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High temperature simulations of the early stage growth of Ge quantum dots on silicon based substrates with the kinetic Monte Carlo code NASCAM.

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For the last 10 years, there has been an increasing interest in semiconductor nanostructures.

This is mainly driven by unique features of nanometric structures whose optical properties strongly depends on their sizes. Recently, it has been demonstrated that nanosized Ge clusters exhibit intense photoluminescence. An interesting method to obtain Ge based highly efficient quantum dots is the self-organization method where atoms are being deposited at high temperature on a substrate and a Stranski-Krastanov or Volmer-Weber growth mode is taking place. To achieve efficient devices, special organization is required and is usually obtained by varying experimental parameters like substrate temperature and flux: if the temperature is too low, the deposited atoms stay at landing sites and no self-organization is happening. On the contrary, if temperature is too high, re-evaporation occurs and detachment from seed-clusters may occur and no big clusters can be formed.

In this work, we model the growth of the first atomic layer of Ge on SiO_2 and Si at high temperature with the help of our kinetic Monte-Carlo code NASCAM.

The current version takes into account the following physical events: deposition at different deposition rates, re-evaporation, diffusion on the substrate, diffusion on the deposited layers, jump from one layer to another one, trapping by defects and detrapping. Substrate can be modelised as a squared or a hexagonal lattice, corrugated or not. Annealing of pre-existing structures can also be performed.

After a short description of NASCAM implementation, we will present results of several modelisations at various temperatures and deposition rates. Method to determine activation energy for re-evaporation of Ge will also be presented.

Keywords
structure modeling
nano clusters
film growth