Integrated Nanomanufacturing and Nanoinformatics for Quality Improvement

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Abstract

Unlike traditional manufacturing, nanomanufacturing (NM) involves product characteristics and process variables at multiple feature scales. However, control of the multiscale process/product variations (MPVs) in NM is constrained by the scarcity of measurement data, a lack of observation during processing, and limited physical knowledge. The article argues that NM and nanoinformatics should be integrated together to address the challenge of MPVs for quality and productivity improvement. We review the works in this new field and illustrate examples of integrated NM and nanoinformatics (INN) research. Finally we will discuss the potential major issues to be addressed in INN.

Keywords (3 maximum):
Multiscale process variations, Multiscale process modelling, Multiscale process control

1 INTRODUCTION

Nanomanufacturing (NM) is the utilization of bottom-up directed assembly or top-down high resolution processing to control matter at the nanoscale in one, two, and three dimensions for reproducible, commercial-scale production [1]. As the key enabler to fulfill the promise of nanoscience and nanotechnology, NM has not been able to achieve scaled-up, reliable, and cost-effective manufacturing of nanoscale materials, structures, and devices. The current yield of nanodevices is 10% or less [2]. In March 2010, the Presidential Council of Advisors on Science and Technology in US responded by recommending to double the research investment in NM over the next 5 years [3].

The emerging nanoinformatics research, on the other hand, focuses on collecting, sharing, visualizing, modeling and analyzing information for comparative characterization of nanomaterials, design and use of nanodevices and nanosystems, and instrumentation development and manufacturing processes [4-5].

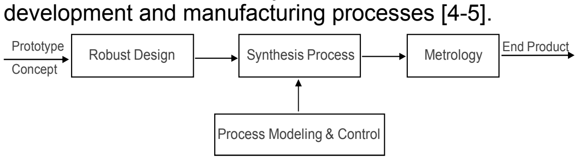

Figure 1: Critical stages in nanomanufacturing.

We argue in this paper that integrated NM and nanoinformatics (INN) is essential to scalable NM. The justification is elaborated as follows.

- High-volume production requires systematic knowledge regarding robust product/process design, synthesis or processing techniques, metrology and inspection, and process modelling and control (Fig. 1). The experience in traditional manufacturing suggests the need of integrating engineering knowledge with advanced statistics in each critical stage (see examples in [6]).
- NM involves product characteristics and process variables at multiple length scales. The process and product variations are therefore across multiple scales as well. This multiscale product/process variation (MPVs) features the multiscale and multiphenomenon challenge in NM. Control of MPVs generally demands more information than variation control at single scale. However, there is a lack of measurement data, observation during processing, and physical knowledge at fine scales.
- The SEM (scanning electron microscope) or TEM (transmission electron microscopy) inspection is extremely time-consuming and costly. Data collection must be guided and optimized for MPV control in order to reduce the inspection cost.
- The current NM research mainly focuses on the processing techniques or synthesis methods of fabricating novel nano materials or devices. NM and nanoinformatics hardly connects with each other to model, control, and reduce the MPVs [7-8].

To summarize, the complexity of MPV control and the lack of information and knowledge demand INN research for quality and productivity improvement in NM. Following the motivation given in Introduction, Section 2 presents an INN framework to integrate available knowledge in NM and points out the major research areas. Section 3 reviews the emerging research related to INN and remaining research issues are discussed therein. Summary and conclusion is given in Section 4.

2 AN FRAMEWORK FOR INTEGRATED NANOMANUFACTURING AND NANOINFORMATICS (INN)

Under the premise that INN is essential for quality and productivity improvement, the subsequent issue is how NM and nanoinformatics are integrated for modelling and control of MPVs. We propose an INN framework illustrated in Fig. 2.

As can be seen, the research in each critical stage is categorized into either NM or nanoinformatics. The key of integration is to establish MPV models that provide realistic description of synthesis processes under manufacturing uncertainties. The foundation of MPV modelling is the process-level understanding of nanomaterial synthesis and characterization (metrology). To address the system-level issues regarding quality and productivity, MPV modelling provides the basis for process monitoring and control, guided inspection and sensing strategy, and more efficient experimental design strategy for robust synthesis of nanomaterials.

