

Wei Yang

Mechatronic Reliability

Electric Failures, Mechanical-Electrical Coupling,
Domain Switching, Mass-Flow Instabilities

With 122 Figures and 9 Tables



Springer

Professor Wei Yang

Tsinghua University
Department of Engineering Mechanics
100084 Beijing
China

E-mail: chenzzh@tup.tsinghua.edu.cn

ISBN 7-302-04768-5 Tsinghua University Press
ISBN 3-540-42283-8 Springer-Verlag Berlin Heidelberg New York

CIP data applied for

Die Deutsche Bibliothek - CIP-Einheitsaufnahme
Yang, Wei: Mechatronic reliability - electric failures, mechanical-electrical coupling, domain switching, mass-flow instabilities / Wei Yang. - Berlin ; Heidelberg ; New York ; Barcelona ; Hong Kong ; London ; Milan ; Paris ; Tokyo : Springer, 2002
ISBN 3-540-42283-8

This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilm or in other ways, and storage in data banks. Duplication of this publication or parts thereof is permitted only under the provisions of the German Copyright Law of September 9, 1965, in its current version, and permission for use must always be obtained from Springer-Verlag. Violations are liable for prosecution act under German Copyright Law.

Springer-Verlag Berlin Heidelberg New York
a member of BertelsmannSpringer Science+Business Media GmbH

<http://www.springer.de>

© Springer-Verlag Berlin Heidelberg 2002
Printed in Germany

The use of general descriptive names, registered names, trademarks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

Typesetting: Data-conversion by author
Cover-design: de'blik, Berlin
Printed on acid-free paper SPIN: 10843426 62 / 3020 - 5 4 3 2 1 0 -

Foreword

Historically, mechanics thrives whenever it participates in advancing a new technology. The language finds new variants, and the tools unravel new mysteries. There are, however, only a finite number of basic mechanics problems in a given technology. When these problems are solved, some of us stay and evolve with the technology, and others move on to newer technologies. In the past two centuries, mechanics has impacted all major technologies: construction, transportation, and energy. The dazzling success makes us feel, at times, intellectually settled. But never should it blind us from new opportunities. Only in confronting new challenges do we realize how immature our science is.

In the coming decades one major source of challenges will be microelectronics and communication systems. The feature size in integrated circuits is now about a tenth of a micron-meter. Nanostructures are being developed for photonic networks. Both technologies involve diverse materials. Each functional part in a device is subject to intense thermodynamic forces—thermal, mechanical, electrical and chemical—all acting within a small dimension. In response, the part evolves by atomic movements along various paths. Maintaining structural stability is a recurring challenge in electronics industry as the size continues to shrink. To meet reliability requirements, all major industrial laboratories are doing testing on various aspects of the problem. A few research groups have appeared in leading universities worldwide. As we explore behaviors of nanostructures, forces of less familiar origins manifest themselves. They assemble the “self-assembled” structures.

Professor Wei Yang is a leader of this exciting field. In the last few years, he and his collaborators have made seminal contributions. Through theses of his students and several review articles, Professor Yang has been shaping this young field. In this book, he focuses on two phenomena: ferroelectricity and electromigration. Both phenomena couple mechanical and electrical actions. This book describes technological background, basic physics, experimental findings, and theoretical developments. The reader is brought from basic concepts to

II Foreword

up-to-date literature. This book is the first in the emerging field. Not only does it synthesize the studies of the two chosen phenomena, it also provides a perspective on how other phenomena might be approached. The study of evolving small structures will position the solid mechanics discipline at the frontier of major technologies of our time. The field is wide open.

