Simulation of Nanowire Growth using Monte-Carlo Method

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Abstract— The proposed work is destined to create an application that can virtually simulate the direction of growth of nanowire with the change in physical conditions like rate of absorption and desorption. To date, the modeling studies using Kinetic Monte-Carlo simulations have been primarily used to understand the crystal growth and etching processes taking place on large surfaces of 3D crystals. These studies typically simulate crystal growth on two-dimensional lattices using periodic boundary conditions. These simulation methodologies were later interpreted for whisker growth to relate growth kinetics with process conditions. The method chosen for the simulations is the Kinetic Monte-Carlo method, well known for its accuracy of the results it produces and the modest computational resources it takes.

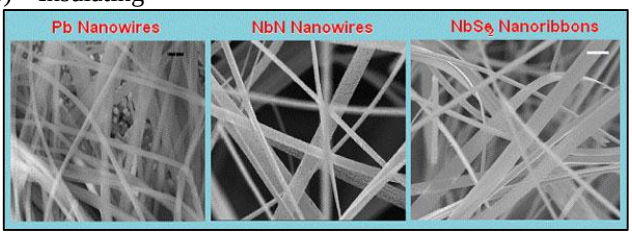
Key words: Kinetic-Monte Carlo, Nanowires, Lattices, Seed

I. INTRODUCTION

Nanowires are one-dimensional form of materials whose diameters range from 1 nm – 100 nm and are gaining importance as building blocks for nanoscale science and technology. Nanowires with sub-100 nm size are useful for re-engineering of products using for optics, electronics, sensors and composites. Furthermore, the nanowires under 20 nm size are considered as low-dimensional solids and could possess new properties due to quantum confinement and surface effects. Consequently, there has been a significant amount of interest in the synthesis and structure-property relationship of sub-20 nm nanowires of technologically important materials such as Si, Ge, Gallium Nitride, diamond etc. The natural progression of the technology dictates a need to synthesize nanowires of such materials systems in a reproducible and controllable manner. Most importantly, the current processes used to synthesize nanowires fail to provide serious insight into the conditions that predictably give rise to different growth directions for nanowires.

Nanowires are of 4 types:

1) Superconducting- Pb, NbN, NbSO2
2) Metallic- Ni, Pt, Au
3) Semiconducting- Si, InP, GaN
4) Insulating



They have following properties:

1) Depending upon what it's made from nanowire can have properties of an insulator, a semiconductor or a metal!
2) Some nanowires are ballistic conductors.
3) At nanoscale, elements can show very different properties than what we expect. For example: -
   1) Gold has a melting point of more than 1000 degree Celsius but if its size is decreased to nanometres then there is a significant decrease in melting point of gold.
   2) Aluminium is not magnetic but very small clusters of aluminium are magnetic.

II. LITERATURE SURVEY

A. Monte Carlo Methods

Monte Carlo method was first proposed by Metropolis and Ulam [5] in 1946. Monte Carlo methods can be defined as numerical methods that employ statistical techniques, which utilize sequences of random numbers, to perform the simulation such that the nature of the system being simulated can be predicted. We should also observe that the sequence of random numbers used obey some property or properties. The Monte Carlo method can be described as a technique of statistical sampling employed to approximate solutions to quantitative problems.

In other words Monte Carlo (MC) method is not very different from the regular statistical method. MC simulations use random moves to explore the search space to find out some information about the space. The random moves are accepted such that a different region of search space is sampled at each step.

This method ensures that events get selected according to their probability. Hence if an event 'e' has high probability of occurrence then the event e will be accepted whenever selected. It also ensures that the real world scenario is simulated as close as possible. The disadvantage of this algorithm is that the events with low probabilities are not selected. But low probability of an event does not mean that the event would never occur. Moreover whenever an event with probability lower than the generated random number is selected, that particular loop yields nothing and wastes computational resources. Various improvements have been made to this algorithm by many others to cover these drawbacks.

1) Metropolis Monte Carlo

The usage of the Monte Carlo method for equilibrium simulations was first proposed by Metropolis [5] for calculating the properties of the substances which are considered to be composed of interacting individual molecules. . This is done so that the Boltzmann average of a property of the system can be easily calculated. This modified Monte Carlo method is known as a Metropolis Monte Carlo simulation. The main reason for the necessity of Monte Carlo in this problem was due to the impracticality involved in calculating the equilibrium value of any quantity of interest in a given model by the traditional numerical methods such as using N-dimensional integral, where N is the number of particles present in that state. MC-simulations were from then used for studying various properties of different systems.

