Single element 2D materials and methods of their epitaxial synthesis

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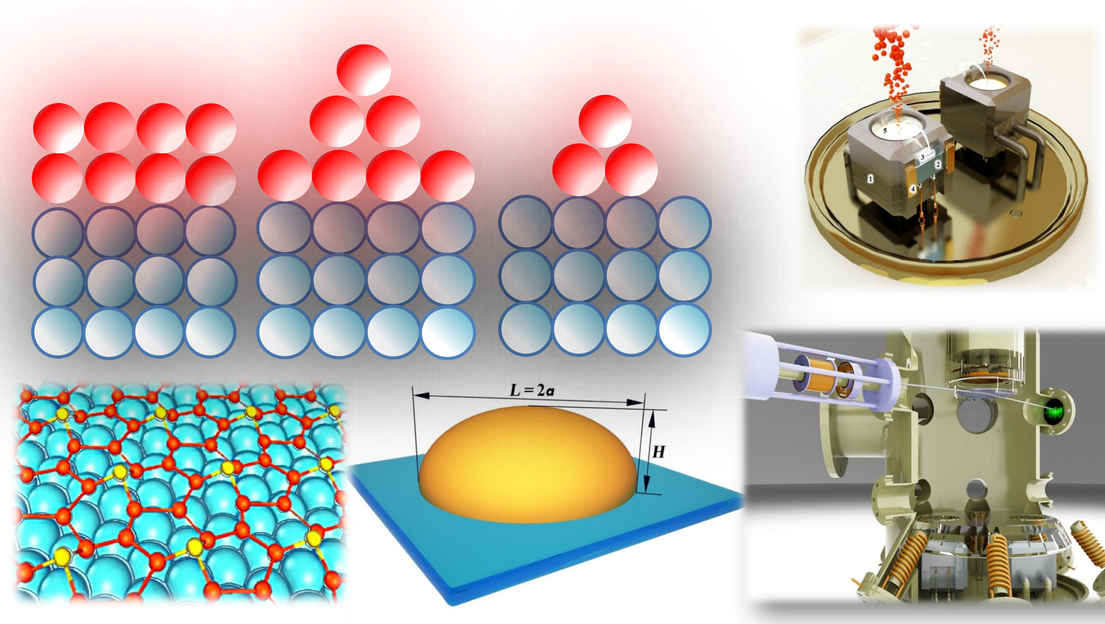
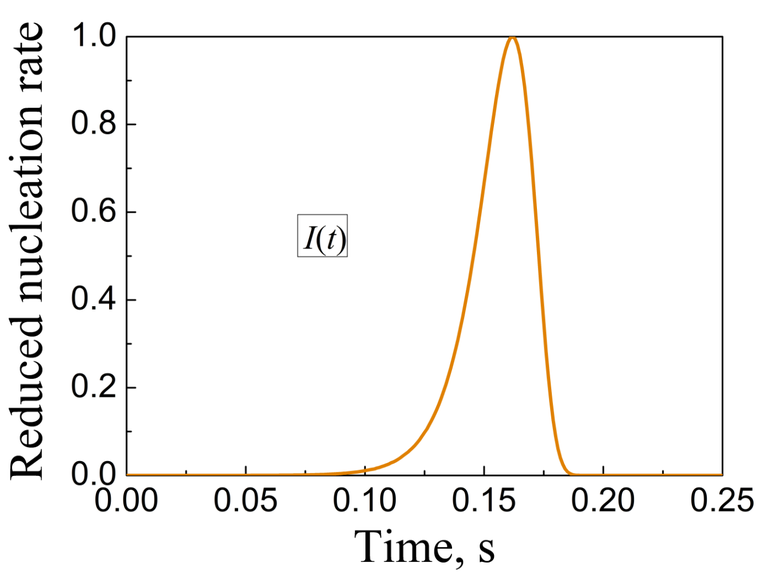
Mechanisms of Epitaxial Growth

- **Frank-van der Merwe (*I*)** growth mode is realized for **homoepitaxial** systems
- **F–M** growth mode is also typical for systems with close values of lattice mismatch ε_0
- **F–M** growth mode may be used for creation of 2D crystals for topological electronics
- **Stranski-Krastanow (*II*)** growth mode is typical for **Ge/Si** and **InAs/GaAs** systems
- 1st stage: **layer-by-layer** (**2D**) growth
- 2nd stage: nucleation of **3D hut-clusters** caused by relaxation of elastic strain
- 3rd stage: emergence of two separate shapes – **hut- and dome-clusters**
- 4th stage: **interaction between islands** and disappearance of small islands
- **Volmer-Weber (*III*)** growth mode is realized for **Ge/SiO_2/Si** and **$A^{III}B^{V}$/Si** systems
- Nucleation of **3D clusters** proceeds on top of the substrate without wetting layer
- Typical for systems with high values of lattice mismatch ε_0



