The Stranski – Krastanov Three Dimensional Island Growth Prediction on Finite Size Model

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Abstract

The Stranski-Krastanov growth theory is important to predict some of the nano-size semiconductor structures such as quantum dots and wires. This growth mode starts from a 2D thin film growth and transits into 3D island growth. The work done is to simulate and study the Stranski-Krastanov growth based on theoretical equations in energy changes. Three main energies involve are the chemical interaction energy, wetting energy and elastic energy. Parameters for various materials are used for the simulation and enable us to understand growth characteristics for certain material undergoing Stranski-Krastanov growth. The selected parameters are then used in actual growth conditions in the laboratory.

Keywords: Stranski-Krastanov, Finite-Size, 2D Growth, 3D Growth

Introduction

Stranski-Krastanov (SK) growth is important when dealing with quantum size structures. The formation of the 3-dimensional (3D) quantum structure (*Volmer Weber equivalence*) is driven by the strain that occur during growth when the deposited 2-dimensional layers (2D) (*Frank-van der Merwe equivalence*) exceed a critical thickness [1]. This growth phenomenon occurs due to the change in interfacial energies of the substrate-vapor namely the free surface energy (γ^{∞}) and the adhesion energy (β^{∞}). For the SK growth mode to occur, it needs large lattice mismatched of different materials between substrate and growth layer but with the same lattice structure. Some common examples are germanium on silicon and gallium arsenide on aluminum gallium arsenide layers.

In a lattice mismatch condition, the vapour of material A is deposited on a substrate of material B (Fig. 1(a)). Initially an ultra thin layer of thin film of material A is formed near the substrate. This stage of growth is called Frank-van der Merwe growth (Fig. 1(b)). When the growth layers reach a certain critical thickness, the growth layers transform to 3D growth instead of 2D growth. This is called Volmer-Weber growth (Fig. 1(c)).

Stranski-Krastanov growth is a 2 phase's growth with phase 1 is the epitaxy layers growth of 3 – 7 % lattice mismatch material (larger lattice) on the crystalline substrate (smaller lattice). The formation of the epitaxy layers will reach supercritical layers, where these layers will have less strain from the substrate layer and relaxation starts. This relaxation results in an island like epitaxy formation.

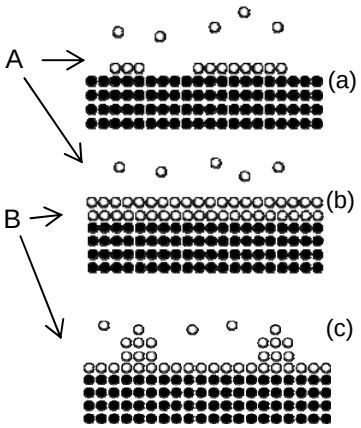

Figure 1

Theory

The Stranski-Krastanov growth mode has been studied extensively by P. Muller [2]. The study based on the finite-size SK growth equation, where the finite-size mentioned is referring to the size of the substrate used in the fabrication. For an SK growth the total stress change ΔF is given by [2]:

$$\Delta F = -\Delta\mu\left(V + L^2 za\right) + \Phi_\infty\left[\left(L^2 - \left(\frac{V}{r}\right)^{2/3}\right)\left(1 - e^{-z}\right) + \left(\frac{V}{r}\right)^{2/3}\right] + 4\gamma_A V^{2/3} r^{1/3} + \varepsilon_0\left(VR + zaL^2\right) \quad (1)$$

There are three parts of stress energy change in Equation (1) i.e.:

