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Perspectives on the design and control of multiscale systems

R.D. Braatz *, R.C. Alkire, E. Seebauer, E. Rusli, R. Gunawan, T.O. Drews, X. Li, Y. He

Department of Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign, 600 South Mathews Avenue, Urbana, IL 61801, United States

Abstract

New applications in materials, medicine, and computers are being discovered where the control of events at the molecular and nanoscopic scales is critical to product quality, although the primary manipulation of these events during processing occurs at macroscopic length scales. This motivates the creation of tools for the design and control of multiscale systems that have length scales ranging from the atomistic to the macroscopic. This paper describes a systematic approach that consists of stochastic parameter sensitivity analysis, Bayesian parameter estimation applied to ab initio calculations and experimental data, model-based experimental design, hypothesis mechanism selection, and multistep optimization.

Keywords: Nonlinear systems; Distributed parameter systems; Complex systems; Stochastic systems; Uncertain dynamic systems; Optimal control; System sensitivity

1. Introduction

New applications in materials, medicine, and computers are being discovered where the control of events at the molecular and nanoscopic length scales is critical to product quality, although the primary manipulation of these events during processing occurs at macroscopic length scales (e.g. temperature of the system, valves on flows into and out of the system, applied potential between two electrodes). These applications include nanobiological devices, micromachines, nanoelectronic devices, and protein microarrays and chips [30,53,72,95,100,113,120]. While many of these devices are designed using highly simplified models or trial-and-error experimentation, recent advances in computer speed and memory, numerical algorithms, and sensor technologies suggest that a more systematic approach to the design and control of these multiscale systems is possible.

The potential applications motivate the creation of tools for the design and control of multiscale systems that have length scales ranging from the macroscopic to the atomistic. This paper describes the challenges to building such multiscale systems tools, which include uncertainties in the physicochemical mechanisms as well as the values of thermodynamic and kinetic parameters, complexities in the simulation of model equations that can span a wide range of time and length scales, lack of manipulated variables and direct measurements of most properties at the nanoscale during processing, and the inapplicability of most existing systems tools to address systems described by noncontinuum and dynamically coupled continuum–noncontinuum models. These challenges specify the requirements for multiscale systems tools.

This paper describes how these requirements can be satisfied by a systematic approach to the design and control of multiscale systems that consists of stochastic parameter sensitivity analysis, Bayesian parameter estimation applied to ab initio calculations and experimental data, model-based experimental design, hypothesis

* Corresponding author. Tel.: +1 217 333 5073; fax: +1 217 333 5052.
E-mail address: braatz@uiuc.edu (R.D. Braatz).

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mechanism selection, and multistep optimization. This enables multiscale systems to be designed and controlled based on the numerical algorithms that are most appropriate for simulating each of the length scales of the process.

2. Challenges and requirements

The challenges associated with the design and control of multiscale systems specify the requirements for multiscale systems tools. To make the description of the challenges as concrete as possible, the manufacture of on-chip copper interconnections in electronic devices is used as an illustrative example. In this process, an applied potential is used to electrodeposit copper on surfaces and in trenches and vias. The product quality of the deposit is a function of nucleation at the atomic scale, surface morphology at the nanoscale, shape evolution at the nano- to micro-length scales, and deposit uniformity over the wafer surface. This electrodeposition process involves phenomena that are simultaneously important over ten orders of magnitude in time and length scales [2–4]. According to the International Technology Roadmap for semiconductors [113], the manufacture of next-generation interconnects will require design and control of all of these length scales.

Fig. 1 is a schematic of the electrodeposition of copper into a trench, in which Cu^{2+} ions in solution diffuse and migrate to the surface in response to a potential applied between the reference and working electrodes. Although the introduction of organic chemical additive cocktails to the solution to produce void-free copper deposits in sub-100 nm trenches is well established [5,6], the precise physicochemical mechanisms of the interactions of these additives with the copper surface are not well understood [21,69,89–91,117,118,122], making it difficult to design new additive cocktails able to produce void-free deposits in smaller features. A challenge in applying systems principles to these and other multiscale systems is that the underlying mechanisms, as well as the thermodynamic and kinetic parameters associated with the steps in these mechanisms, are uncertain. *Multiscale systems tools are needed that can handle uncertain mechanisms, as well as uncertain parameters.*