The main disadvantage of this implementation is that the events with high rate are selected more often than those with small rates, even if the events with low rate are high in concentration. Another main disadvantage is that

there are chances that none of the events are picked before we reach the completion of this loop.

Much later, the MC-simulations are used for the study of kinetic processes. The kinetic MC algorithm allows us to model the site-dependent surface chemistry and also allows us to visualize the evolution of resulting surfaces. In the absence of site-dependence of surface chemical reactions, it is possible to model the growth via reaction modeling without ever resorting to atomistic aspects. In most crystal growth problems, the surface chemistry set could involve tens of known reaction steps whose rates depend upon the site and its neighborhood. So, kinetic MC treatment is the only way to understand the evolution of crystals.

2) BKL Algorithm

One of the most popular versions of Monte Carlo algorithm that is used for kinetic processes is the BKL algorithm [6], which was actually devised to perform Monte Carlo simulations of Ising spin systems. It used a new method called the n-fold way, where N numbers of particles are classified into n groups based upon their rates, which significantly reduced the computation time required for the simulations. Please see review by Levi and Kotrla [7] about different variations of the KMC algorithms.

3) Other Improvisations

Schulze [10] proposed a variation of KMC where the selected event is accessed in constant time instead of searching it. When events are divided in to groups, a separate list is maintained for each group indexing each event of the group when a group is selected, an integer random number r1 is generated. The event with the index r1 is selected. By following method described by Schulze, i.e., to maintain a separate list of sites with same rate constant and picking one of them at random utilizing the random number generated, we can further reduce the computation time in the KMC algorithm.

III. METHODOLOGY

The initial design considered for the simulation is the one implemented by Radhika [11]. The reason behind selecting it as our base model is the similarity of the problems being simulated by that model and our model. It was designed to study the 3D growth process of the diamond structures while we have to design a model to simulate the 1D crystal growth process of the diamond structure. The main changes that are made to adapt those for suiting the current situation is to control the growth of the surface area.

The synthesis of nanowire is done by removing the site from the active growth surface list if it lies at the distance greater than the diameter from another site on the active growth surface.

For further computation we follow the following procedure:-

1) Read the input data (rate of constants of reaction) and initialize all variables.

Type ←0, R[i] ←0, Csp[i] ←0

2) Categorize type of sites-

If parent [bond]==1 and occupied_sites == 1:

Type← 1

Else if (parent[bond] == 2 and second_neighbour >=1) or (parent[bond] == 3 and second_neighbour[bond] >= 2):

Type← 2

Else if parent[bond] == 3 and second_neighbour == 1:

Type← 3

Else if distance[parents]<=0.05 and parent[bond]== 1 and second_neighbour[bond] ==1:

Type← 4

Else if parent[bond] == 3 and third_neighbour[bond] == 1:

Type← 5

Else if parent[bond] == 2 and third_neighbour[bond] >= 1:

Type ← 6

Else if site[bond] == 2 or site[bond] == 3:

Type← 7

Else:

Print no site

3) Identifying site fraction using-

X[i] ← S[i]/ N, Where N is the total no. of sites, S[i] is sum of each type of sites.

4) KMC loop:-

a) Calculation of rate of each reaction i :-

$r_i = \mu_i * X_i$ (if absorption) or

$r_i = \lambda_i * X_i$ (if desorption)

where μ_i and λ_i are the constants taken input from the user.

b) Calculation of probability of each reaction:-

$P_i = r_i / R$, where $R = \Sigma n$

c) Find cumulative site probability:

Csp[i] ← Csp[i-1] + Pi

d) Select a random X number between 0 and 1 and pick reaction I from 1 to n.