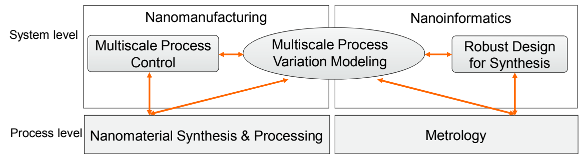

Figure 2: An INN framework

The MPV modelling bridges NM and nanoinformatics and connects with other critical activities in scalable NM. In Section 3 we will review the emerging research related to INN, particularly show examples of MPV modelling. As pointed out in Introduction, the current NM research mainly focuses on the process-level synthesis of nano materials and device, review on that area is omitted because it can be found elsewhere.

3 INN RELATED RESEARCH

3.1 MPV modelling

The objective of MPV modelling is to describe the NM process variations at multiple features scales. Using nanowire (NW) synthesis as an example (Fig. 3), the process variation can be measured by the average NW length over the entire substrate (macroscale) the average NW length of a local region (fine scale). The macroscale NW length measures the substrate-to-substrate variations, while the length at fine scales evaluates spatial variations on the substrate with different degrees of resolution [7].

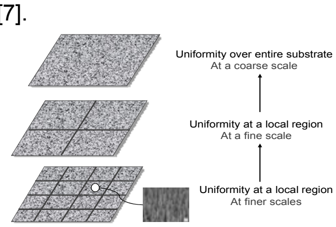

Figure 3: MPVs in nanowire growth.

A more complicate case is that the quality feature varies with scales. For nanocomposite manufacturing (Fig. 4), the process variation at the nanoscale can be measured by the dispersion of nanoparticles in the polymer matrix, while quality features at coarse scales can be material properties.

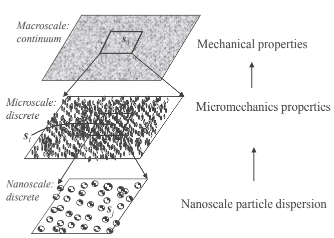

Figure 4: MPVs in nanocomposite manufacturing.

Modeling of MPVs needs (1) to describe process variation with integration of physical knowledge at each scale, and (2) to couple process models between scales.

Integrating physical knowledge into process models should consider the fact that knowledge disparity at different scales, i.e., limited understanding of growth kinetics at the fine scales (greater uncertainties) vs. relatively established work at coarse scales (less uncertainties). Huang (2011)[7] proposed three principles for MPV model development:

- Openness: In light of the rapid advance in nanoscience, the modeling framework should be open enough to integrate the forthcoming knowledge at fine scales without dramatic changes in model structures.
- Separation: The model components with different degrees of uncertainties should be separable so that during model estimation the model structures with less confidence in physics will have no or little impact on those with better physical knowledge.
- Structured simplicity: Due to limited measurement data, it is preferred to have a simple process model (containing less unknown parameters) with a physical structure embedded with growth knowledge.

To describe the NM process variation at each scale, Huang (2011) [7] developed a space-time random field modeling approach. The nanostructure feature such as NW length or nanoparticle dispersion can be generally represented by a space-time random field $\boldsymbol{X}(\boldsymbol{s},t,j)$ at the scale j, where $\boldsymbol{s}$ denotes a collection of regions or sites on a substrate at time t. To integrate the physics into the statistical model, $\boldsymbol{X}(\boldsymbol{s},t,j)$ is decomposed into a global profile component $\boldsymbol{\eta}(\boldsymbol{s},t,j)$, and local component $\boldsymbol{\varphi}(\boldsymbol{s},j)$ [7]

$$\boldsymbol{X}(\boldsymbol{s},t,j) = \boldsymbol{\eta}(\boldsymbol{s},t,j) + \boldsymbol{\varphi}(\boldsymbol{s},j) + \boldsymbol{\varepsilon}(j) \quad (1)$$

The rationale of this decomposition is the knowledge disparity across scales. Because of the relatively good understanding of global behaviors, physical model structures can be embedded into $\boldsymbol{\eta}(\boldsymbol{s},t,j)$. Since limited physical knowledge is available for area-specific variability due to latent and unobserved factors, pure statistical models are more suitable for $\boldsymbol{\varphi}(\boldsymbol{s},j)$ to characterize local variations. Figure 5 summarizes the modeling approach for process variation at each scale.