Another challenge to engineering multiscale systems is that the codes used to simulate these systems are computationally expensive. For example, consider Fig. 2, which is a schematic of a multiscale simulation model for the electrodeposition of copper into trenches. Chemical reactions and the diffusion and migration of species in the solution boundary layer are described by a system of partial differential–algebraic equations, which are typically simulated using the finite volume or finite element method. The height of the boundary layer is typically ~50 μm and a typical time step for such a code is ~1 ms. The nucleation, surface chemistry, and roughness evolution of the trench surface are more accurately simulated using noncontinuum methods such as kinetic Monte-Carlo (KMC) simulation [12,27,52,73,103,124]. KMC methods are used to simulate structural properties of matter that cannot be represented by a macroscopic continuum description. A KMC simulation is a realization of the master equation [33]:

$$\frac{\partial P(\sigma,t)}{\partial t} = \sum_{\sigma'} W(\sigma',\sigma)P(\sigma',t) - \sum_{\sigma'} W(\sigma,\sigma')P(\sigma,t) \quad (1)$$

where σ and σ' are successive states of the system, $P(\sigma,t)$ is the probability that the system is in state σ at time t, and $W(\sigma',\sigma)$ is the probability per unit time that the system will undergo a transition from state σ' to σ. For a particular system being studied, the KMC code chooses randomly among the possible transitions of the system and accepts particular transitions with appropriate probabilities defined by the kinetic rate laws for each

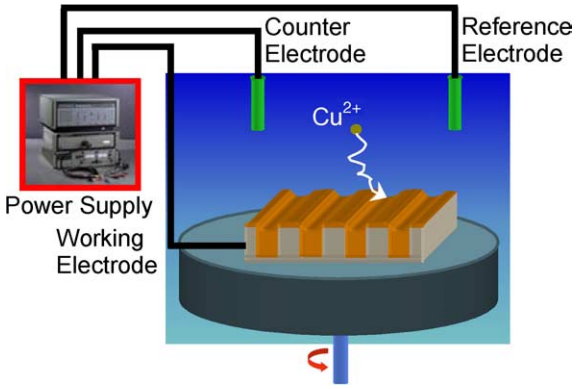

Fig. 1. Electrochemical process for manufacturing on-chip copper interconnects, in which a rotating disk creates a boundary layer above the wafer surface (not drawn to scale).

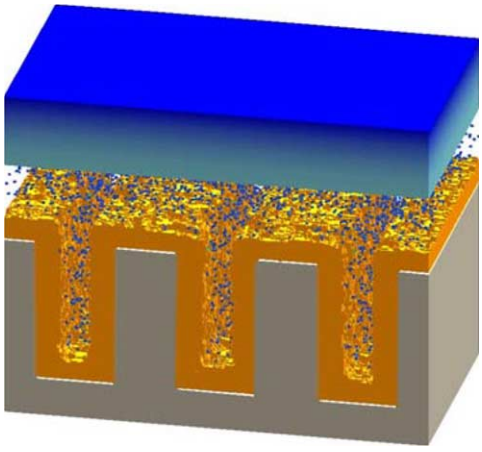

Fig. 2. Multiscale simulation of the electrochemical process for manufacturing on-chip copper interconnects (not drawn to scale). The dots represent Cu^{2+} ions in solution, with the film on the surface being metallic copper.

allowed event in the simulation [27]. After each accepted or attempted transition, the time variable is incremented by one Monte-Carlo time step (typically the time step is ~1 ns), and the process is repeated. By selecting the probabilities to satisfy certain conditions, the real time variable t corresponding to the number of Monte-Carlo time steps can be computed.

The bottom part of Fig. 2 shows the infill of several trenches simulated using a three-dimensional (3D) KMC code, that tracks adsorption, desorption, bulk and surface diffusion, and chemical reactions [28,29]. To reduce the computational load, the 3D KMC code was coarse-grained [41,55,56,60,78,114], such that clusters of molecules were tracked instead of individual molecules [25,66,67,98,99], and periodic boundary conditions were used at all sides (but not the top or bottom) of the simulation domain. Even with these simplifications, it takes ~1 day to perform one simulation run. This greatly limits the number of simulation runs that a systems tool is allowed to make in a coupled simulation–optimization algorithm such as used in control vector parameterization [105]. Further, systems techniques that write the simulation code as an algebraic system of equations to be embedded into a structured nonlinear program [59], are not computationally feasible for multiscale systems, as there would be $>10^{16}$ algebraic equations in the structured nonlinear program. *Multiscale systems tools must be much more computationally efficient than most existing systems tools.* Note that the state dimension of KMC codes is very high, while the numbers of simulation inputs (e.g., applied potential) and outputs (e.g., surface roughness, fraction of voids) are much lower. *This motivates the creation of multiscale systems tools that act directly on simulation inputs and outputs*, to keep the computational cost low.

