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Nucleation simulation using a model of hard/soft discs

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HIGHLIGHTS

- Computer study of the nucleation probability is described by different disk models.
- Percolation probability is described as probability of forming a spanning cluster.
- The HCSS model and continuous percolation explain the beginning of the nucleation.

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ABSTRACT

In this paper we present a computer study of the quantum dot (QD) nucleation probability with three possible models of particle interaction; Soft Core (SC), Hard Core (HC) and Hard Core/Soft Shell (HCSS) model. Computer analysis of the nucleation probability is performed on a 500 by 500 lattice with 2000 simulations per event. If a matrix is assumed to represent an SiO_2 substrate in which a pure Si quantum dot can grow, it is demonstrated that nucleation centers are more easily distinguished and initially more likely to form in the SC and HCSS models rather than in the HC model. If particles are allowed to move, nucleation centers can appear even in the HC model independent of a preexisting local density. A low probability of nucleation in the HC model and a high probability of nucleation in the SC model are evident from the system entropy curve. The probability of nucleation, therefore, depends on the local density change, percolation probability and system entropy. Low probability of nucleation in the HC model is in accordance with a lower probability of percolating clusters forming in a given model.

1. Introduction

In recent scientific research, silicon quantum dots' physical properties have been studied and simulated in order to help the development of high quality, next generation electronic and optoelectronic devices. The nucleation process and the formation of a quantum dot (QD) are not yet fully understood and are still subject to numerous discussions [1–3]. Quantum dot nucleation origins from spinodal decomposition of SiO_x layers, which further leads to the formation of SiO_2 matrix supersaturated with Si atoms [4]. Si atoms tend to cluster and form the nuclei for further QDs growth, which is believed to occur spontaneously at a random site of the matrix (preferred heterogeneous nucleation [5]), due to a density variation or stress caused by structural differences of decomposing materials [6]. For example, nuclei can form in a supersaturated

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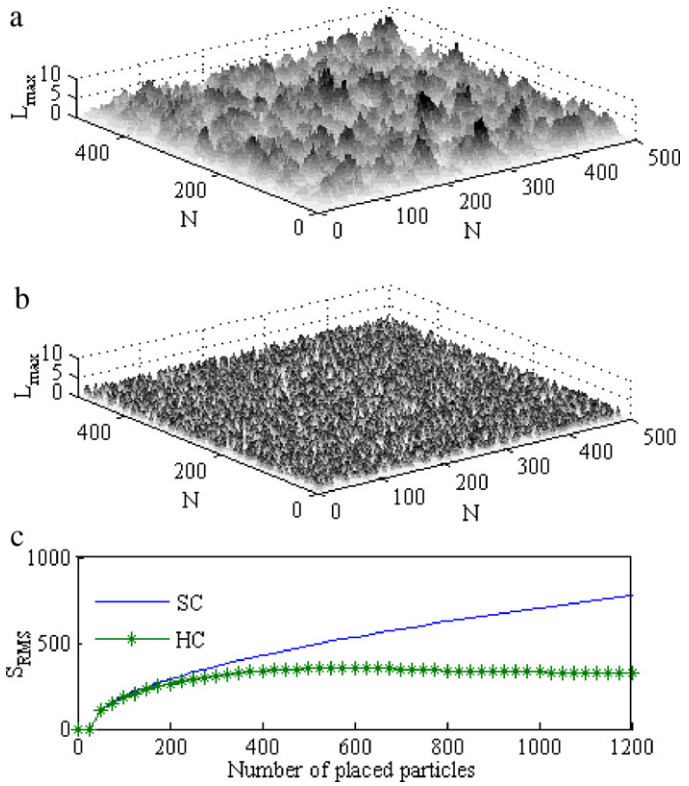

Fig. 1. Example of the overlap amplitude distribution: (a) a random SC model, (b) a HC model; and (c) amplitude intensity measure calculated as the roughness parameter S_{RMS}.

solution depending on the local temperature and Gibbs free energy (for the adding particle) at each site [7]. But, whether a nucleation site will develop into a quantum dot depends on yet another set of conditions such as critical cluster radius or density, and even the distance and size of the neighboring clusters [8].

In computer simulations an indicator of nucleation can be extracted from the particle overlapping amplitude. If each overlap appearing between two or more particles is marked with an integer, this measure produces a 3D view of the overlap amplitude distribution within the matrix. The distinguishable local maxima, visible in Fig. 1(a), indicate the places in the matrix where multiple particles are clustered. If clearly defined maxima do exist in the 3D overlap distribution view for a particular interaction model, it can point to the nucleation center position.

These distinguishable maxima can be observed in simulated Soft Core (SC) and Hard Core/Soft Shell (HCSS) particle interaction models. On the other hand, particles in the Hard Core (HC) model homogeneously cover the surface eliminating the possibility of random particle overlapping or clustering, Fig. 1(b). The measure of intensity of overlapping can be calculated using the surface roughness model. The most common measure parameters used to describe the roughening process are arithmetic averages (S_a) of the absolute value of vertical distances from the mean line (f_i) and the root mean square (S_{RMS}) of f_i in the considered matrix. The roughness profile is then defined as:

$$S_{RMS} = \sqrt{\frac{1}{n}\sum_{i=1}^{n} |f_i^2|}, \tag{1}$$

where n is the number of points in the matrix.

To be in close agreement with the physical picture, simulation takes into account the processes and conditions that contribute to QD nucleation. Therefore, a variation in the local density of silicon suboxide and randomness in the creation of Si atoms as a result of its decomposition reflects in a random placement of discs in our model, as governed by a pseudo-random generator. Experiments have shown that QDs in real superstructure based systems have a narrow size distribution [9] which leads to the conclusion that processes such as small particle aggregation have to be minimized in simulations. Another way to achieve a narrow size distribution is to assume that nucleation and growth are two separate processes which exist independently [10].

If isolated particles in a matrix are allowed to follow random Brownian movement (which is characterized by particle movement in a random direction with a constant distance step) or a random Kinetic MonteCarlo (KMC) process (which is characterized as the time evolution of the particle movement in a random direction with distance step depending on