Initial Stages of 2D Layer Growth and 2D-3D Transition



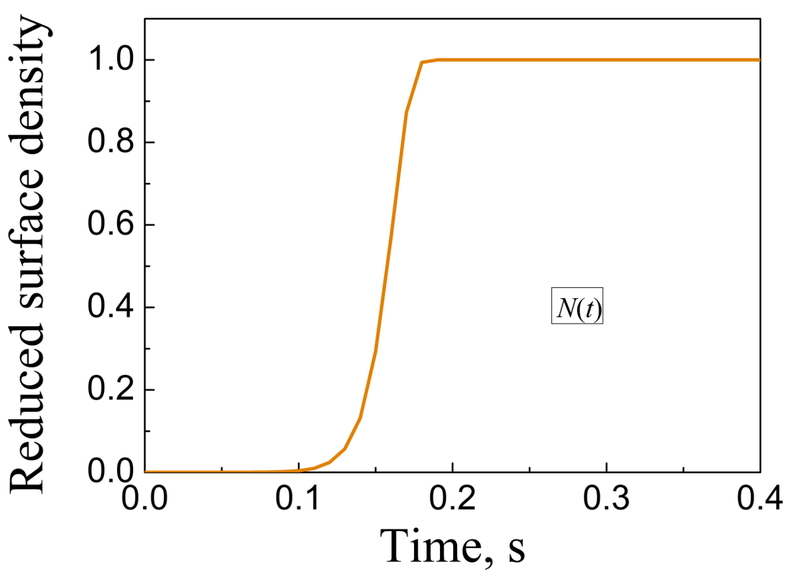


Figure 1. **Dependencies of the 2D islands nucleation rate and surface density on time (or the effective thickness of the deposited material).**