As a further complication, the codes in Fig. 2 must be dynamically coupled when dilute additives are included in the simulation, as the surface chemistry and transport determines the amount of depletion of additives in the boundary layer, and the boundary layer influences the rate that chemical species reach the surface. *Multiscale systems tools are needed that can handle models described by dynamically coupled continuum and noncontinuum codes.*

Another characteristic of noncontinuum codes is that their outputs typically have significant stochastic fluctuations, which can be nonGaussian. For example, Fig. 3 is the current density response from a dynamically coupled KMC-finite difference simulation of copper electrodeposition in response to a staircase function of the applied potential [109]. The current density only takes on discrete values, which are associated with electron transfer at the copper surface (e.g., as a Cu^{2+} ion gains two electrons to form copper metal). The values of the current density are computed by dividing the sum of the amount of charge passed within a given time interval

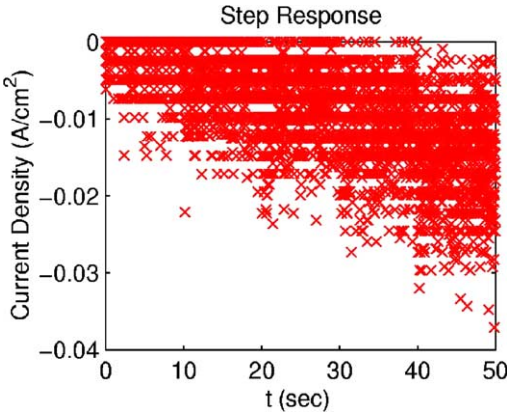

Fig. 3. Current density response to a staircase function of applied potential for the dynamically coupled simulation of the electrochemical process for manufacturing on-chip copper interconnects (each step of the staircase was 10 s long).

by the length of the time interval, which is highly noisy as this calculation essentially involved taking the derivative of a noisy signal (charge passed with a short time interval). This response is in sharp contrast to the typical step and staircase responses reported in the controls literature [74,105]. Although most existing systems tools are applicable to stochastic models with Gaussian fluctuations, these tools always assume that the deterministic part of the model is known. *Multiscale systems tools must be able to address models with large amounts of nonGaussian noise, for which a deterministic model is unavailable.*

Another challenge in multiscale systems is the lack of key measurements during processing at industrially relevant operating conditions. While there are some on-line measurements available, most of these measurements are only available *after* processing is completed. For example, the only on-line measured variables for the copper electrodeposition process are temperature and current. There are no on-line concentration measurements at the surface, where the uncertain chemical mechanisms and most of the uncertain parameters are located. The key measurement data, which are atomic force microscopy images, are only available at the end of the process (see Fig. 4). *Multiscale systems tools must include experimental design methods that maximize the*

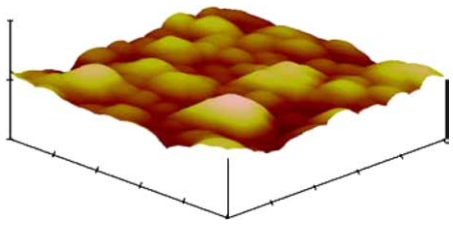

Fig. 4. Atomic force microscopy image of an electrodeposited copper surface.

information from the available sensors, to create models that are predictive.

Another characteristic of multiscale systems is a lack of manipulated variables at the molecular and nanoscopic length scales during processing. For example, the only variable manipulated during the electrodeposition process in Fig. 1 is the applied potential, which does not provide enough degrees of freedom to produce void-free copper in the 0.13 μm trenches used in modern microelectronic devices. This is why industrial practice is to introduce additional degrees of freedom in the initial conditions, which is done through the selection and concentrations of organic chemicals added to the solution. In general, *most multiscale systems require that molecular and nanoscale manipulation be treated as a design focus, to exploit self-assembly during processing*.

3. Complex systems tools

Before looking at multiscale systems tools, it is useful to review some systems tools developed for complex continuum models that address most, but not all, of the challenges of multiscale systems (see Fig. 5). Before carrying out model identification for a complex system, an identifiability analysis should be carried out to determine whether the available measurements are sufficient to enable the estimation of model parameters and competing hypothesized mechanisms (see [57], and references cited therein). The next step is the identification of the model, which is an iterative procedure. The first experiment is designed using engineering judgment on how to excite the dynamics of the system, or is computed using initial estimates of the model parameters and some experimental design objective such as minimizing the uncertainties in the parameters [8,11,13]. Improved estimates of the parameters and an associated uncertainty description are computed from the dynamic data collected from the experiment. This can be augmented with ab initio computational chemistry calculations (such as density functional theory) using Bayesian parameter estimation techniques [48]. While DFT calculations have a high computational cost and limited accuracy for complex chemical systems, they have been very useful for computing prior parameter estimates that are improved by applying Bayesian parameter estimation to experimental data.