1. The stress change due to chemical work

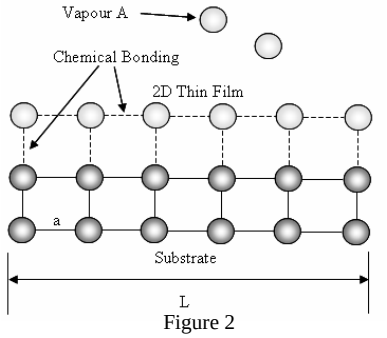

Figure 2

$$\Delta F_1 = -\Delta\mu\left(zaL^2 - hl^2\right) \quad (2)$$

$\Delta\mu$ is the supersaturation per unit volume of the deposited vapor, *z* is the deposited layer thickness in term of molecular layers (ML), *a* is the lattice constant of the deposited materials in nanometer (nm), *L* is the length of the substrate in nanometer (nm), and *h* and *l* are the height and length of the 3-diamensional islands respectively in nanometer (nm).

2. The stress change due to surface contributions

$$\Delta F_2 = \Phi_\infty\left[\left(L^2 - \left(\frac{V}{r}\right)^{2/3}\right)\left(1 - e^{-Z}\right) + \left(\frac{V}{r}\right)^{2/3}\right] + 4\gamma_A V^{2/3} r^{1/3} \quad (3)$$

Where Φ_∞ is the wetting energy between the vapor and the substrate in joule (J), *V* is the volume of the 3-diamentional islands, r is the aspect ratio between the height, *h* and the length, *l* of the 3-dimensional island (*h/l*), and γ_A is the surface energy of vapor A in joule (J). The wetting energy, Φ_∞ is given by:

$$\Phi_\infty = \gamma_{AB}\left(n_A, n_B\right) = \gamma_A^\infty\left(1 - e^{-n_A/\zeta}\right) + \gamma_B^\infty\left(1 - e^{-n_B/\zeta}\right) - \beta^\infty\left(1 - e^{-n_A/\zeta}\right)\left(1 - e^{-n_B/\zeta}\right) \quad (4)$$

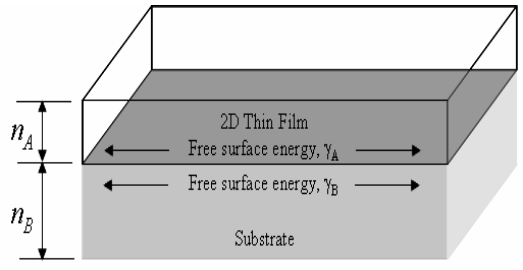

Figure 3

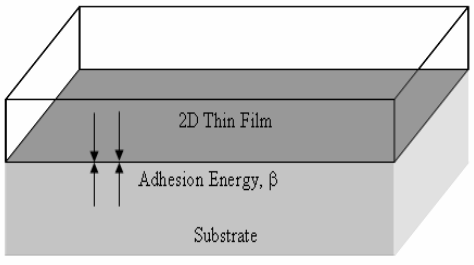

Figure 4

Where γ_A is the surface energy of vapor A and γ_B is the surface energy for substrate B, β is the adhesion energy between the vapor A and the substrate B, n_A and n_B are the layers thicknesses of the deposited layers and of the substrate respectively.

Double layers zeta potential of the thin film is given by [3]: $\varsigma = \frac{u\eta}{\varepsilon_w \nabla\phi}$ (5)

u is average velocity which is given by [4]: $u = \sqrt{\frac{8kT}{\pi m}}$ (6)

η is the viscosity of the vapor A, ε_w is the permittivity and the ϕ is the electric potential of the vapor A. All variants are assumed equals to 1 except the temperature that was calculated from the equation below:

$$\Delta F = -\Delta\mu\left(V + L^2 za\right) + \Phi_\infty\left[\left(L^2 - \left(\frac{V}{r}\right)^{2/3}\right)\left(1 - e^{-z\varepsilon/\eta\sqrt{\frac{8KT}{\Pi m}}}\right) + \left(\frac{V}{r}\right)^{2/3}\right] + 4\gamma_A V^{2/3} r^{1/3} + \varepsilon_0\left(VR + zaL^2\right) \quad (7)$$