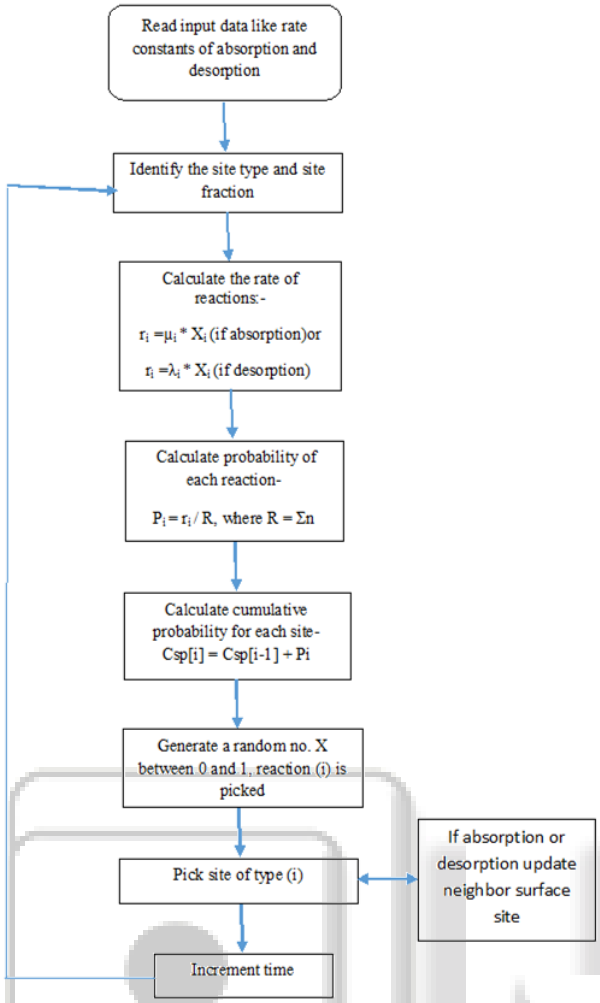
Site i is picked :- If desorption or absorption, update neighbors and surface sites

e) Increment time: - $\delta t = -\ln(X)/R$

$T = t + \delta t$

f) Go to step 2 until a desired length of wire if formed

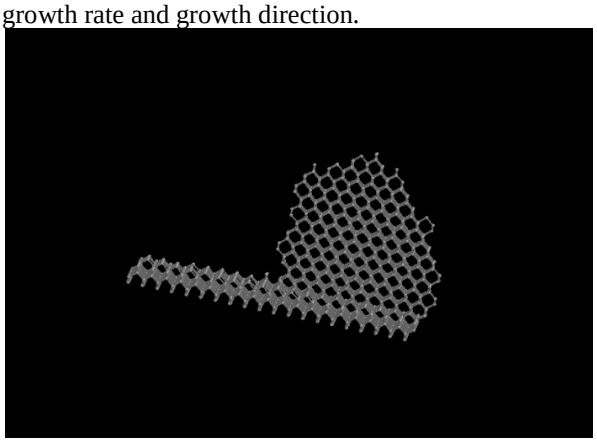
There are many improvements when compared with previous simulations. One of the major improvements is the speed of the simulations. The length of simulation always depends on the rate constant of the crystal. The number of loops taken to form a crystal cannot be minimized. In order to gain speed in simulations the time taken for each loop is minimized. In each loop there are different processes which have different computation complexity of $O(n^2-n)$. The time taken for each loop is reduced to O(n), from exponential to linear. The length of the simulation is always not a measure of the speed of the simulations. The number of KMC loops that are performed in a given time is a good measure of the speed of the simulations.



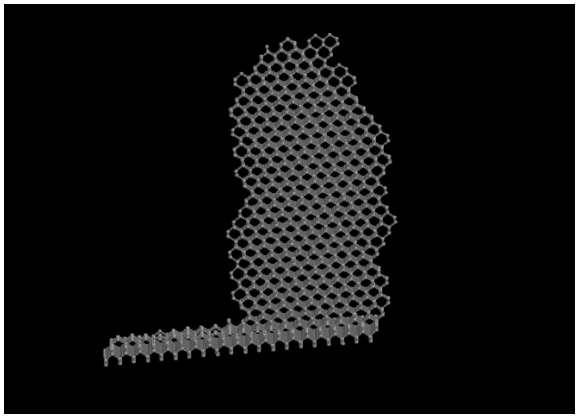
Flow chart of the Kinetic Monte Carlo algorithm used in the initial design

IV. SIMULATION RESULT OF NANOWIRE GROWTH

For visualization of the dataset the open source data visualizer RASMOL is used. The results of simulations are interesting in more than one way. The primary target of simulating 1D growth is achieved. Throughout the entire simulation crystal is maintained constant. This is due to growth surface area control. The simulations are stopped either if the desired number of atoms is reached or if the steady state is observed in growth rate and growth direction.



Ball and stick models of simulated 1D Crystals (3500 atoms) obtained using different sets of rate constants



Ball and stick models of simulated 1D Crystals (7000 atoms) obtained using different sets of rate constants.

Three primary planes (<111>, <100>, <110>) are considered in our simulations. The number of sites available on each plane gives us site concentrations. It can be considered as a measure of growth rate. A steady state in site concentrations indicates that the growth rate has reached steady state.

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