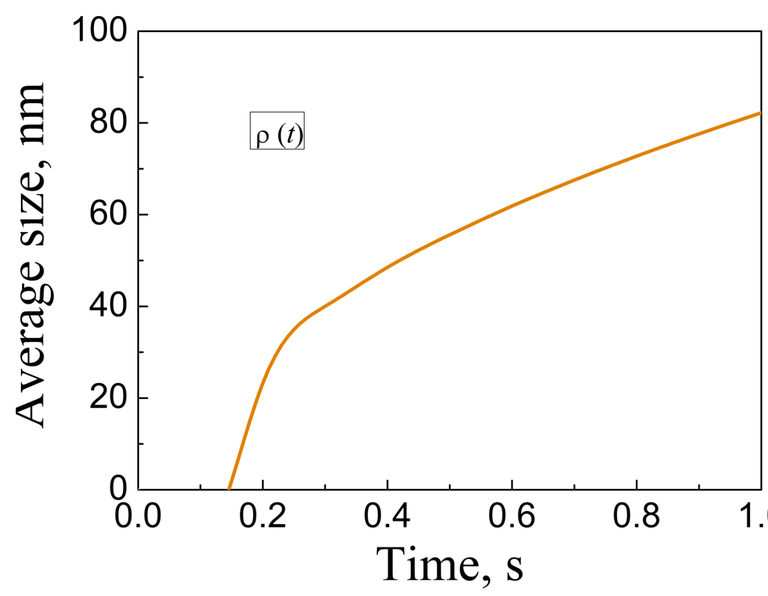


Figure 2. **Dependency of the average size of 2D islands on time.**

Nucleation and Evolution of Epitaxial Quantum Dots

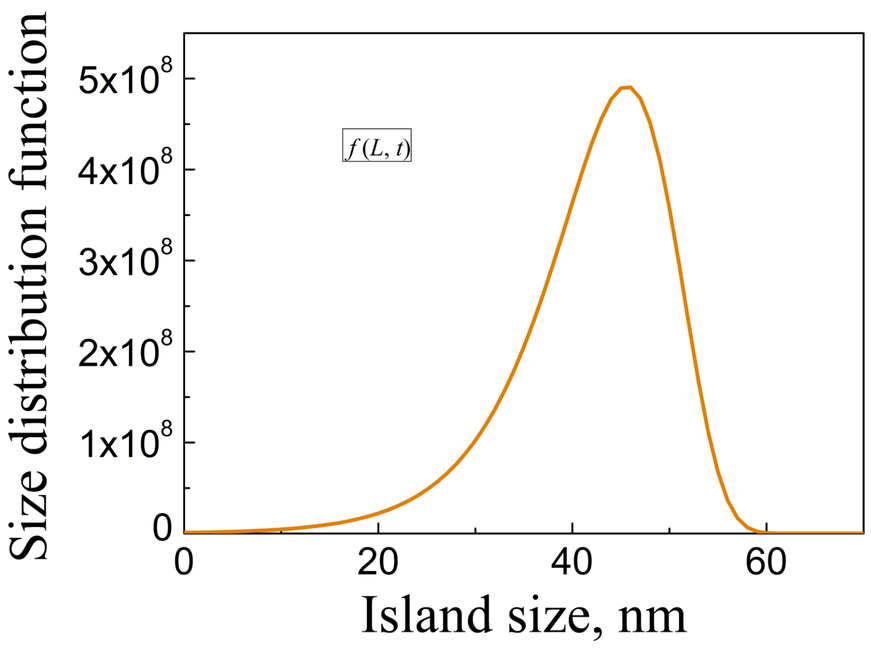
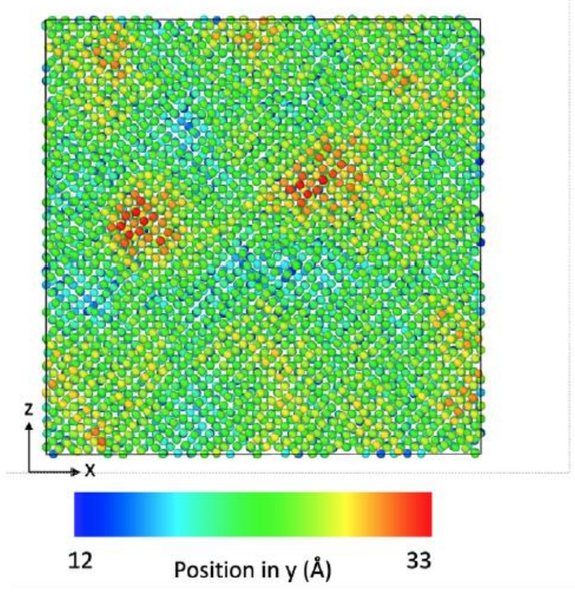


Figure 3. **Size distribution function of quantum dots.**

Zhou Y., Lozovoy K. A. et al. // Surface Science. – 2020. – V. 696. – P. 121594 (1-9).



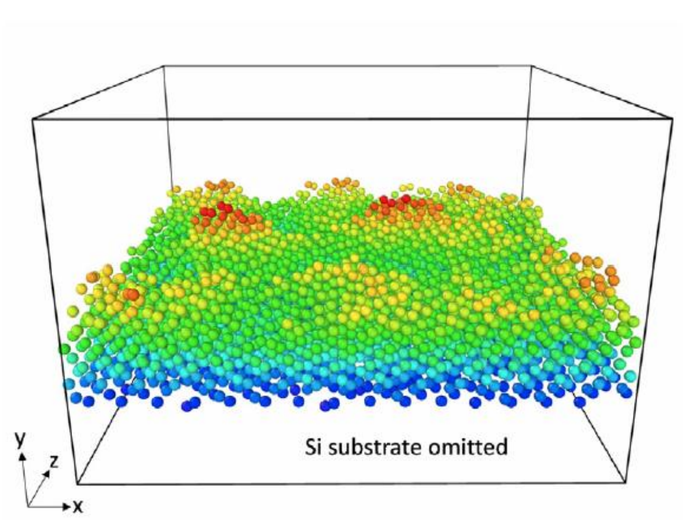


Figure 4. **The formation of 2D layer and small Ge islands after 4900 deposited Ge atoms at 1000 K. The atoms are deposited every 0.1 ns, normal to the surface with an energy of 1 eV. The initial stages of the growth of germanium on the dimer reconstructed Si(100) surface is modelled using molecular dynamics. Pyramidal island structures are observed to form despite molecular dynamics simulations being carried out at a deposition rate faster than experiment.**

Conclusions

As a result, different stages of formation of two-dimensional layers with the thickness from one to several monolayers, including possible nucleation of 2D and 3D islands are described. Physics and mathematical model of thin film growth and islands nucleation in the considered systems is proposed. The possibilities of decreasing the surface roughness, suppressing the nucleation of islands and preventing the transition to undesirable three-dimensional growth are identified.