When several hypothesized physicochemical mechanisms are available, model discrimination techniques are used to select which mechanism is most consistent with the experimental data techniques (e.g., [15,50,106]). The model parameters and uncertainty description are used to design the next laboratory experiment, which can be constructed to further reduce the model uncertainties or to maximize the ability to distinguish among the multiple hypothesized mechanisms [8]. Parameter estimates obtained from this iterative procedure can be many orders-of-magnitude more accurate than estimates obtained from data collected from trial-and-error experimentation. Once the model parameters

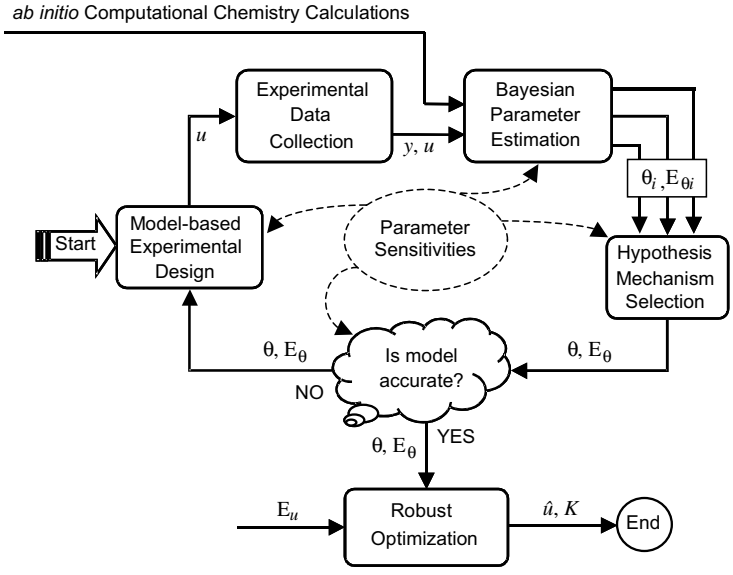

Fig. 5. Iterative process of model identification and robust optimization of complex systems: u represents all experimental design variables (e.g., initial conditions, processing conditions, actuator and sensor locations), y represents the measurements, θ_i is the vector of model parameter estimates and $E_{\theta i}$ is the confidence region for the ith hypothesized mechanism, θ is the vector of parameter estimates and E_θ is the confidence region for the most likely mechanism, $\hat{u}$ is the optimal control policy (including initial conditions, equipment specifications, operating conditions, actuator and sensor locations, etc.), K is the optimal controller, and E_u is the uncertainty in the implementation of the optimal control policy, including the effects of disturbances.

are accurate enough, the simulation model is incorporated into an optimization algorithm to compute the physical design variables, initial conditions, startup procedures, setpoint trajectories, and the feedback control system.

These complex systems tools are well established for continuum models described by general integro-partial differential algebraic equations (IPDAEs), and have been applied to the manufacture of photographic chemicals [88], pharmaceuticals [14,34], and semiconductors [49]. These applications include a wide range of real physical systems at Merck, Eastman Kodak, and Sematech (an international consortium of semiconductor companies), indicating the wide applicability of these tools. The key to the generality of these complex systems tools is that they act directly on the inputs and outputs of simulation codes, rather than requiring a particular form for the equations or the numerical algorithm used to simulate the equations. Also key to providing generality is that the numerical algorithms implemented in the steps in Fig. 5 incorporate parameter sensitivity methods based on finite differences (e.g., [13,18,65]) or automatic differentiation [16,17,32,35,75] and can handle correlations between parameter estimates [77]. The parameter sensitivities improve the numerical conditioning of the systems tools while focusing the modeling effort towards only the key parameters whose values must be known with high certainty to produce predictive models. This is critical when the number of parameters is large, as is typical for semiconductor processes ([48,86]).

In recent years fast techniques have been developed to quantify the effects of model uncertainties on all states and outputs for the batch and semibatch processes used to manufacture the most complex systems [9,31,83,87], and to integrate robustness into all design variables. Some of these techniques have little restrictions on the zero dynamics, the integro-differential structure of the equations, the simulation algorithms, or the form of the nonlinearities or uncertainties [81,93,94,96,97,119]. The uncertainties can be defined by joint probability distributions or upper and lower bounds on parameter estimates, with most robustness analysis methods applying either semi-analytical techniques or Monte-Carlo simulation to carefully constructed low-order approximations for the simulation models. These analysis algorithms have been used to determine how much accuracy is needed to achieve an effective design or control strategy [82], and have been incorporated into optimization algorithms to produce designs and controllers that are robust to the uncertainties [92,94].

To illustrate the complexity of systems that can be addressed by these systems tools, consider their application to the manufacture of ultrashallow junctions. The current technology for the formation of ultrashallow junctions in microelectronic logic devices relies almost exclusively on ion implantation to introduce dopants into the substrate (see Fig. 6). Although junctions can be made shallower by reducing the implant energy, the effectiveness of this approach has been limited by the need to anneal the resulting structure to over 1000 °C both to activate the dopant electrically and to eliminate implant-induced defects in the crystal structure (see Fig. 7 for an example temperature trajectory). Defects mediate unwanted diffusion of dopants during the anneal process, which leads to a significant undesired increase in the junction depth. The aforementioned systems tools have been applied to the post-implant annealing process, to construct a simulation model and to minimize the junction deepening while maximizing dopant activation.