Z. Suo
Princeton, New Jersey
June 2000

Contents

Introduction	1
0.1 Mechatronic failure of information devices.....	1
0.2 Three levels of mechatronic coupling.....	3
0.3 Bottlenecks for reliability of information devices.....	4
0.4 Mechatronic reliability.....	7
0.5 Book outline.....	10
 Part I Electric Failures	13
Chapter 1 Electric fracture	15
1.1 Cracking under electric field.....	15
1.2 Fracture toughness anisotropy	19
1.3 Asymmetric field effect on fracture toughness	21
1.4 Grain size effect of fracture toughness.....	25
Chapter 2 Electrically induced fatigue cracking	29
2.1 Fatigue crack growth above coercive field	29
2.2 Fatigue crack growth below coercive field	37
2.3 Models for electrically induced fatigue cracking.....	44
Chapter 3 Current induced mass-flow instability	49
3.1 Electromigration	49
3.2 Mass-flow instability of polycrystalline lines	57
3.3 Mass-flow instability of bamboo lines	66
 Part II Mechatronic Coupling	69
Chapter 4 Piezoelectrics	71
4.1 Piezoelectric behavior	71

4.2	Governing equations for linear piezoelectrics.....	75
4.3	Defects and boundary conditions	78
4.4	Two-dimensional crack solutions.....	82
4.5	Crack kinking.....	88
Chapter 5	Relaxor ferroelectrics.....	97
5.1	Physics of relaxor ferroelectrics.....	97
5.2	Constitutive relations of relaxor ferroelectrics.....	100
5.3	Field concentration near defects and electrodes.....	106
5.4	Stress concentration	111
5.5	Cracking and stress intensity factors.....	114
Chapter 6	Ferroelectrics.....	120
6.1	Atomic model of ferroelectrics	120
6.2	180 ° and 90 ° domain switching	129
6.3	Domain characterization	132
6.4	Constitutive laws of ferroelectrics	138
Part III	Reliability in Domain Switching	147
Chapter 7	Theory and experiments of domain switch.....	149
7.1	Switching criteria	149
7.2	Domain bands	153
7.3	Crack tip domain switching	170
7.4	Indentation of ferroelectric single crystals.....	179
Chapter 8	Fracture toughness and polarization.....	182
8.1	Small scale domain switching.....	182
8.2	In-plane poling	187
8.3	Effect of permeability	200
8.4	Anti-plane poling	206
8.5	Fracture toughness modified by polarization	214
8.6	Vickers indents for poled ferroelectrics	216
Chapter 9	Cyclic switch and fatigue cracking	219
9.1	Crack tip switching under positive and negative fields.....	219
9.2	Stress intensity factors under positive and negative fields.....	222
9.3	Fatigue cracking driven by cyclic switch.....	225
9.4	Steady state model	232

Part IV Mass-Flow Reliability	237
Chapter 10 Mass-flow under mechatronic fields	239
10.1 Mass-flow formula.....	239
10.2 Chemical potential and energetic forces	241
10.3 Distributed dislocations for constrained mass-flow	244
Chapter 11 Microstructural evolution	248
11.1 Buckling of dislocation loops.....	248
11.2 Evolution and instability of voids	253
11.3 Waviness of interconnects.....	260
11.4 Hillocks and sinks	267
Chapter 12 Mass-flow instability	276
12.1 Passivation cracking.....	276
12.2 Voiding within interconnects.....	278
12.3 Open circuit failure for single crystal and bamboo lines.....	283
12.4 Open and short circuit failures for polycrystalline lines	291
Concluding Remarks	298
Acknowledgements	300
References	302
Subject Indices	319

Introduction

0.1 Mechatronic failure of information devices

Mechanics and electricity have been nourishing the advances of sciences and technologies in the past 500 years. In the dawn of the new millennium, information science emerges as a major driving force in the horizon of science and technology. Intertwined with electronics, a fully blossomed discipline of mechanics engages new frontiers such small structures, smart structures, active control, miniature space technology, and microelectronic devices and packaging (Freund, 2000).

For instance, the development in very large scale integration (VLSI) brings about the emergence of sub-micron technology. The development drives the miniaturization of microelectronic devices as predicted by Moore's law. The configuration of microelectronic devices shifts from the thin film and substrate structures to the three-dimensional architectures, featuring skyscrapers of hundreds of multi-layers. The stereotype sub-micron processing enables the manufacturing of micromachines or highly integrated microsystems of millimeter size. Micromachines of ever-smaller dimensions emerge, such as a helicopter weighing a few grams, a miniature automobile with a dimension of 3 mm, a micro-pump of micron size, and an electromagnetic generator of 1.5 mm diameter. With micro-sensors of versatile sensing abilities, electronic chips of data processing, storage and control functions and micro-actuators to carry out mechanical functions, a micro-electronic-mechanical system (MEMS) can be assembled. The system encompasses the sensing, thinking and acting perspectives. The electronic-mechanical integration concept promoted a new discipline called "mechatronics" (Bradley *et al.*, 1991).