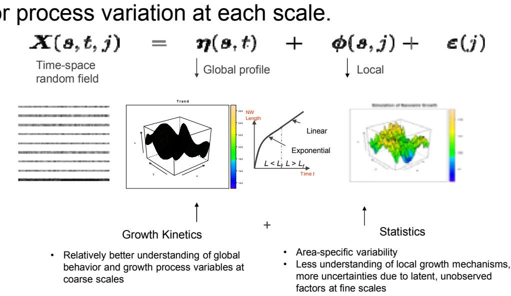

Figure 5: Space-time random field modeling of process variation at each scale.

Once the physical model structures are embedded, a Bayesian hierarchical framework can be used for model estimation [7]. In addition, prior knowledge regarding process physics and process parameters can be integrated through specifying prior distributions of parameters $\boldsymbol{\xi}$ in $\boldsymbol{X}(\boldsymbol{s},t,j)$. Statistical theory and methods are then applicable to the model estimation and inference.

The research on coupling the process variation models across scale is very limited. Since the NM process model in Eq. (1) has a statistical form, one viable approach to integrate model across scale is to use the Bayesian multiscale framework developed in [10]. But little research work has been reported. The main reason is that the development of MPV models is still the major focus at this stage.

In a different example shown in Fig. 4, we developed the nanoparticle dispersion model at fine scales [9]. Figure 6 illustrates the cross-section view of a nanocomposite material at a fine scale [9]. The number of nanoparticles/clusters in a unit area or volume varies from region to region, and it reveals the degree of uniformity of nanoparticle dispersion on the surface observed.

Therefore, we used a nonhomogeneous Poisson random field with site-dependent intensity function to establish the particle dispersion model

$$\log[\lambda(\boldsymbol{s}, \boldsymbol{\beta})] = \mathbf{x}^{T}(\boldsymbol{s})\boldsymbol{\beta} + \Psi(\boldsymbol{s}) \tag{2}$$

where $\mathbf{x}$ are process variables such as pH value, $\boldsymbol{\beta}$ are coefficients to be estimated, and Gaussian random field $\Psi(\boldsymbol{s})$ characterizes the particle-particle interactions. To integrate process physics, Bayesian hierarchical modeling was adopted for model estimation and prediction.

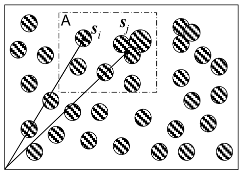

Figure 6: Nonhomogeneous Poisson random field model for particle dispersion [9].

More research efforts are needed for MPV modeling to address (1) formulating and modeling NM process at each length scale; (2) embedding physical knowledge into NM process models; (3) coupling of process models across multiple length scales; and (4) process variation modeling at fine scales.

3.2 Robust design for nanomaterial synthesis

Development of efficient NM processes demands systematic investigation of conditions under which nanostructures are synthesized. Statistical design of experiment is an important tool to identify the robust and optimal synthesis conditions or recipes with minimal number of experimental runs [11].

Study on the growth of one-dimensional CdSe nanostructures through statistical modeling and optimization of the experimental parameters required for synthesizing desired nanostructures was reported in [12]. A 5x9 full factorial experiment was conducted with five levels of temperature and nine levels of pressure. The observed response $\mathbf{Y} = (Y_1, Y_2, Y_3, Y_4)$ represents the numbers of nanosaws, nanowires, nanobelts, and no morphology. By assuming $\mathbf{Y}$ follows a multinominal distribution with probability vector $\mathbf{p} = (p_1, p_2, p_3, p_4)$, the multinominal logits $\eta_j = \log(p_j/p_4)$ was model as

$$\eta_j = \mathbf{x}^{T}\boldsymbol{\beta} \tag{3}$$

where $\mathbf{x}$ represents the collection of process variables.

With the model, a two-step procedure was adopted to maximize the yield and minimize the variability [12].

