Microelectronics Reliability xxx (2017) xxx–xxx

Contents lists available at ScienceDirect

Microelectronics Reliability

journal homepage: www.elsevier.com/locate/microrel

Uncertainty quantification in nanowire growth modeling – A precursor to quality semiconductor nanomanufacturing

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ARTICLE INFO

Article history:
Received 19 May 2017
Received in revised form 22 June 2017
Accepted 19 July 2017
Available online xxxx

Keywords:
Nanomanufacturing
Nanowire growth model
Semiconductor reliability
Sensitivity analysis
Uncertainty quantification

ABSTRACT

Mitigating the uncertainties associated with nanowire growth models have significant ramifications for the quality and reliability of nanomanufacturing of semiconductor nanowires. This research is focused on the development of a sectional-based mechanistic model of nanowire growth and the determination of the level of impacts the model parameters have on the growth of nanowires, characterized in terms of their weight, diameter and length. After testing the model with experimental growth data of silica (Si) nanowire weight, ZnO average diameter and length, it was observed that the direct top impingement growth coefficient (α_{im}) had the largest influence on the nanowire growth, in comparison to other model parameters → sidewall diffusion growth coefficient (α_{sw}), maximum allowable growth weight or length ($W^{(\max)}$) and initial weight or length (W_0). The knowledge of the impact of uncertainty in these parameters on the overall growth of the nanowire can be leveraged on for robust design of the nanofabrication process that will impact on the quality, reliability, yield and cost of nanomanufacturing.

1. Introduction

Nanomanufacturing has gained a lot of interest in recent years due to the immense contributions of nanoparticles to revolutionizing computation, data storage, actuation and sensing for several applications. The popularity and influence of nanostructures have made it the focus of many research activities in the fields of engineering, healthcare, agriculture, space and earth sciences [1–2]. However, despite the proliferation of research in nanotechnology, there have been considerable problems with high cost of nanofabrication [3] due to the numerous uncertainties associated with the physics, measurement and experimental control in nanofabrication [4]. Nanowires, which are pivotal to nanotechnology advancements, have unfortunately not been reliably fabricated due to the complexities in modeling, experimentation and replication of experimental and mathematical model results [4–5]. Imperatively, the cumulative effects of these problems can be mitigated with the characterization, quantification and minimization of the uncertainties.

Understanding the effects of uncertainties in nanowire growth will facilitate the nanofabrication process via appropriate decisions on parametric application that will improve the quality and minimize the cost of nanomanufacturing [6]. Hence, achieving reliable nanomanufacturing will entail making proper decisions on parametric applications in growth modeling and equipment calibration during nanofabrication [6–7].

Many researchers have worked on nanowire growth modeling from different perspectives → physical, statistical and cross domain modeling [4,8–10]. Diffusion based modeling, which centered on the concentration gradients of the growth materials that cause the growth of nanowires have also been published widely [11–13], whereas the focus on growth rates of the direct top impingement and sidewall diffusion events have been the focus of other researchers [8,11]. Despite the advances made by these numerous authors on nanowire growth modeling, there is still a need for understanding the parametric uncertainties associated with nanowire growth models, based on a discrete sectional growth configuration. This is because this sort of model will not only capture the localized growth conditions inherent in a section of the nanowire, but will also aid in the characterization of the growth parameters in those sections.

The objective of this research is to develop a contributory sectional nanowire growth model that will utilize the growth rate coefficients of the direct top impingement and sidewall diffusion mechanisms to establish the growth trend of nanowires. We will also quantify the effects

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http://dx.doi.org/10.1016/j.microrel.2017.07.085
0026-2714/

Please cite this article as: C.I. Ossai, et al., Uncertainty quantification in nanowire growth modeling – A precursor to quality semiconductor nanomanufacturing, Microelectronics Reliability (2017), http://dx.doi.org/10.1016/j.microrel.2017.07.085

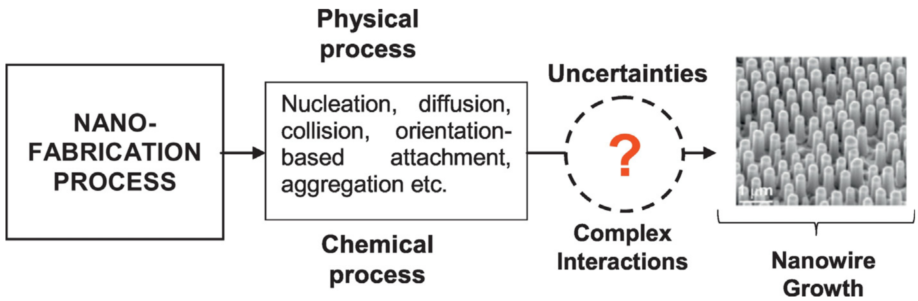

Fig. 1. Diagram describing the complex interactions of the physical and chemical processes in nanowire growth.

of the model parameters on the growth of nanowires, to determine their behaviors at different time limits in the nanofabrication process. This knowledge will help to improve the quality of nanowires. This work will therefore develop a model that:

i. Will capture the inherent uncertainties associated with nanowire growth at different times.
ii. Provide for a unified approach that will distinguish the growth characteristics of the direct top impingement and sidewall diffusion growth in the nanofabrication process.
iii. Give a better overall growth perspective of nanowires, since the model will capture the growth behavior of the nanowire sections.
iv. Assess the impact of variability in the nanowire growth model parameters on the growth of nanowires.