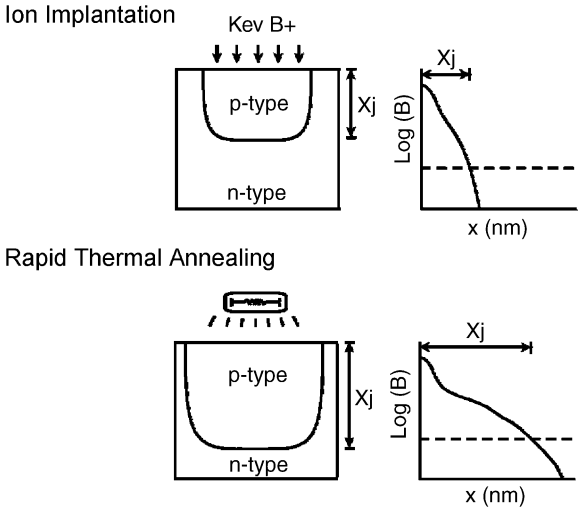

Fig. 6. Schematic diagram of the junction increase that takes place during rapid thermal annealing after ion implantation of dopant.

The simulation model includes the coupled mass balance equations for interstitial atoms, interstitial clusters, and related defects. These equations have the general form for species i :

$$\frac{\partial N_i}{\partial t} = -\frac{\partial J_i}{\partial x} + G_i \tag{2}$$

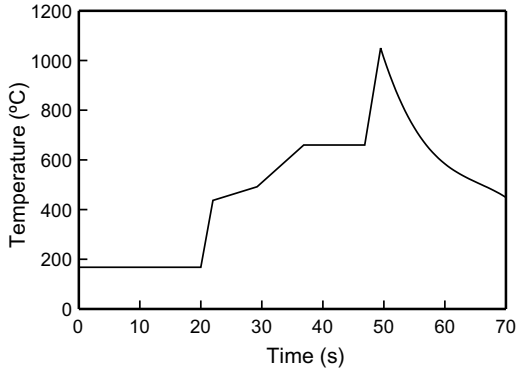

Fig. 7. A typical rapid thermal anneal temperature program, which consists of a stabilization step and a spike-anneal (i.e., a fast linear heating step followed by a natural cool down step).

where N_i denotes concentration and G_i is the net generation rate. The flux J_i incorporates terms due to diffusion and drift in response to electric fields. The model also includes Poisson's equation describing the electric field generated by spatial imbalance of the charge density. The simulation model consisted of ~25 partial differential equations which were nonuniformly spatially discretized using between 200 and 800 points in the depth direction, resulting in up to 20,000 extremely stiff ordinary differential equations that were solved using the public domain software FLOOPS [71], which integrates the equations using a combination of the one-step trapezoidal rule and the multiscape backward differentiation formula [10].

The activation energies in the expressions for G_i and J_i were obtained by Bayesian parameter estimation, which incorporated information from density functional theory (DFT) calculations, past experimental studies, and boron secondary ion mass spectroscopy data from the International Sematech consortium of semiconductor companies [48]. A combination of parameter sensitivity analysis and kinetic insights was used to select the physical mechanism [47,46], in which the most important part was the specification of the network of chemical reactions for the clusters. Parameter sensitivity analysis was a necessity in the construction of the physical mechanism, as the number of kinetic parameters was large, including 18 activation energies associated with the interstitial diffusion, cluster association, and cluster dissociation reactions.

The complex systems tools in Fig. 5 permitted the construction of a clear picture of the fundamental kinetic processes that govern diffusion and electrical activation of dopant [61,62,64]. The agreement between the simulated and experimental boron dopant profiles was within 2 nm for the entire junction (see Fig. 8). To provide further validation of the simulation model, the junction depth and sheet resistance (this is a measure of dopant activation) were computed for a wide range of temperature profiles, and compared to a large number of experimental values reported in the literature and to the "Sematech curve," which summarizes additional experimental values (see Fig. 9). The predictions of the simulation model are highly consistent with reported experimental values.

The simulation model was incorporated into an optimal control problem to compute an annealing temperature trajectory that minimized the junction depth while maintaining a desirable level of boron activation [49]. Robustness analysis as shown in Fig. 5 was applied to rigorously quantify the performance degradation from uncertainties in the feedback control implementation and the model parameters. The analysis indicated that limited improvement in product quality is achievable using existing metrology and rapid thermal processing controllers.

As discussed in Section 2, the limited actuation available at macroscopic length scales motivates the application of *molecular design*, and it was argued that the potential impact of such design optimization can be much greater than the potential benefit of improved feedback control. As it is highly advantageous in terms of electronic device properties to restrict the chemistry to dopant and silicon molecules, we have been keeping the atomic species unchanged, but using the simulation model to change the bond structure at the silicon surface [63]. We have shown that the effects of the structure of bonds at the silicon surface have a substantial effect on the junction depth due to a change in the effective surface boundary condition for interstitials. These simulation studies have motivated discrete changes in processing conditions, which are being evaluated experimentally [22] and form the basis of a patent disclosure [112].