In [13], a sequence of factorial designed experiments toward growing aspect ratio enhanced ZnO NW arrays was conducted to identify the optimal recipe. In another example [14], a three-level full factorial experimental design on force and speed was carried out with AFM (atomic force microscopy) tip being a third noise factor. The combined effects of these three parameters on the output of nanogenerator and optimal parameter settings were examined using a statistical model.

Since large number of experimental runs is cost-prohibitive in nanomaterial synthesis, the need to reduce the run size is imperative. On the other hand, more data is preferred to study the effects of parameters on synthesis. Therefore, the proposed INN strategy (Fig. 2) is to conduct experiments guided by MPV models. Since the MPV models embed physical model structures, theoretically the model-guided experiments will need less runs to understand the input-output relation. In [15] we demonstrated the experimental strategy of estimating parameters in growth process models.

More research effort is needed in this direction, particularly for robust design to analyze the responses at fine scales.

3.3 Multiscale process control

Since material properties such as uniformity, composition, and micro/nano structures are depedent on the process conditions, real-time process control and optimzation for distributed and multiscale process systems becomes increasingly important in order to meet the stringent requirements on the quality of nanomaterials and reduce process variability. Regulation of spatial process variables (temperature, concentration, etc) has been conducted in advanced materials processing applications.

Physical multiscale modeling has been mainly developed in computational physics, chemistry, and materials [16-18]. Different scale techniques are implemented sequentially in computational domains at different levels of discretization ranging from discrete atoms to continuum elements. Macroscale property (uniformity, composition) control can accomplished on the basis of continuum-type distributed parameter models. Microscale precise control of microstructure requires multiscale distributed models that predict how the microscopic scale property is affected by changes in the controllable process parameters (macroscopic scale) [19-20].

In this line of research, the models at each scale are mainly built upon the first principles. Real-time control faces computational challenge. We believe that the MPV modeling, which embeds physical model structures into a statistical framework to describe process variations, provides a viable alternative base to develop multiscale process control methods. It is an important direction in need of more research.

3.4 Metrology and other nanoinformatics research

In order to reduce the MPVs, quality inspection of nano products is a prerequiste. Features and patterns related to design specification should be obtained quickly and automatically in order to achieve effective quality control.

Current metrology practice relied on characterization techniques such as microscopies. It is a tedious, time-consuming, and costly process for large-scale manufacturing. In addition, images from microscopies cannot be directly used for quality control. First, morphology features such as dimension and density require automatic image processing. Second, normally a few sites on a substrate are sampled, the images do not necessarily represent the condition of a whole substrate.

Therefore, the nanoinformatics research in metrology needs to address issues from two aspects (1) automatic feature extraction through image analysis, and (2) optimial sensing strategy to reduce the characterization cost.

The work in [21] provided a statistics-guided approach to characterize the lengths, diameters, orientations, and densities of ZO nanowires. This approach has three key components. First, a geometric model was proposed to recover the true lengths and orientations of nanowires from their projective scanning electron microscope images, where a statistical resampling method is used to mitigate the practical difficulty of relocating the same sets of nanowires at multiple projecting angles. Second, a sequential uniform sampling method for efficiently acquiring representative samples in characterizing diameters and growing density. Third, a statistical imputation method was developed to incorporate the uncertainty in the determination of nanowire diameters arising from nonspherical cross-section spinning.

The work in [22] aims to study the morphology of nanoparticales that are overlapping with one another and overcrowded.

For effective control of MPVs in nanomanufacturing, MPV models should guide metrology studies. No research has been reported in this direction.

4 SUMMARY AND CONCLUSION

The scale up nanotechnology advances, NM should reduce process variations at multiscale scales at all critical stages (robust design, synthesis, process control, and metrology). INN research is a must to control MPVs under process uncertainites.

We proposed a framework for INN research and provided examples of INN research in MPV modeling and robust design. We reviewed the related works in this new field and discussed the potential major issues to be addressed in INN. We believe that INN is an emerging field worthy of great research efforts in order to improve quality and productivity in NM.

5 ACKNOWLEDGMENTS

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