2. Mechanistic sectional-growth model of nanowires

The growth of nanowire, which is caused by physical and chemical interactions of nanoparticles [2,14] can be depicted by Fig. 1.

This growth is affected by uncertainties in physics, measurement and experimental control [4,10,15] because of the heteroepitaxy [16–17], which culminates in non-uniform nanoparticles deposition. It is assumed that a constant (ω) that determines the growth uncertainty in nanowires, results in the variation of sectional growth. Hence, the ith nanowire sectional growth influencing factor (ω_i), can be related to the sectional area (A_i) by Eqs. (1) and (2).

$$A_i \propto W_i^{\omega} \tag{1}$$

$$\begin{cases} \omega_i = f\left(\alpha_{im}^{(i)}, \alpha_{sw}^{(i)}\right) \\ \omega_i = \alpha_{im}^{(i)} + \alpha_{sw}^{(i)} \end{cases} \tag{2}$$

where W is the growth weight or length, (α_{im}) is the direct top impingement growth coefficient and (α_{sw}) is the sidewall diffusion growth coefficient.

If the growth of a nanowire (due to the nanoparticle deposition from direct top impingement and sidewall diffusion) is contributed from n discrete sections as shown in Fig. 2, then, the growth weight or length of each section can be represented by W_i, whereas the maximum allowable weight or length (equilibrium weight or length) can be represented by $W_i^{(\max)}$.

Considering the varied sectional dimensions, which result in the variability of the maximum allowable sectional growth weight or length, the growth rate of the ith nanowire section and the entire nanowire can be expressed by Eq. (3).

$$\begin{cases} \dfrac{\partial W_i}{\partial t} \propto \left(W_i^{(max)} - W_i\right) \\ \dfrac{\partial W}{\partial t} \propto \left(W^{(max)} - W\right) \propto \displaystyle\sum_{i=1}^{n} \left(W_i^{(max)} - W_i\right) \end{cases} \tag{3}$$

If the influence of the sectional growth factor that determines the growth characteristics of the sections at a given time in the nanofabrication process is considered, the contributory sectional growth of the nanowire, due to the direct top impingement growth at the sections and the entire nanowire can be represented by Eq. (4).

$$\begin{cases} \dfrac{\partial W_i}{\partial t} = \alpha_{im}^{(i)} \left(W_i^{(max)} - W_i\right) \\ \dfrac{\partial W}{\partial t} = \displaystyle\sum_{i=1}^{n} \alpha_{im}^{(i)} \left(W_i^{(max)} - W_i\right) \end{cases} \tag{4}$$

For a circular cross-sectional area of the nanowire with radius r, assumed to be constant in the growth process, the sidewall diffusion

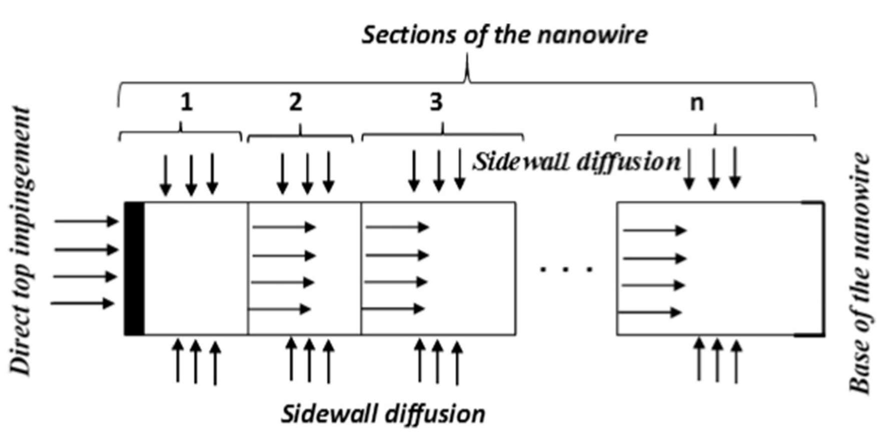

Fig. 2. Schematic showing the nanowire sectional growth due to direct top impingement and sidewall diffusion of atoms.

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