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Kinetic Monte Carlo simulation of low-pressure chemical vapor deposition of silicon nitride: Impact of gas flow rate and temperature on silicon cluster size and density

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ABSTRACT

In the present study, the deposition process of SiN_x thin films obtained by a low-pressure chemical vapor deposition technique with a mixture of disilane (Si_2H_6) and ammonia (NH_3) was simulated by using the kinetic Monte Carlo method. A new pattern describing the distribution of ammonia molecules in the simulation matrix was proposed. The influences of the NH_3/Si_2H_6 gas flow ratio and the deposition temperature on the obtained films structure in terms of silicon cluster size and density were analyzed. The simulation results indicate that an increase in the gas flow ratio leads to the deposition of amorphous silicon clusters characterized by small sizes. Nevertheless, an increase in the temperature values of the process provokes an enhancement in the silicon cluster size along with a decrease in their density.

1. Introduction

During the last few years, an intense research activity has been focused on the formation of silicon nanocrystals (Si-nc) in SiN_x thin films [1–10] due to the huge potentiality of these nanocrystals in nanoelectronic applications for example channel layer of thin film transistors leading to a great enhancement in carrier mobility [11], and in optoelectronic applications, because Si-nc is expected to exhibit a quantum size effect. Indeed, the wavelength of luminescence can be controlled by changing the size of Si-nc [7]. Nevertheless, the production of the light emission from Si-nc was also studied in silicon (Si) oxide films [12–15]. However, the large barrier height of the Si oxide prevents the injection efficiency of the carriers, which reduces the properties of the devices. In this context, the SiN_x thin films receive considerable attention due to its lower barrier height than silicon oxide.

Different chemical vapor deposition (CVD) techniques have been used for Si-nc formation in the SiN_x thin films, like low-pressure chemical vapor deposition (LPCVD) [1,9], plasma-enhanced chemical vapor deposition (PECVD) [3–5,16], and catalytic chemical vapor deposition (Cat-CVD) [7,8]. Indeed, the deposition parameters (temperature, total pressure, gas flow ratio…) of these films strongly control the physical properties of the obtained nanocrystalline thin film [4–7,9,17,18]. Therefore, the simulation of the deposit step is necessary for designing the material with the required properties.

In this work, we aim to simulate the deposition process of SiN_x thin films obtained by a LPCVD technique with a mixture of disilane (Si_2H_6) and ammonia (NH_3) by using the kinetic Monte Carlo (KMC) method. To simulate this process, we propose a new simulation pattern to describe the distribution of the NH_3 molecules in the simulation

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matrix. Indeed, by reserving sites for NH_3 molecules in the system, the structures of the deposited films can be studied by varying the NH_3/Si_2H_6 gas flow ratio and the temperature values of the process.

2. Simulation procedure

2.1. Kinetic Monte Carlo algorithm

The KMC method has been widely and successfully used for exploring the evolution and properties of a wide range of problems and systems. It is a powerful tool for modeling the process of chemical vapor deposition, which involves the adsorption, desorption, evolution, and incorporation of vapor species at the surface of a growing film.

Our work concerns the simulation of the deposition process of SiN_x thin films. To do this, molecules and radicals are assumed to have discrete positions within a two-dimensional triangular lattice representing the surface structure of the film. The simulation lattice contains a fixed number of sites ($N=40{,}000$) while the diameter of the silicon atom was given to be around 0.25 nm [19]. During the simulation procedure, a lattice site is selected randomly from the simulation matrix. In the present 2D simulation, the deposition of a molecule (or a radical) occurs at the condition that the selected site is empty. The corresponding deposition rate was given by the following expression [20]:

$$V_d = V_{d_0}\exp\left(-\frac{E_a}{K_B T}\right) \tag{1}$$

where V_{d_0} parameter depends only on the deposition total pressure P and on the wafer-to-wafer distance δ, K_B is the Boltzmann constant, T is the deposition temperature, and E_a is the deposition activation energy which was estimated to be 2.25 eV [18].