3. The stress change due to lattice strain or elastic energy storing.

$$\Delta F_3 = \varepsilon_0\left(VR + zaL^2\right) \quad (8)$$

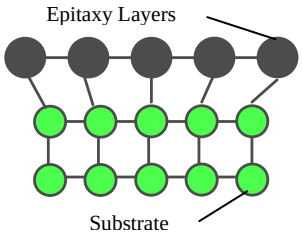

Figure 5

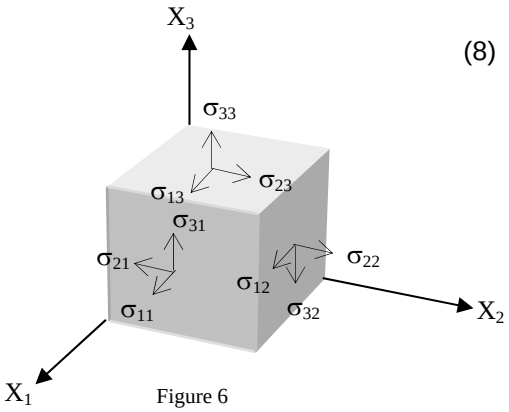

Figure 6

ε_0 is the strain in a 3-D system and given by: $\varepsilon_0 = \frac{\sigma}{M}$ (9)

Where σthe stress of the 3-dimensional system and M is is the elastic modulus. R is the elastic relaxation factor with values between 0 and 1. *Substrate smaller lattice compare to larger lattice of the deposition layers.* Strain result from this lattice misfit in all three directions is shown in figure 5.

Result and Discussion

I. *Stress change due to chemical contributions*

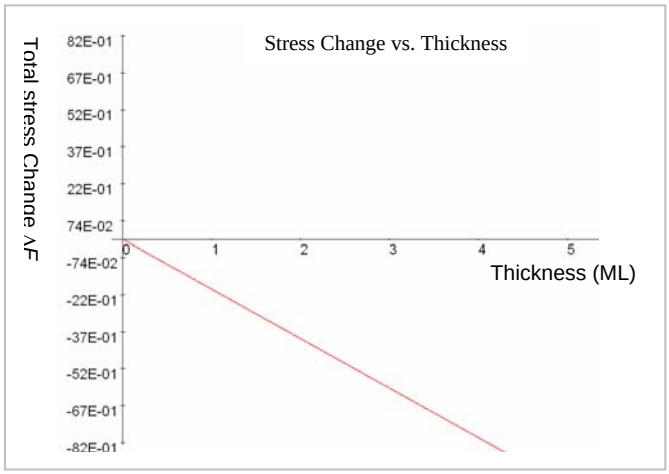

Figure 7

The simulation due to the chemical contributions shows that the total stress change increases with the deposition layers (Fig. 7). Negative values in the graph means that the stress is relax when the deposited vapor form chemical bonding.

As the thickness of the deposited layers increase surface re-construction starts to occur. The chemical bonding binds the atomic vapor together closer to the original lattice structure and without lattice strain. This results in elastic relaxation.

