

Preface

Nearly three decades ago, it was uncovered that silicon can be an excellent mechanical material. The excellent electronic properties of silicon combined with the excellent mechanical properties led to revolutionary advances in the development of microelectromechanical technology. Microelectromechanical systems (MEMS) are miniaturized sensors, actuators, devices and systems with a critical dimension of the order of micrometers. Even though many initial concepts for MEMS were based on silicon, a variety of other materials and fabrication techniques have been developed over the last two decades for applications in mechanical, electrical, chemical, biological and other disciplines. MEMS devices such as accelerometers, gyroscopes, high performance mirror displays, pressure sensors, micro motors, micro engines, RF switches, valves, pumps, ultra sensitive membranes, single-chip microfluidic systems such as chemical analyzers or synthesizers, single-chip micro total analysis systems (also referred to as lab-on-a-chip) and many more devices and systems have been designed and fabricated over the last one to two decades. MEMS technology has already impacted many industries (*e.g.*, defense, aerospace, health care, etc.) even though a number of fundamental and practical challenges still remain. On the other hand, advances in nanotechnology as well as in nanomachining techniques over the last decade have enabled development of novel nanoelectromechanical systems (NEMS). Nanoelectromechanical systems (NEMS) are nanometer scale sensors, actuators, devices and systems with critical feature sizes ranging from 100 nanometers to a few nanometers. The effective masses, heat capacities and power consumption of NEMS are proportional to the critical feature size, either linearly or nonlinearly, while the fundamental frequencies, mass/force sensitivities, mechanical quality factors are inversely proportional to the critical feature size.

A number of experimental and fabrication approaches, and computational design tools have been developed over the last decade to accelerate progress in the area of MEMS. In the area of NEMS, fundamental aspects are slowly being understood and experimental measurement techniques and computational design tools are starting to emerge. While many NEMS devices can be modeled using MEMS

physical theories or MEMS computational tools, a large class of NEMS devices demand new simulation capabilities because of the new physics encountered at nanoscale. In addition, the break-down of a continuum approximation for some NEMS devices poses new challenges. As a result, the development of quantum, atomistic, multiscale and continuum simulation tools based on advanced physical theories becomes critical.

Covering at length computational techniques for both classes of devices in one single book is not realistic and we have chosen to focus on the more mature world of MEMS, with several openings towards the NEMS world. In particular, we privilege fundamental aspects and computational design tools. Moreover, a few chapters addressing experimental techniques for MEMS and NEMS have been included. Indeed, not only numerical models have to be validated against experiments, but it is also true that experiments at the micro/nanoscale often give access to the quantities of interest often in an indirect way and data-reduction procedures strongly relying on numerical simulations are required. The thin borderline between experiments and simulation becomes immaterial at these scales.

Many experts have written excellent chapters in this book summarizing the state-of-the-art, fundamental issues, computational methods, experimental measurements, validation and future challenges. In the first part of the book (Chapters 1-6) focus is set on micro/nanofluidics, while in the latter (Chapters 7-12) more emphasis is given to truly multiphysics analyses concerning mainly advanced topics of solid mechanics and electrostatics.

Microfluidics has deep roots in MEMS and NEMS. Microducts are used in infrared detectors, diode lasers, miniature gas chromatographs and high-frequency fluidic control systems. Micropumps are used for ink jet printing, environmental testing and electronic cooling. Potential medical applications for small pumps include controlled delivery and monitoring of minute amount of medication, manufacturing of nanoliters of chemicals and development of artificial pancreas. Moreover, microfluidics affects the dynamical behavior of almost all microsystems through dissipation even when it is not the mechanical phenomenon of direct interest. Hence, flows in micro and nanochannels have always attracted and deserved considerable attention in the scientific community, even though many open challenges remain, as stressed in Chapter 1. The customary continuum, Navier–Stokes modeling is ordinarily applicable for flows in macrodevices. Even for common fluids such as air or water, such modeling is bound to fail at sufficiently small scales, but the onset for such failure is different for the two forms of matter. Moreover, when the no-slip, quasi-equilibrium Navier–Stokes system is no longer applicable, the alternative modeling schemes are different for gases and liquids. For liquid flows, the dense nature of the matter precludes the use of the kinetic

theory of gases, and numerically intensive molecular dynamics simulations are the only alternative rooted in first principles, as discussed in Chapter 1.