These complex systems tools address most of the requirements for application to multiscale systems, in that nonGaussian stochastic behavior and uncertain mechanisms and parameters are taken into account; the tools are computationally efficient, general purpose,

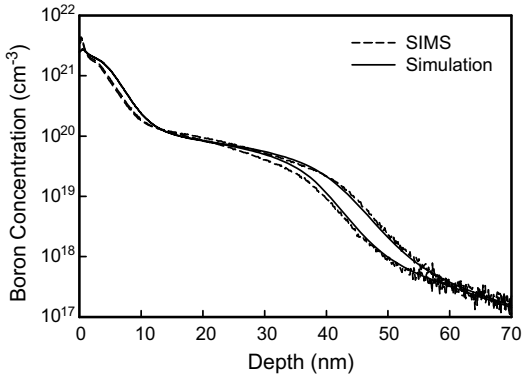

Fig. 8. Experimental and simulated boron dopant profiles, for two batch operating recipes [48].

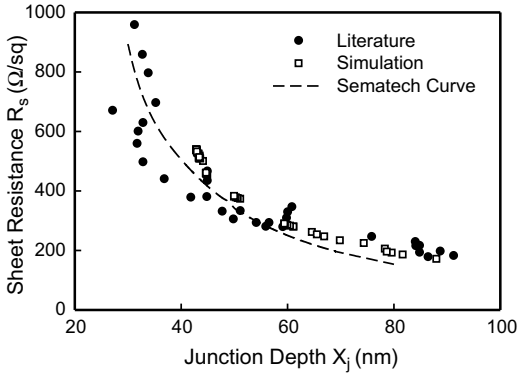

Fig. 9. Comparison of junction depth-sheet resistance pairs from various published experimental papers and TED simulations employing various heating and cooling rates, and annealing temperatures. The Sematech curve summarizes the sheet resistance and junction depth data in experimental studies performed by International Sematech [48].

and act directly on simulation inputs and outputs; experimental design methods are included that maximize the information from sensors to create predictive models; and that design and control are optimized simultaneously, which enables molecular and nanoscale manipulation in the design problem to be considered jointly with the manipulation of the on-line variables by feedback controllers during processing. The complex systems tools, however, do not consider all of the issues particular to models described by noncontinuum and coupled continuum and noncontinuum simulation codes, namely, the lack of an underlying deterministic model for the noncontinuum simulation codes, and the additional numerical stability issues that can arise when codes are linked. The next section discusses efforts to extend these complex systems tools to address these two additional requirements of multiscale systems.

4. Noncontinuum and coupled continuum/noncontinuum codes

For the noncontinuum models that describe complex systems, the optimizations that occur in the model-based experimental design, Bayesian parameter estimation, hypothesis mechanism selection, and optimal design and control steps in Fig. 5 are stochastic with no closed form expression for the underlying deterministic system. For KMC codes, it has been proposed to construct reduced-order models by truncating unlikely configurations and grouping probabilities that evolve together [37–39], using smaller lattices [79,80], approximating fast reactions either deterministically or as Langevin equations [51], or applying least-squares model identification methods [36,40]. Similar reduced-order models have been defined for dynamically coupled continuum/noncontinuum codes [102,109]. Although such approaches are acceptable for controller design, one of the main points in Section 2 is that molecular and nanoscale manipulation should be treated as a *design* problem, to exploit self-assembly during processing—*not* primarily as feedback controller design. For design purposes, the reduced-order models must be a function of the physicochemical parameters in the simulation codes to be manipulated in the design optimization, which can be changed through modifying the chemistry of the system, rather than as a function of macroscopic manipulated variables such as temperature. Developing reduced-order models that are globally applicable and a function of both the physicochemical parameters and the macroscopic manipulated variables is a challenging problem, considering the high computational cost of the simulation codes.

Another consideration is that simulation codes which include molecular-scale phenomena are stochastic, which implies that averaging techniques [109] or stochastic optimization algorithms such as simulated annealing are appropriate [1]. We have shown that even the finite difference calculation of parameter sensitivities typically used in systems engineering algorithms must be formulated as a stochastic optimization, to obtain estimates of the highest accuracy [24]. More specifically, the finite difference expressions for sensitivities reported in textbooks and papers are derived assuming that the underlying system can be described as a deterministic Taylor series expansion, whereas this assumption is invalid for simulations that include noncontinuum models, whose outputs are stochastic. A much more accurate and appropriate formulation is to include a stochastic term in the series expansion, and determine the finite difference expression by solving an optimization problem whose objective is to compute either the minimum variance or maximum likelihood estimate of the parameter sensitivity. As in continuum models, these parameter sensitivities are a key step needed to reduce the complexity and improve the numerical conditioning of the stochastic optimizations that define the systems tasks in Fig. 5.