II. *Stress change due to surface contributions*

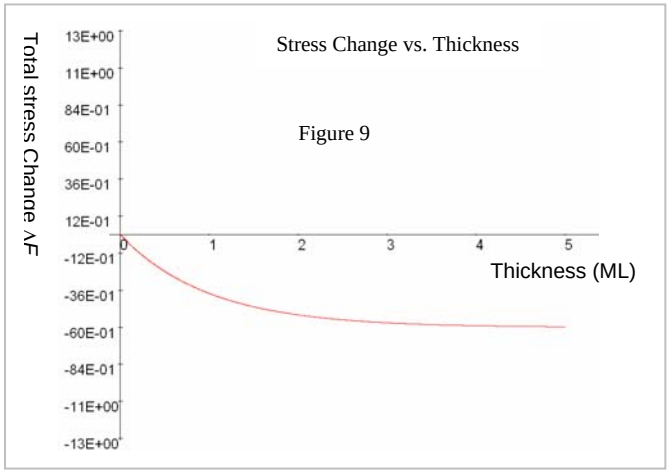

Figure 8

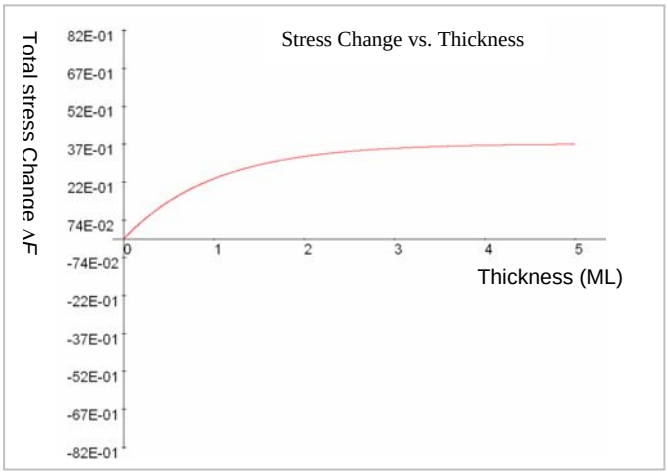

Figure 9

The total stress change due to surface contributions increases exponentially initially (Fig. 8 and 9). It reaches constant value at a certain layer thickness (at about 2.5 ML in this case). Wetting energy can be either negative or positive depending on the growth condition, i.e. the wetting energy is negative in a 2-dimensional thin film growth (Fig. 8), but is positive in a 3-dimensional island growth (Fig. 9). This is because the energy change is control by the free surface energy (γ) and the adhesion energy (β).

In a 2-dimensional growth, lattice strain in the system increases with layers thickness and causes the surface energy increase. In a 3-dimensional growth, surface reconstruction occurs as the deposited layers thickness increase. Elastic relaxation occurs in the atomic structure when it reaches a certain critical thickness value. During relaxation, the surface energy will be minimized and balance out by the adhesion energy and the total stress becomes constant. [5]

III. *Stress change due to lattice strain*

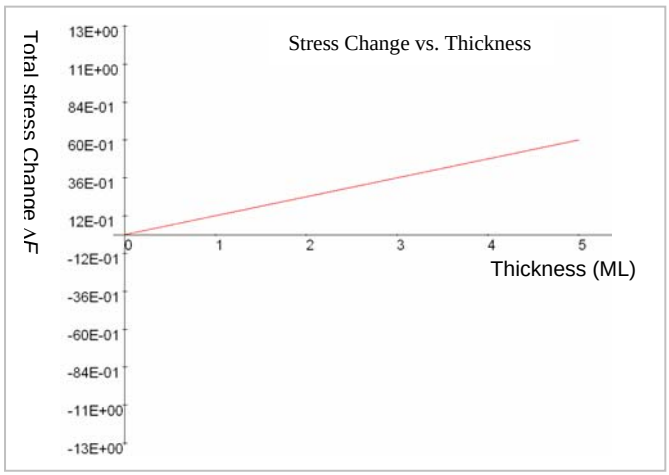

Figure 10

From the simulation, the total stress change due to elastic strain increases with the deposited layers (Fig. 10). This is due to the growth on lattice misfit system. As more layers are deposited, more strains are stored into the lattice system and the lattice system will seek elastic relaxation. he meaning of relaxation is the atomic layers of the epitaxy layers getting less strain effect from the substrate layers, thus the epitaxy layers can relax to forming it orginal larger lattice structure.

Conclusion

In conclusion, the result from the simulation for 2-dimensional and 3-dimensional growth is in accordance with the result given by P. Müller. This simulation can be used to predict the growth of uniform thin film or island structure when given appropriate parameters such as supersaturation, material elastic strain, lattice constant, and the most important are the free surface energy and adhesion energy of the material.

Reference

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