understanding the kinetic roughening of the growth species with anisotropic interactions.

FIG. 1. (a) Growth of interface width with time for BD model for a system of patchy particles for different patch size (b) The surface morphology of the film for the patch size $p = 0.6$. The tree like growth of the surface is observed.