For dilute gases, statistical methods are applied and the Boltzmann equation is the cornerstone of such approaches. This topic is addressed in Chapter 2. The application of kinetic theory methods is first illustrated by deriving a generalized Reynolds equation from the linearized Boltzmann equation. The analysis, valid for arbitrary Knudsen number, is based on two different kinetic models of the collisional operator: the Bhatnagar, Gross and Krook (BGK) model and the ellipsoidal statistical (ES) model. The semi-analytical results described also form the basis for the *modified viscosity approach*, a simplified technique discussed in Chapter 5 and frequently applied to extend the validity of continuum models to the transition regime. In Chapter 2 it also shown that gas flows occurring in inertial MEMS having a complex geometry can be successfully studied by numerical deterministic solution of linearized kinetic model equations (BGK) whose predictions are in very good agreement with the experimental data presented.

The most well-known numerical tool for the solution of the Boltzmann equation in general strongly nonequilibrium conditions is the Direct Simulation Monte Carlo (DSMC) approach, analysed in detail in Chapter 3. Even DSMC is computationally more demanding than most continuum CFD methods it is shown that this problem can be partially alleviated by its superior parallel performance. Another feature of DSMC is the lack of numerical instabilities even for the most physically and geometrically complicated problems which, together with its unmatched accuracy, makes DSMC a unique method to study physical phenomena at the mean-free-path level. Besides the cases for which DSMC is the only applicable method, DSMC can be used concurrently with continuum methods and analytical approaches to develop empirical models that can be implemented in engineering codes.

However, using DSMC for subsonic-flow MEMS simulations is not without issues. A problem arises when the characteristic velocities of the micro-gas flow become very small since the use of conventional DSMC in such instances often incur in large statistical errors. Unfortunately, the typical gas flow velocities in most MEMS devices are in the low velocity range. This issue has stimulated many investigation and novel numerical approaches, like the multiscale coarse-grain molecular block (or “big molecule”) described in Chapter 4. Molecular blocks are used to replace the particles in the DSMC method, and a molecular block direct simulation Monte Carlo (MB-DSMC) method is established. As the mass of the molecular block is larger, the statistical error of the MB-DSMC method is expected to be sensibly smaller.

Even if all the approaches presented in these chapters are rooted in the molecular nature of fluids, the evaluation of gas damping for MEMS working at ambient pressure can be still conveniently addressed by means of continuum models. Estimating dissipation in air-packaged MEMS like inertial sensors seems, for several reasons, to be an ideal application for fast integral equation methods as shown in Chapter 5. First, the micromechanical structures are innately three-dimensional and geometrically complicated. Second, in order to provide an estimate of the mechanical dissipation, the only quantities of interest are velocities and forces on the structure surface. Surface-only integral equations have a dimensional advantage over volume methods in such a setting. Third, the velocities and displacements for many MEMS of interest are small enough, and the surrounding air is viscous enough, that the flow, at moderate frequencies, can be often described by a linear quasi-static Stokes model with slip boundary conditions. For the above reasons, there have been a number of experimentally-verified successes in evaluating gas damping for air-packaged MEMS as discussed at length in Chapter 5.

As a conclusion for the microfluidics section and as a transition towards the second part of the book, Chapter 6 reviews experimental techniques that are suitable for quality factor measurements of in-plane, out-of-plane and torsional vibrations of microresonators and comments on optical techniques applicable to nanoresonators.

Interestingly enough, one major open issue for MEMS working in near vacuum-conditions, is that dissipation predicted by experiments is much larger than expected for resonators having high aspect ratios and there is strong evidence that it should be linked to surface phenomena even if no reliable physical models are available. The classical theory of thermoelastic coupling can however explain intrinsic dissipation in specific conditions and is the object of several investigations and extensions, as done in Chapter 7. A full-Lagrangian multiphysics Newton method is proposed for the dynamic analysis of electrostatic MEMS in the presence of damping. This new scheme has several advantages over conventional MEMS simulation tools in terms of speed and convergence rates and is used to explore new nonlinear dynamic properties of electrostatic MEMS. Complex nonlinear oscillations and the period doubling route to chaos are observed under superharmonic excitations and the effect of these complex oscillations on thermoelastic damping in electrostatic MEMS is also studied.