Recently we incorporated our stochastic parameter sensitivity algorithm into a multistep optimization algorithm [101] that uses sensitivity analysis to determine the key parameters, followed by solution mapping to parameterize the responses of the simulation model as low-degree polynomials of the key parameters, and simulated annealing to optimize the key parameters. The low-order parameterization is used to reduce the number of runs of the computationally expensive stochastic simulation code required to converge to the parameter estimates. This revised algorithm (see Fig. 10) has been used to estimate kinetic parameters associated with copper electrodeposition from measurements of the applied potential and the surface using atomic force microscopy images (see Fig. 4), where the simulation model consisted of a coarse-grained KMC code dynamically coupled to a finite difference continuum code [26].

This application coarse-grained the KMC code to further reduce the computational expense; other acceleration methods such as the tau-leaping [44,45,104] and gap-tooth methods [41] could be applied, in isolation or in addition to coarse-graining.

Another important consideration is that the coupling of simulation codes can induce an additional systems issue—linkage instabilities. While numerically stable codes are available for simulating each length scale, numerical instabilities can be induced in the coupling of such codes by temporal and spatial mismatches at the interfaces between the codes. For the coupling of continuum codes, one approach to numerically stabilize the coupling codes is by passing *both* boundary conditions and *associated sensitivity information* between the codes [19]. The approach cannot be applied to dynamic couplings that include noncontinuum codes; however,

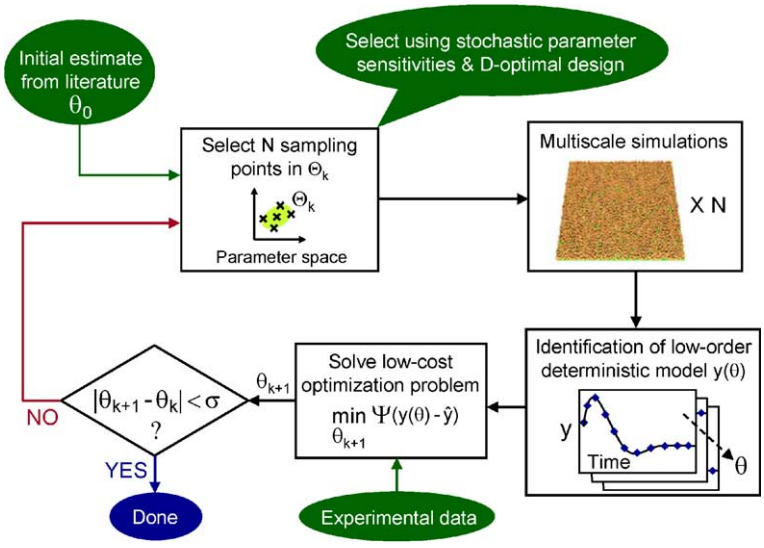

Fig. 10. A simplified schematic of the multistep optimization algorithm for parameter estimation in stochastic simulation codes. Kinetics from ab initio calculations such as DFT are included using a Bayesian formulation [48].

since the associated sensitivities cannot be computed to high enough accuracy for such codes. We have used control systems theory to design numerical linkage algorithms that modify the dynamic information passed between the simulation codes to numerically stabilize their coupling, and to increase the numerical accuracy of the simulation results [29,110,111]. In this approach, the simulation codes are represented by deterministic or stochastic discrete-time nonlinear operators, with mismatches at the interfaces between simulation codes modeled as norm-bounded perturbations, as is commonly done in robust control theory (see Fig. 11). Dynamic coupling algorithms are exactly modeled as additional operators inserted into the block diagram, which are designed by optimal control theory [110, 111]. A constructive procedure for testing whether an arbitrary interconnection of simulation codes is well-posed is provided by nonlinear systems theory [110, 111], which also provides general conditions regarding

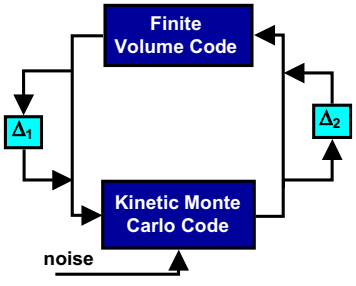

Fig. 11. Time- and length-scale mismatches at interfaces between simulation codes can be modeled as perturbations Δ_i on the information passed between simulation codes. The effects of these mismatches and uncertainties in kinetic parameters in the individual simulation codes on the simulation outputs can be analyzed using nonlinear systems theory and uncertainty-based simulation techniques.

the numerical stability and accuracy of dynamically coupled simulation codes. The dynamic coupling algorithms designed by this control theoretic approach have been analyzed using the classical methods of numerical analysis (e.g., such as described in the textbook by [7]) and compared to previous algorithms such as direct coupling [29,107]. Nonlinear control theory and numerical analysis are complementary approaches for drawing clear and direct comparisons between the various dynamic coupling algorithms described in the literature (e.g., see [23,58,86,95,102,121]; and references cited therein).