The growth process of SiN_x thin films considered in this paper includes two microscopic processes: an adsorption process, in which molecules and radicals are incorporated into the film from the gas phase, and a migration process, in which silicon adatoms move to their adjacent sites. In the migration process, a silicon adatom having six nearest neighbors is associated with an adatom that is fully surrounded by other adatoms and cannot migrate [21,22]. However, when a silicon adatom has one to five nearest neighbors, it can jump to a vacant neighboring site with a rate that depends on its local environment [21,22]. Indeed, a silicon adatom with only one nearest neighbor is considered unstable [21–23] and is subject to migration. During the simulation, a silicon adatom overcomes the energy barrier of the site and moves to its most stable neighboring vacant site, which is defined as the site with the most nearest neighbors with a migration rate (probability) that depends on the local environment of the silicon adatom; i.e. the number of the nearest neighbors of the silicon adatom selected for a migration event [21,22,24]. The corresponding migration rate of the ith silicon adatom is calculated as follows [19,21,22,24]:

$$r_{m,i} = \upsilon_0\exp\left(-\frac{n_i E_0}{K_B T}\right) \tag{2}$$

where υ_0 represents the pre-exponential factor, n_i is the number of the nearest neighbors of the ith silicon adatom, and E_0 is the contribution to the activation energy barrier. In this work, the pre-exponential factor and the energy barrier contribution in Eq. (2) take the following values $\upsilon_0=10^{13}\ s^{-1}$ and $E_0=0.6$ eV [25]. In the case of multiple neighboring

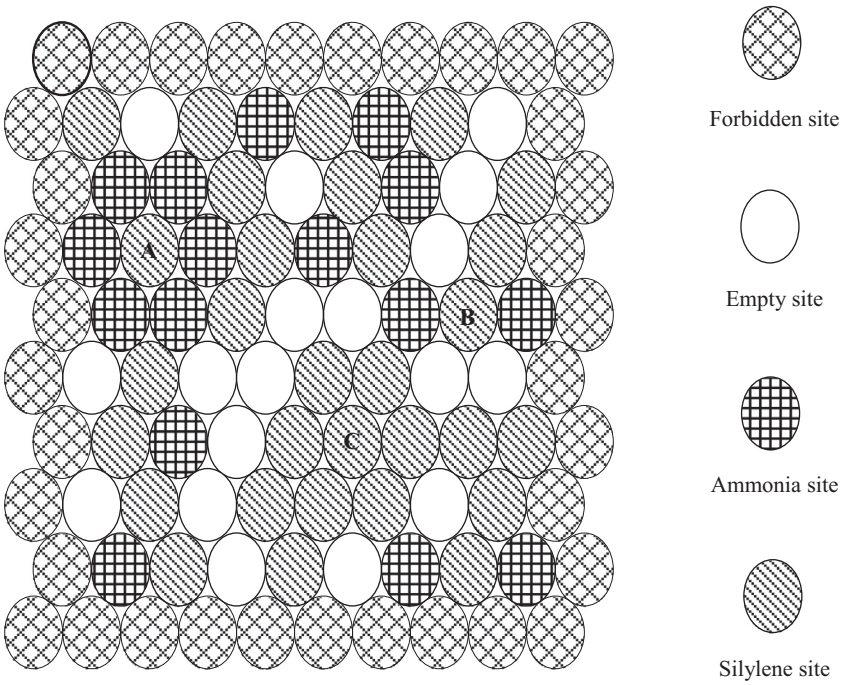

Fig. 1. Schematic design of the deposition process of a SiN_x thin film. A: silylene (SiH_2) site enclosed by ammonia (NH_3) molecules in all directions. B: SiH_2 site having less than six nearest neighbors. C: SiH_2 site enclosed by SiH_2 radicals in all directions.