A similar approach to electromechanical coupling is addressed in Chapter 8 which focuses on the quasi static response behavior of MEMS devices made up of very thin conducting plates. A convenient way to model such a problem is to assume plates with vanishing thickness, solve for sum of the charges on the upper

and lower surfaces of each plate and adopt a full-Lagrangian scheme both for the solid-mechanics and electrostatics analysis.

One major and truly multiphysics issue in vibrating MEMS is pull-in instability, which is investigated in Chapter 9 for MEM membranes subjected to Coulomb and Casimir forces. The Casimir force represents the attraction between two uncharged material bodies due to modification of the zero-point energy associated with the electromagnetic modes in the space between them. An important feature of the Casimir effect is that even though its nature is quantistic, it predicts a force between macroscopic bodies. This nonlinear multiphysics problem is analyzed by the meshless local Petrov-Galerkin (MLPG) method. It is shown that beyond a critical size, the geometric effect modeled by the Casimir force becomes dominant over the Coulomb force, and the device collapses with zero applied voltage.

Dielectrophoresis, addressed in Chapter 10, is an effective tool for particle separation and manipulation which is increasingly used in various BioMEMS applications for the analysis and separation of biological particles, such as cells, bacteria, viruses and DNA. The term alternating current (AC) electrokinetics refers to the particle movement arising from the interaction of non-uniform AC electric field with polarizable particles. One of these techniques is the dielectrophoresis (DEP), which arises from the interaction of AC electric field and the induced dipole in a particle. One of the DEP techniques is the field flow fractionation (FFF) method, in which DEP force levitates different particles to different vertical heights above the surface, and hydrodynamic force drives the particles traveling at different speed according to their heights from the surface to achieve the separation. Another well-known DEP technique is the traveling wave dielectrophoresis (twDEP), in which the particle motion is induced by traveling electric field. Both these techniques are simulated by means of a novel meshfree method named the linearly conforming point interpolation method (LC-PIM).

Chapter 11, the last contribution of the book addressing specific numerical techniques, discusses topology optimization issues emerging in the context of MEMS and focuses, in particular, on two problems related to manufacturing constraints in surface-micromachined structures and in protein sequence design.

All the numerical methods detailed in previous chapters make indeed use of material parameters which have to be evaluated from experiments. As in other technologies, the ability to exploit materials in MEMS and NEMS is limited by our knowledge of their properties. In particular, the successful fabrication and the reliable use of micro/nanostructures is strongly contingent on a sufficiently rigorous understanding of their length scale-dependent and process-dependent mechanical properties. In turn, such understanding requires the ability to perform mechanical measurements on microstructures. Hence, the challenging task of

mechanical characterization requires an entirely new set of techniques to achieve the force and displacement resolution required. The issue of mechanical characterization of polysilicon often used in MEMS is discussed in Chapter 12. An innovative approach based on a fully on-chip testing procedure is described and three ad hoc designed electrostatically actuated microsystems are here used in order to determine experimentally the Young's modulus and the rupture strength of thin and thick polysilicon. The accurate data-reduction procedure relying on electromechanical numerical simulations is discussed. The rupture values are interpreted by means of the Weibull approach and statistical size effects and stress gradient effects are taken into account thus allowing for a direct comparison of the data obtained from the different test structures.

Curiously enough, MEMS can be adopted as test machine for nanostructures, as demonstrated in Chapter 13. The need to characterize nanometer-scale materials and structures has grown tremendously in the past decade and a brief review of some of the methods used in mechanical characterization of nanoscale specimens, is presented first, followed by a detailed description of a MEMS-based material testing system. This MEMS-based system allows for continuous observation of specimen deformation and failure with sub-nanometer resolution by scanning or transmission electron microscope while simultaneously measuring the applied load electronically with nano-Newton resolution. Special emphasis is placed on modeling and analysis of a thermal actuator used to apply a displacement-controlled load to the tensile specimen as well as the electrostatic load sensor. Finally, experimental results demonstrating the advantages of the MEMS-based system are presented.

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