Feasibility Study of Directed Self-Assembly of Semiconductor Quantum Dots

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ABSTRACT

Strain mismatched semiconductors are used to form Self-Assembled Quantum Dots (SAQDs). An important step in developing SAQD technology is to control randomness and disorder in SAQD arrays. There is usually both spatial and size disorder. Here, it is proposed to use spatially varying heating as a method to direct self-assembly and create more ordered SAQD arrays or to control placement of single dots or dot clusters. The feasibility of this approach is demonstrated using a 2D computational model of Ge dots grown in Si based on finite element analysis of surface diffusion and linear elasticity.

Keywords: self-assembly, quantum dots, semiconductor heterostructures, Si/Ge

1 Introduction

Self-assembly of quantum dots represents an important step in the advancement of semiconductor fabrication at the nanoscale that will allow breakthroughs in electronics and optoelectronics. The two most studied systems are Ge_xSi_{1-x} dots grown on a Si substrate and $In_xGa_{1-x}As$ dots grown on a GaAs substrate. The former being most interesting for electronic applications and possibly even optoelectronic applications, and the latter being most useful for optoelectronic applications. An important step in developing SAQD technology is to control randomness and disorder in SAQD size and SAQD position. One would like to direct self-assembly to either a) generate large arrays of regularly spaced and/or regularly sized SAQDs or b) be able to place SAQDs in desired locations. Three examples of directed self-assembly of quantum dots are the preferential nucleation of SAQDs above intersection points of an array of misfit dislocations [1], nucleation of quantum dots on etched mesas [2], and the ability to nucleate SAQD clusters using a FIB (focused ion beam). [3]

Here, spatially varying heating is proposed as a method to direct self-assembly. The underlying principal is quite basic. Surface diffusion is required for formation of SAQDs. Surface diffusion is a thermally activated process. Thus, dots will form more quickly where the temperature is high and less quickly where the temperature is low. By selectively controlling the hot spots, the sites for SAQD formation can be chosen. This selection is enhance by ripening. Dots that get a "head start" will ultimately absorb the material of slower forming dots.

Possible methods of spatially varying heating are using a laser interference pattern to generate spatially periodic temperatures as in [4,5], and heating with low energy ion bombardment or an electron beam might also be possible. A spatially periodic temperature profile can produce an array with greatly enhanced spatial and size ordering, or a focused hot spot can produce a quantum dot cluster (similar to a quantum fortress [6]) or even a single dot. The feasibility of using spatially varying heating to direct self-assembly is demonstrated through computational experiment using a 2D numerical model of elasticity and surface diffusion similar to [7, 8].

2 Modeling/Method

The physical model is based on surface diffusion, similar to [7]. The film surface evolves and ultimately forms SAQDs via surface diffusion and deposition of new material. The surface diffusion is driven by a chemical potential $\mu = \mu_{surface} + \mu_{elastic} + \mu_{wetting}$. All calculations are fully non-linear except for the stress-strain portion that uses linear isotropic elasticity. For developmental convenience and computational efficiency, the model is implemented in two-dimensions with a 1D evolving surface (Fig. 1). The model is implemented via finite element analysis using FEMLAB [9].

3 Results

Three growth processes are simulated and reported on (Fig. 1). *Simulation 1* uses spatially uniform temperature. *Simulation 2* uses a spatially periodic temperature profile of periodicity $\lambda = 185$ nm. *Simulation 3* is growth in the presence of a gaussian shaped hot spot of width 371 nm.