For information structures, the integration of mechanics and electronics has mixed blessings. On one hand, the exploitation of mechatronics is fruitful,

with advantageous functions such as piezoelectricity, ferroelectricity, memory, actuation, sensing and energy band modulation [see Gandhi and Thompson (1992), Wang *et al.* (1995)]. On the other hand, the mechatronic coupling can be lethal to the devices, with many mechatronic reliability concerns (Yang, 1996). This book is not tempted to explore the wonders of mechatronics, but rather aimed at unveiling various mechatronic reliability issues.

Mechatronic failures share three common features: small in length scale; coupling of stress and electric fields; and mass transport influence. The readers will be provided a glimpse of these features through the examples of MEMS and microelectronics devices.

A micro-electronic-mechanical system typically has a film/substrate or a multi-layer architecture. The main structural characteristics are tiny scale, layered inhomogeneity, and coupling of fields from different physical origins. The tiny scale calls for the applications of micromechanics, and drives researches on microstructural evolution (Suo, 2000). In a film/substrate or a multi-layers structure, stress as high as 0.001 or even 0.01 of its Young's modulus appears; the characteristic time required for a substantial shape change is much shorter in a thin film than in a bulk material; miscellaneous damage modes may present; and reliability is typically the bottleneck for the development of new technological structures. The investigations on the stress, morphological evolution, damage modes and reliability of the thin film structures bear important implications.

Failure in sub-micron integrated circuits is attributed to the coupling of mechanical, thermal and electrical fields. Mass transport in interconnects under intensive current is termed electromigration. Interconnects of vast amount are used in a semi-conductor device, and they may be stacked in three dimensions. The open circuit failure of a single interconnect, or the short circuit failure of two neighboring interconnects is enough to crimple the whole device; and the failure of one device may cause malfunction of the entire system. A mass diffusion process is intrinsically non-uniform. The non-uniformity induces local stresses, and consequently causes other failure problems. For example, it was found (Zhao and Yang, 1997) that the processing of one-micron width integrated circuit in China led to sub-micron tubular grains in interconnects, and that would raise severe electromigration reliability issues.

Information technology is in a transition era from invention to competitive manufacturing. In the endless spin-offs of information materials and IT

architectures, the ones that survive the competition are the quality products of high reliability. Upgrading the devices and packaging reliabilities becomes a key technology to survive the competition of new generation IT products. The reliability research to prevent failure of mechatronic coupling will be addressed in an increasing pace in the future.

0.2 Three levels of mechatronic coupling

Force can generate electricity, and vice versa. The mechatronic coupling can be examined in three different levels, namely from microscopic, mesoscopic and macroscopic perspectives.

From a microscopic perspective, the force is originated from the interaction of electron clouds, while the electricity is originated from the collective movements of electrons in a certain direction. The intensity of electron cloud interaction would bear influence on the collective and directional flow of the electrons; and vice versa, the directional flow of electrons would bear influence on the interaction of electron clouds. The mechatronic coupling comes as a natural consequence of the microscopic behavior of electron clouds.

From a mesoscopic perspective, two types of mechatronic coupling exist: (1) the incompatible strains activated by the electric field lead to incompatible stresses; and (2) the mass transfer activated by electric field, as well as its non-uniform presence, cause incompatible stresses. The mechanisms for the latter are less transparent, but they can nevertheless be dealt with by the method of mesomechanics.

