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Senior Research Fellowship

Multiscale models for strain-controlled diffusion problems

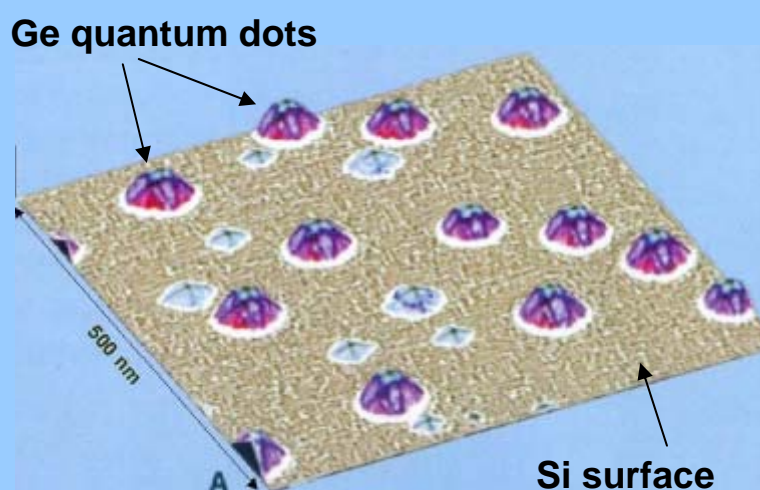
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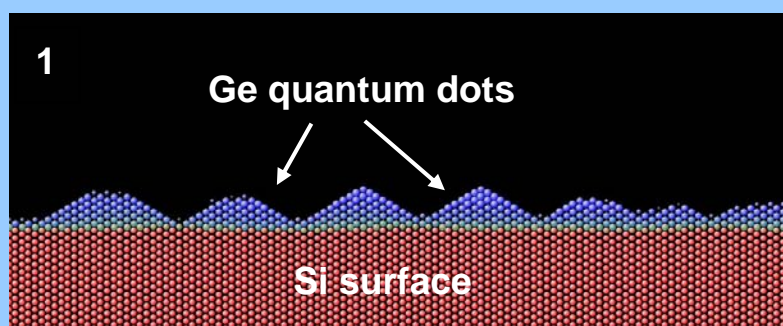
Self-organised Nanostructures



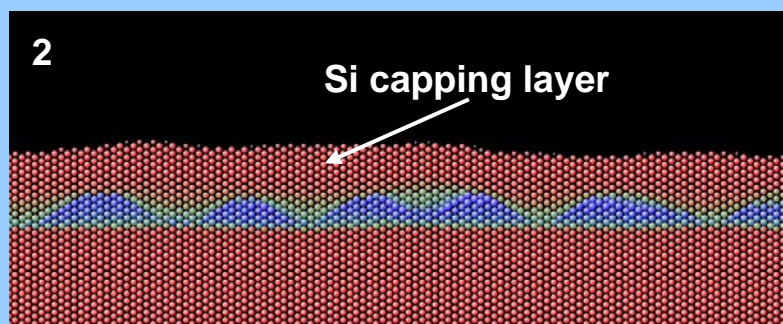
Example

- Vaporised germanium (Ge) condenses onto silicon (Si).
- Ge assembles into regular structures by diffusion of atoms over the Si surface due to -4.2% elastic mismatch strain.
- Atomic clusters below 20 nanometers (nm) in size are known as *quantum dots*.
- Capped dots used in optoelectronics and have possible uses in memory storage and quantum computers.
- Atomistic models such as molecular dynamics function at femtosecond timescale. Diffusive timescale is seconds.
- Need to develop new *diffusive molecular dynamics* method to simulate these systems.

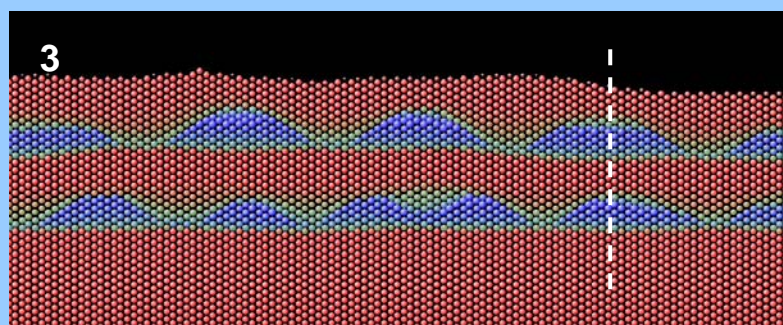
Diffusive Molecular Dynamics Model



1. Ge (blue) is deposited onto Si (red). Elastic mismatch promotes self-organisation. Mismatch is reduced at the Ge/Si interface by intermixing (green).



2. A capping layer of Si is deposited on the Ge dots to stabilize them. The top of the pyramidal dots dissolves into the capping layer as seen experimentally.



3. Further deposition of Ge followed by Si generates another layer of dots. Dots in the second layer grow above the ones below creating a vertically aligned *superlattice* as seen in experiment.

Shape and composition of simulated quantum dots (left) similar to that of real dots (right).

