Materials and Design 160 (2018) 119–130

Contents lists available at ScienceDirect

Materials and Design

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

Messily grown nanowires: Simulation, geometrical characteristics and microstructural dynamics

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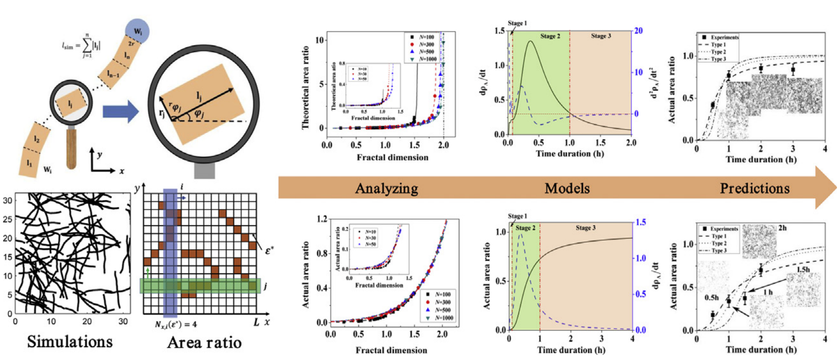
HIGHLIGHTS

- Morphology of messily grown nanowires is simulated by Monte Carlo method.
- The area ratio is used to describe the microstructure of messily grown nanowires.
- Microstructural dynamic models are obtained based on Monte Carlo simulations.
- The time varying area ratio shares S type growth mechanism.
- The dynamic of area ratio is determined by growth type of nanowire parameters.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 1 May 2018
Received in revised form 5 August 2018
Accepted 31 August 2018
Available online 06 September 2018

Keywords:
Monte Carlo simulation
Fractal characteristics
Messily grown nanowires
Microstructural dynamics

ABSTRACT

The geometrical characteristics and microstructural dynamics of messily grown nanowires were investigated by the means of Monte Carlo simulations and fractal geometry. Firstly, the simulated morphologies of messily grown nanowires are generated by Monte Carlo simulations. The fractal dimensions of simulated morphologies were calculated and found to be significantly determined by the quantity, radius and length of the simulated nanowires. Then, factors called theoretical and actual area ratio were proposed to describe the structure of simulated morphologies. Based on the new factors and the simulation results, a series of empirical models describing the actual area ratio varying with nanowire growth time were proposed. Finally, the proposed model was used on the time varying morphologies of messily grown Si nanowires synthesized by experiments. Predictions provided by the model show good agreement with experiments. The best fits appear when the nanowire quantity shows the saturated growth mode. Further simulations also show that the growth dynamic of actual area ratio shares the S type growth and is influenced by the growth modes of nanowire length, quantity or radius.

1. Introduction

Nanowires (NWs) are very potential one-dimensional nanomaterials with a variety of applications, including advanced functional sensors, electrodes, and promised reinforcements in nanocomposites or coatings [1–7]. The unique properties such as magnetic, conductivity and mechanical behaviors of nanowires are mainly determined by their specific physical and morphological structures [5–10].

According to the growth conditions, nanowires can form two categories of morphologies – aligned grown morphologies and messily grown morphologies. The aligned nanowires which are with uniform length and directions such as nanowire arrays, have found their

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https://doi.org/10.1016/j.matdes.2018.08.060
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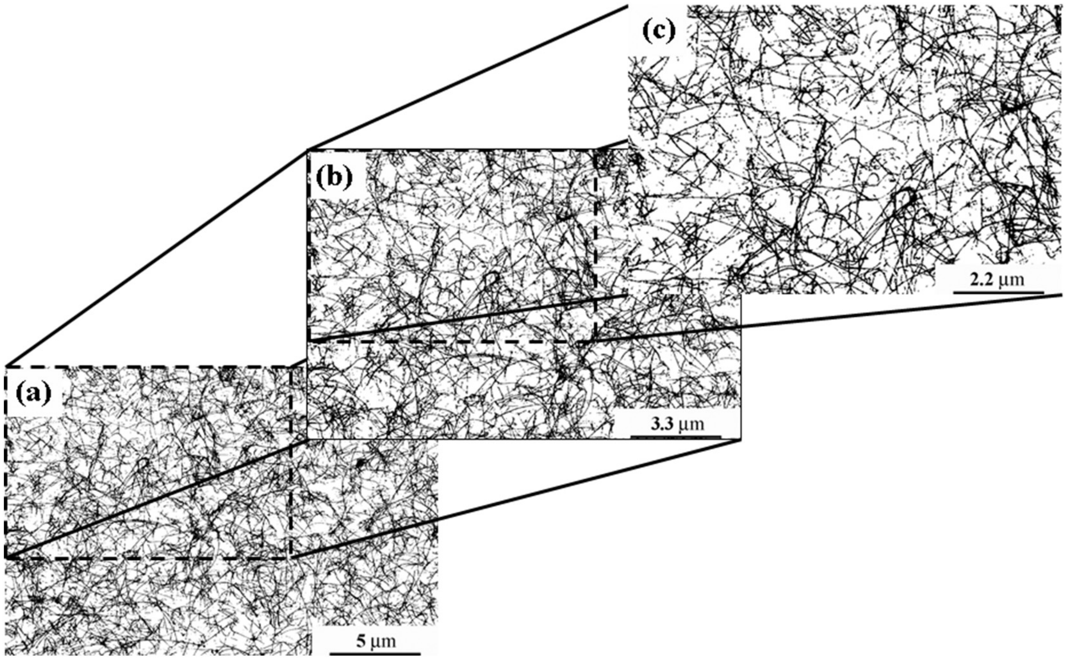