From a macroscopic perspective, the mechatronic coupling refers to the interference between the mechanics field and the electric field. The coupling can be further distinguished as the unilateral coupling or the bilateral coupling. For unilateral coupling, the coupling is strong in some directions, but weak in the other directions. For examples, the stresses induce electric signals in linear piezoelectrics, but the influence of the electric signals to the stress field is secondary; on the other hand, the electric field can induce substantial deformation in a ferroelectric material, but the effect of the deformation to the electric field is rather insignificant. Therefore, the mechatronic coupling in a linear piezoelectric material appears in the direction from the stress field to the electric field; while in a ferroelectric material appears in the direction

from the electric field to the stress field. For a bilaterally coupled problem, the expression of either the strain or the electric field depends jointly on the stress and electric displacement fields, and the decoupling of any forms is impossible.

0.3 Bottlenecks for reliability of information devices

0.3.1 Bottleneck of smart structures: fragile ferroelectrics

Increasingly severe requirements are imposed to materials to transform mechanical and electric properties. Linear piezoelectrics are capable to output sensitive electric signal under a brushing contact force, but cannot offer noticeable actuation under moderate electric field. Ferroelectric ceramics of perovskite structure, on the other hand, are capable of delivering large actuation under realizable electric signals. Ferroelectrics are widely used in microelectronic technology due to their awesome mechatronic transformation efficiency and accurate controllability. Today, ferroelectric ceramics have been widely used in smart devices such as actuators and micro-positioners [see Cross (1993), Uchino (1997)]. In the late 80s, the breakthrough in ferroelectric thin film manufacturing enabled an integration between the ferroelectric thin films and semi-conductor devices. The integration led to the developments and applications of ferroelectric memories in information devices and systems of the new generation (Scott and Araujo, 1989). The smart structures by alternating electrodes and layers of ferroelectric ceramics and can realize enough actuation under conventional voltage range. The statistics in 1990 showed that in the electronic applications alone, the ferroelectric ceramics shared 60% of the high-tech ceramics market in the world (Cross, 1993).

On the other hand, ferroelectric ceramics is fragile, with fracture toughness typically in the order of $1\text{MPa} \cdot \text{m}^{1/2}$. That weakness often leads to various failures in applications involving electric loading. In many applications, ferroelectric components are subjected to intensive direct or alternating current. Intensive field concentration and stress concentration are induced near an internal electrode or a processing defect in a ferroelectric device. The failures include the fracture under an intensive electric field—known as electric fracture, and the fatigue crack propagation under alternating electric field—termed hereafter the electrically induced fatigue cracking. The issues of electric fracture and electrically induced fatigue cracking limit the

applications of ferroelectric ceramics and undermine the upgrading for the performance of microelectronic devices. The importance for the reliability of ferroelectric ceramics gives a strong impetus for the researches on the mechanisms of electrically induced failures [see Winzer *et al.* (1989), Yang (1996), Suo (1998)], and for the proposals of the corresponding toughening mechanisms.

0.3.2 Reliability in microelectronics: electromigration in aluminum lines

Nowadays VLSI semi-conductor integrated circuit typically assembles $10^6 \sim 10^7$ units, and they are connected solely by interconnects. Vast amount of interconnects may occupy as high as 80% of the chip area. Further improvements on the degree of integration and the circuit speed demand a shorter mean pass of interconnects, and an adoption of multi-layered architecture (Wang *et al.*, 1991). In a complicated interconnect structure, the open circuit failure of one line or the short circuit failure of two neighboring lines may fail the whole device. Though most interconnects may enjoy a very long life, but the line of the shortest life dictates the device life.

The most severe issue for an interconnect is to sustain high density operating current of unchanged direction, and that inevitably leads to the electromigration issue. For conducting wires and cables made of bulk materials, the phenomenon of electromigration is less severe due to relatively low current density. However, thin film interconnects used in semi-conductor devices confront a different situation. The superior heat transfer property of a silicon substrate enables the metal lines deposited on it to sustain an operating current density as high as 10^{10} A/m^2 without melting the line.

The low resistance and good processing capability render the aluminum line an advantage with respect to RC delay and allow for higher performance circuit design. In the integrated circuits, interconnects have small cross-sections (less than $0.1 \text{ } \mu\text{m}$ wide), carry intensive electric current (above 10^{10} A/m^2), and may operate at a temperature nearly half of the melting point (933 K) of aluminum. The flowing electrons exert a force (the electron wind force) on aluminum atoms, which drives aluminum atoms to diffuse. Mass diffusion under electric current, known as electromigration, raises the reliability concerns.