More recently we have been using nonlinear systems theory to guide the design of much more complex dynamic coupling of simulation codes than shown in Fig. 11. An improved multiscale simulation model for the electrochemical process used to manufacture copper interconnects (shown in Figs. 1 and 2) is shown in Fig. 12. The multiscale simulation model couples multiple instances of a solid-on-solid KMC simulation code [27] to an internally coupled moving boundary (MB) finite-volume/level set continuum simulation code [20,76,123] to simulate the filling of on-chip features (trenches) by electrodeposition in the presence of additives. The KMC and MB simulations dynamically pass interface conditions during the simulations. The MB code sends surface concentrations and the solution potential to each KMC code, which computes reaction rates from the simulation of the chemistry and physics that occur at the electrode surface. The KMC codes send species fluxes to the MB code which are used as surface boundary conditions. The MB code advances the copper-solution interface using the level-set method, and simulates the chemistry and physics in the electrolyte in and above the trench using the finite volume method.

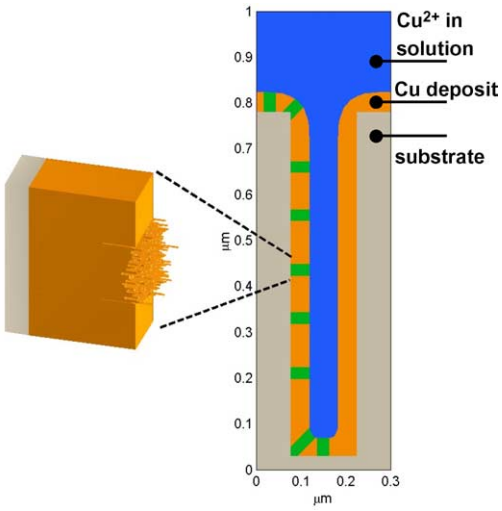

Fig. 12. A coupled simulation with "master-worker" computational paradigm. The stripes in the copper deposit denote the location of KMC simulations. The zoom-in picture of the copper deposit shows the distinction of the actual surface morphology and the surface seen by the MB code in the simulation.

It is useful to relate the multiscale systems approach described in this paper to coarse microscopic time-stepper-based methods for constructing bifurcation maps [70,115,116]. These methods satisfy one of the key requirements for multiscale systems tools described in Section 2, in that they act directly on the inputs and outputs of simulation codes. Although originally developed for continuum codes, these methods can be applied to noncontinuum codes [43,42,54,68,84,85,115]. It is straightforward to show that these methods apply to dynamically coupled continuum/noncontinuum codes as well. The main assumption underlying these time-stepper methods is the requirement of a clear separation of time scales [43,108], which holds for some but not all physical systems (note that the aforementioned methods in Sections 3 and 4 do not require a clear separation in time scales). For systems in which this assumption holds, these time-stepper methods enable the analysis of the nonlinear dynamical behavior of multiscale systems, which can be used for an initial assessment of whether the qualitative dynamic behavior of a hypothesized mechanism is consistent with experimental observations. Hypothesized mechanisms with qualitative dynamics that are consistent with experiments are removed from further consideration in the mechanism selection step in Fig. 5.

5. Conclusions

This paper describes the characteristics of multiscale systems, using the manufacture of on-chip copper interconnections as a specific example to illustrate the key points. These characteristics specify the requirements for multiscale systems tools. One of the key points was that limitations in manipulations available during processing for most multiscale systems imply that *a much larger impact on product quality can be achieved from molecular design* rather than on designing better feedback controllers. Systems tools applicable to complex continuum models were summarized that satisfy the requirements for multiscale systems, except for issues specific to dealing with noncontinuum and coupled noncontinuum–continuum codes. This was illustrated in an application to the manufacture of ultrashallow junctions. An extension of the complex systems tools to deal with the requirements of multiscale systems was described, that incorporates stochastic sensitivity analysis within a multistep optimization algorithm.

Although the systems principles are the same for multiscale systems as for macroscopic systems, the problem formulations and the numerical algorithms designed to solve these formulations are different. Further, a new issue arises in multiscale systems, which is how to address numerical instabilities that can arise during the linkage of individual simulation codes. Some results in applying nonlinear control theory to design numerical linkage algorithms were described. More theory is needed to provide a systematic methodology for the numerical stabilization of multiscale simulation codes, and on algorithms for Bayesian parameter estimation, model-based experimental design, hypothesis mechanism selection, and robust optimization.

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