Fig. 1. Self-similar network structures of the messily grown nanowire morphology. The morphology is formed by messily grown Si nanowires synthesized at 1100 °C for 2 h. (a) Binary image of the original morphology; (b) magnified image of the region within the dashed line in (a); (c) magnified image of the region within the dashed line in (b).

potential applications on novel electronic devices like nanoscale transistors and quantum dots [11,12].

Morphologies formed by messily grown nanowires are usually with uniform nanowire network structures. The messily growth, which means nanowires growing towards random changing directions in a relatively high speed, leads to the bending, overlapping of the nanowires and forms net-structures with complex, disordered but uniform geometrical features [4,7,13]. Though the nanowire network structures may not find their applications on precise nanoscale devices, they are great candidates for advanced electrodes, reinforcements of structural composites or functional coatings [4–7,14,15]. For instance, in the designation of nanowire reinforcements for the composites or coatings, the relative fraction and distribution of messily grown nanowires have significant influence on the properties of the synthesized material [7]. To control the distribution and fraction of the reinforced nanowires, it is necessary to understand the microstructural dynamics and develop mathematical methods to predict the evolution of geometrical structures of messily grown nanowires. The structural formation of messily grown nanowires starts with the free growth of single nanowire. At the initial growth stage, massive nanowires growing out of the substrate are short, separated, and with random distributed growth directions. As the growth continues, the bending or intertwined long nanowires with different growth directions then form the complex network structure.

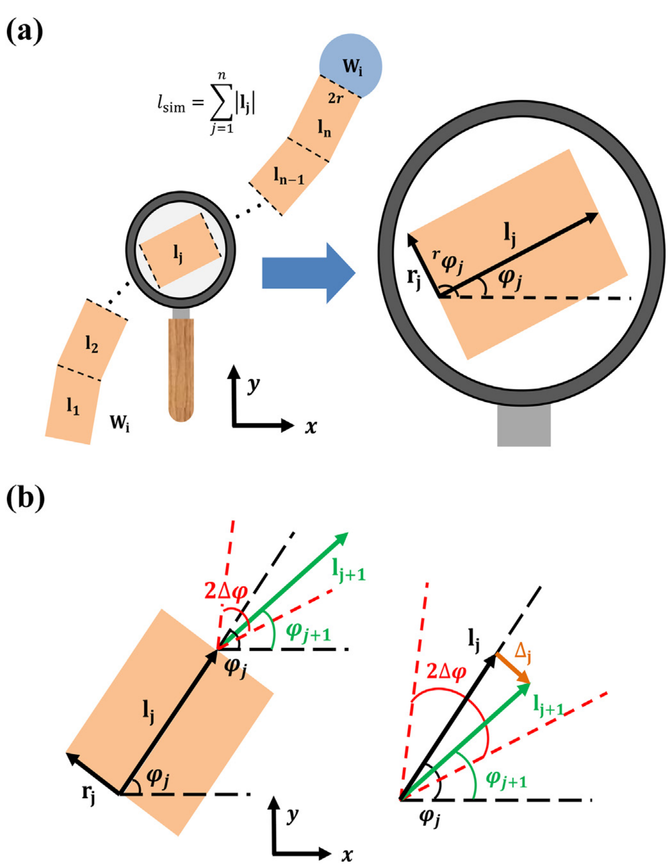

Fig. 2. The structure and growth algorithm of the simulated nanowires. (a) The structure of the simulated nanowire. (b) The growth algorithm of the simulated nanowire.

From the above discussions, we can find that the basis of describing the microstructural dynamics of messily grown nanowires is the modeling of mono nanowire growth. Fortunately, many efforts have been devoted to analytical describing the growth mechanism of mono nanowire. One of the most discussed growth mechanisms is the vapor-liquid-solid (VLS) mechanism, which is the main cause of nanowire grown with the assist of metallic catalyst [16]. In 1970s, E.I. Givargizov firstly established an exponential kinetic model to explain the dependence of nanowire growth rate and radius at steady growth stage [17]. Afterwards, the detail growth models describing the axial and radial growth kinetics of mono nanowire are developed by many researchers [18–23]. However, there are few studies focusing on the modeling of microstructural dynamics of massive and messily grown nanowires, which is important in designation of nanowire reinforcements, functional sensors, or novel electrochemical electrodes.

In this work, the geometrical characteristics and microstructural dynamics of messily grown nanowires were studied by means of Monte Carlo simulations and fractal geometry. Large numbers of simulated messily grown nanowire morphologies which are similar to those