The situation is further accentuated by the continuing trend toward miniaturization in integrated circuits, especially in the VLSI and power

semiconductor devices. The research on 1 Gb DRAM employing 0.18 μm line technology succeeded in 1995, and its product was put on market in 1999. Modern microelectronic technology has matured the sub-micron lines, and those lines are currently in the massive production stage. The trend to shrink the line width continues. INTEL Group is developing microelectronic circuits of 0.13, 0.10, 0.08, and even 0.06 μm line widths. The endless drive for higher degree of integration continuously narrows the thin film interconnects, with the consequence of ever-increasing current density through the lines. The increasing current density in interconnects makes the interconnect failure by electromigration a persistent bottleneck for the reliability of microelectronic devices.

The usage of aluminum lines or copper lines in integrated circuits remains a fundamental technology debate concerning investment in the order of 100 billion US dollars. As earlier as in the seventies, d'Heurle (1971) pointed out that the adoption of metals (such as copper, silver, gold and molybdenum) with high melting temperature, low diffusivity and high activation energy would substantially improve the resistance of an interconnect against electromigration. However, aluminum and its alloys possess the following advantages for interconnects [see Wang *et al.* (1991)]: (1) good conductivity for high IC speed; (2) low resistance for Ohm contact between aluminum and silicon; (3) good adhesion with insulators such as SiO_2 ; (4) corrosion resistance; (5) good deposition and etch properties; and (6) bonding ability and the endurance of bonding spots. These advantages have granted the leading edge of aluminum and its alloys as the first pick materials for interconnects in semi-conductor industry. In IC technology, above 90% of metalizations use aluminum based lines, and they can function properly in a temperature range below a half of the melting point (933 K) of aluminum. The weakness of aluminum and its alloys lies in their low melting point, and consequently their poor resistance to electromigration. That raises the issue to replace aluminum lines by copper lines. Though copper has a higher melting point and consequently a better resistance to electromigration, it has a poor adhesion with SiO_2 that gives a high cost in copper technology. It is only in the case of sub-micron lines that copper may be used as the base material of interconnects. In 1999, the pronounced electromigration issue in sub-micron lines led IBM Corporation to introduce IC chips of copper interconnects.

The interconnect failure under electromigration is not an isolated problem. Failure in interconnects usually attributes to the combinational effect of stress migration, thermal migration and electromigration. The stress field that induces stress migration originates from thermal mismatch and the field

transients during the operation of the device. Joule heat effect induced by current crowding cannot be ignored. It may induce temperature gradient and lead to thermal migration. By electromigration, the electric field dictates the mass transport and redistribution in interconnects, and those processes cause stresses in the line [see Blech (1976), Blech and Herring (1976), Thouless *et al.* (1996)]. Huang *et al.* (1996) reported the stress within a line covered by stiff passivation may exceed several times of the yield stress of the interconnect material, high enough to cause void nucleation. The stress field within the line has the counter effect on mass transport. Electromigration and other mass transport processes produce morphological changes, and henceforth perturb the electric and the stress fields.

0.4 Mechatronic reliability

Since the nineties, the researches in mechatronic reliability have surged as a rapidly developing front in the interface of solid mechanics, material science and electronics (Yang 1993, 1996). Mechatronic reliability studies various failure modes of information materials under electric or mechatronic loading. Though the electric loading causes the failure, the stress-induced fracture consists of the underlying mechanism of the failure. Under the framework of mechatronic reliability, the failure modes under mechatronic loading are identified; the failure mechanisms are elucidated; new approaches of analysis are pursued; and comprehensive guidelines of reliability are assessed, under the objective to raise the service lives of information materials and MEMS structures. The development of mechatronic reliability is still at its early stage, but it is a new field full of opportunities.

