Nonequilibrium diffusion of reactive solid islands

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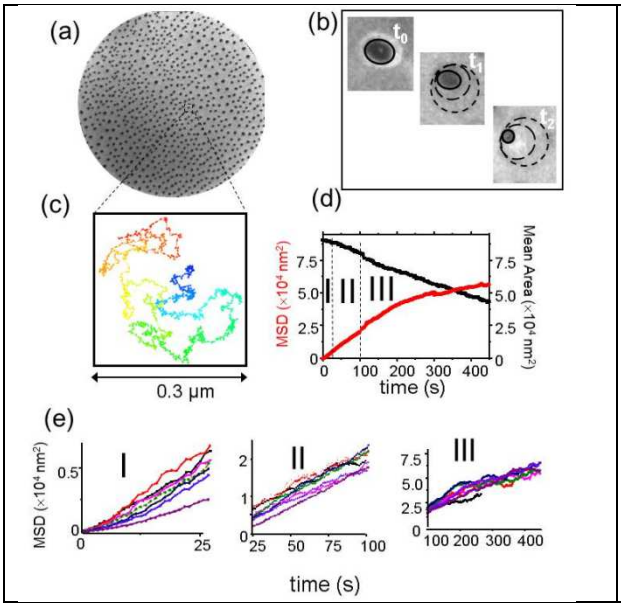
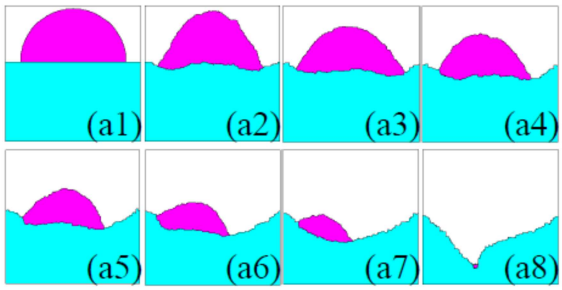
In this paper we report on the combined effects of reactivity, wetting, and shape changes on the random motion of crystalline Si islands on amorphous SiO_2 substrates during annealing. For this purpose nanoparticle motion and size evolution are studied both experimentally (*in situ* and real time experiments) and theoretically [kinetic Monte Carlo simulations (KMC) including chemical reactivity).We show that the time dependence of the mean square displacement. behaviors: (I) an equilibrium Brownian motion consistent with existing equilibrium theories, leading to strong size dependence of the diffusion constant, (II) an unexpected regime characterized by a linear time dependence of the MSD roughly independent on the nanoparticle size, attributed to a repeated pinning depinning of the triple line in ring-shape trenches formed by chemical reaction, and (III) a self-trapping regime where the reactive islands are trapped in the pit they drill in the substrate, leading to a saturation of the MSD.

The experimental observations are supported by the KMC simulations, based on interface reaction of Si with SiO2, interface diffusion of oxygen, and evaporation of SiO.





On left: *Experimental results (a) LEEM image of 3D islands, (b) means square displacement of a given island, (c) sequence of LEEM pitures for an island, (d) MSD versus time for a given island, (e) time evolution of the MSD for different island radius.*
On top: *snapshots of KMC simulations*

Reference:

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