4 Analysis/Conclusions

For $t = 100$s, the uniformity of the dots using a periodic temperature are compared with the results of the control uniform temperature simulation. Uniformity in height, width and spacing are compared. It should be

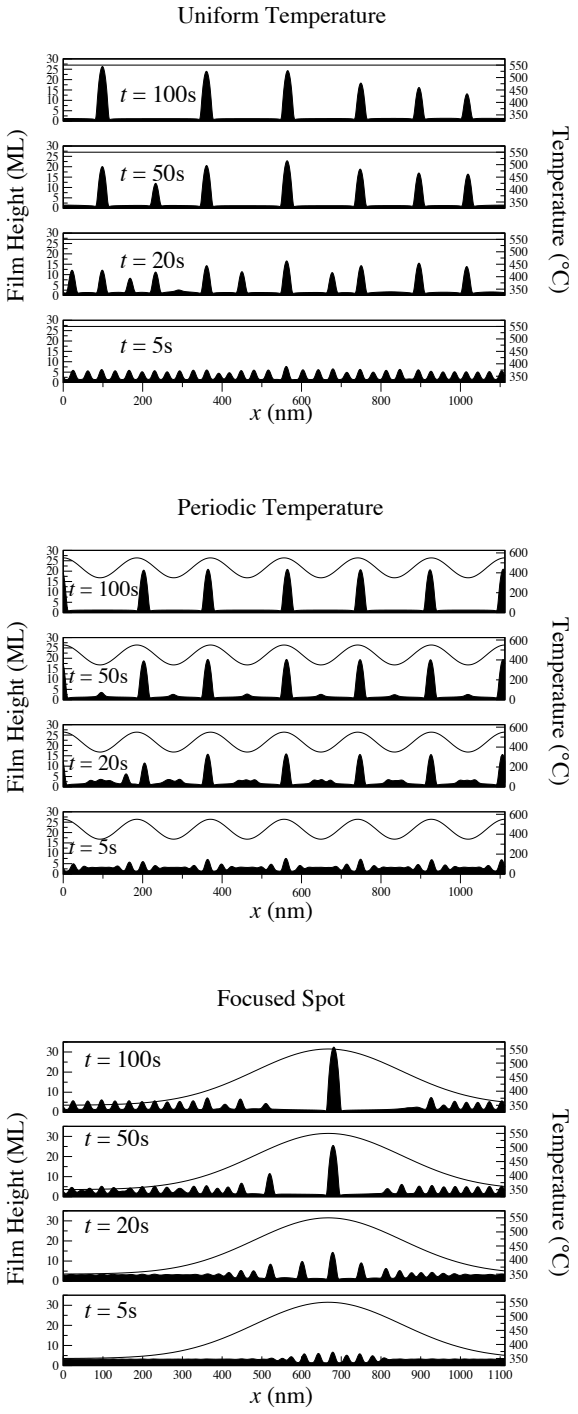

Figure 1: *Simulation Results.* Solid line (—) indicates temperature profile. Filled pattern indicates film height. The graphs are not to scale as the dot aspect ratios are stretched in the vertical direction for clarity.

noted that the mean values for each simulation are essentially the same while the percent standard deviations show that the periodic temperature profile gives vastly superior uniformity.

measure	system	mean	% std. dev.
height (nm):	uniform	5.52	25.8%
	periodic	5.62	0.32%
width (nm):	uniform	28.2	11.57%
	periodic	28.4	0.32%
peak-peak	uniform	185	26.3%
spacing (nm):	periodic	185	8.80%

The spatially varying heating gives smaller improvements in spacing-scatter than it does for size-scatter, but the spacing scatter for the periodic case is relative to the temperature profile, and it will maintain its coherence over the same length scale as the temperature profile. Thus, spacing regularity could be guaranteed over the coherence length of a laser.

The gaussian-shaped hot spot, *simulation 3*, produces a central dot surrounded by smaller dots. For the realization shown in Fig. 1, the central dot peak is located 14.0 nm from the temperature peak. That is a misalignment of 3.8% of the full peak width or 40% of the full dot width. The surrounding dots have heights of 1.5 ± 0.24 nm compared with the central dot's height of 8.8 nm. Thus, there is sufficient separation to prevent optical spectrum overlap or similarity in capacitance.

The success of spatially varying heating to produce ordered or controlled SAQDs in this simple simulation has not yet been confirmed experimentally, and it should be followed up by both more detailed modeling and experimental trials.

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