Mechatronic reliability extends the mechanics formulation from the traditional structural materials to the new arena of information materials and MEMS. It promotes three thrusts in the interface of mechanics and material science. The first thrust pursues the active design and prediction of MEMS. A sequence of developing stages beyond the empirical design unfold as follows: modeling the mechatronic coupling behaviors; qualitative design guided by the reliability principles; quantitative design, optimization and simulation incorporating mechanical and electric factors; intelligent and predicative design with high reliability and recoverability. The second thrust endeavors a formulation of mechanical, electrical and thermal actions in a unified model based on forces of different physical origins. That unified model can explore the failure mechanisms under coupled fields. The third thrust explores the

multi-scale perspective linking the continuum and atomistic approaches. The macroscopic and microscopic link of the mechanical and electric fields holds the key of the basic understanding of mechatronic reliability.

0.4.1 Phenomena of failure: electric reliability

Electric reliability reveals various failure phenomena under electric loading. It encompasses electrically induced failure phenomena such as electric fracture, electrically induced fatigue cracking and electromigration. The investigation is conducted by the combination of mechanics and electromagnetics.

The objective for electric reliability is to prevent the electrically induced failures of various forms, and to propose pertinent device designs to assure reliability. Typical examples are listed as follows. How to design a ferroelectric actuator to prevent electric fracture and electrically induced fatigue cracking? How to design smart crack arresters according the principle of electrostriction? How to proceed in a mechatronic design so that the failure of a thin film or multi-layer film is prevented? How to stabilize the mass-flow during electromigration? And so on.

0.4.2 Cause of failure: mechatronic coupling

Coupling between the mechanical field and the electric field is the intrinsic cause for mechatronic failure. Mechatronic coupling can be studied from the constitutive relations of the materials. Typical constitutive laws featuring mechatronic coupling include: linear piezoelectric constitutive relation; relaxor ferroelectrics constitutive relation; and ferroelectric constitutive relation with domain switching. In ferroelectrics, the incompatible strains induced by electric field manifest in two mechanisms: the gradually increased incompatible strains under electric field in terms of electrostriction; and the abruptly varied incompatible strains by domain switch when the electric field exceeds a critical value. Of fundamental importance are the field characterization and the controlling parameters near a defect under three different mechatronic coupling characteristics.

0.4.3 Mechanism of failure: mechatronics of domain switch

The fracture toughness of ferroelectrics exhibits intricate dependence on

electric field: not only the electric field applied during the testing, but also the history of electric field prior to the testing. The accumulated testing data indicate two intriguing phenomena. The first is the fracture toughness anisotropy induced by the poling field: the cracking along the direction of the polarization encounters higher fracture resistance than that for cracking normal to the polarization. The second is the fracture toughness asymmetry with respect to the applied field: the fracture toughness exhibits an unpredictable change if the electric field is applied along or against the direction of the polarization during the test.

Domain switch holds the key to unlock the failure mechanisms of ferroelectrics. Local domain switch is activated near a flaw by the stress and electric field concentration. The crack-tip switching zone dictates the above-mentioned experimental data (Yang and Zhu, 1998a, b). Highly concentrated stress field near a crack tip may cause 90° domain switch in the crack tip vicinity. The electric field is perturbed by the low permeability of the defect, and the field concentration reconfigures the domain structure near a crack tip. The change in the apparent fracture toughness is highly sensitive to the defect electric boundary condition.

Predictability on the electric field influence to the fracture toughness may serve as the guidance for the failure resilient design and the operation of ferroelectric actuators. For instances, proper poling can be exploited to improve the fracture toughness of ferroelectrics in the principal loading direction; negative field may be applied to the ferroelectric actuators in operation to raise their fracture toughness.

0.4.4 Failure during mass-diffusion: mass-flow reliability

Any factor that contributes to the change of the chemical potential of a mass system may drive the mass-flow. In an operating aluminum-based interconnect, current of flowing electrons acts as electron wind that blows over the aluminum atoms to drive them to diffuse along the line. Other driving forces for mass-flow include stress gradient, curvature effect, and interface energy. The kinetics of mass-flow is controlled by temperature, the mobility of mass diffusion, and the activation energy of mass diffusion. Mass-flow reliability studies the mass-flow instabilities under electric field, stress gradient, surface energy, and other causes. Typical research issues include the instabilities of unconstrained and constrained mass-flows in a

s i n g l e - c r y s t a l