

Abstract Title**Multiscale Scientific Simulations of Materials Integrity in Aerospace Microsystems****Symposium Track****Fundamental Modeling in Nanomechanics****Authors' names***Wing Kam Liu, Cahal McVeigh, and Albert To***Authors' affiliations***Northwestern University***Abstract body**

It is fair to say that microsystems have become an integral part of our lives nowadays – computers, cell phones, iPods¹, automobiles, aerospace systems, and biomedical systems all consist of these ever-shrinking microsystems. For example, a hard drive in a computer/cell phone/iPod is a micromachined cantilever system that reads and writes information. An accelerometer microsystem in a car is used to activate the airbag when a preset threshold acceleration is reached. A gyroscope microsystem in an aerospace system such as satellite and space station is utilized for stabilization and navigation. Microfluidic devices are used to collect and analyze blood samples. The advances in microsystem technologies have brought and will continue to bring convenience to our daily lives, enhance health and safety, and help to make major scientific discoveries, among many other advantages. In 2004, annual sales of microsystems have exceeded 5 billion dollars, and an annual growth rate of more than 20% is expected in the rest of the decade². From either the health, science, technology, and economics point of views, microsystems are of significant national importance and interest.

Major hurdles remain in ensuring the long term performance and reliability of microsystems in aerospace applications despite the redundancies with which the microsystems are often designed. Microdevices on satellites and other spacecrafts are subjected to harsh environments that include the following sources of damage: solar radiation, extreme thermal cycling, residual atmosphere, electrons and ions associated with plasma sources, cosmic rays, and particles from meteoroids and debris. The nature and relative importance of these environmental hazards depends on the position of the spacecraft and the level of shielding. For example, the thermal cycling that occurs as the satellite orbits the earth results in material degradation that can lead to mechanical/electrical failure such as fracture, stiction in contacting components, failure of electrical contacts in switches and many other modes. For example, in the International Space Station, “gyroscope failure [is] likely caused by lack of lubrication³.” In the Hubble Space Telescope (HST), “electronic glitches and the corrosion of electrical wires have previously knocked some gyros out of commission... Since then, two of those gyros have failed - apparently because clumps of lubricant or small particles have prevented their bearings from turning smoothly⁴.” It is estimated that by 2008 only one will remain, leaving the system unusable. Designing using novel materials and new microsystem technologies by demonstrating the long term system reliability in hostile environments with our integrated multiscale analysis system.

¹ iPod is a trademark of Apple Computer, Inc.

² Microelectromechanical Systems (MEMS) Technology: Current and Future Markets by Andrew McWilliams, Feb 2006

³ in Florida Today, June 26, 2002

⁴ in Newscientist.com news, May 19, 2005

Our major aim is to achieve a *paradigm shift* from empirical approaches of microsystem modeling and design to one which is based on multi-scale predictive science. While the former relies on tests on prototypes, the proposed approach can treat situations where full duration system level tests are not feasible. This change in paradigm will offer many benefits in the design and maintenance of microsystems, because it is neither possible nor practical to pretest new designs for the long lifetimes and the environmental conditions that are required. It is anticipated that these approaches will be applicable throughout science and engineering.

A focus problem is conceived to drive research and to demonstrate the predictive science-based simulation system. The proposed research program is based on six pillars:

1. Multidisciplinary Predictive Science – the development and advancement of predictive theory and methodologies for thermal-mechanical-chemical-electrical aging and materials instability, radiation damage and radiation-enhanced diffusion, materials damage, fatigue, and fracture, and energy dissipation mechanisms, culminating in constitutive models that can be used for prediction of the performance of microsystems in aerospace applications.
2. Multiscale Modeling, Simulations, and Computational Mathematics – the development of multiscale, multiphysics field equations and constitutive equations based on coupling first-principles methods, molecular dynamics simulation, Monte Carlo methods, and phase-field models.
3. A program that addresses challenges in validation, verification, and uncertainty quantification.
4. Integrated Computational System and Software – the aim is to integrate science/engineering, computational mathematics, and computer science to develop scalable parallel algorithms both at the application and systems levels for petaflop computation.
5. Prediction of Thermal-Mechanical-Electrical Performance and Long Term Reliability of the Focus Microsystem.
6. Design of Novel Materials for Future Microsystems.

Keywords

Nano mechanics and materials, thermo-mechanical-chemical-electrical, predictive Science

References

W.K. Liu, E G. Karpov, H S. Park. Nano Mechanics and Materials: Theory, Multiscale Methods and Applications. Wiley, New York, 2005.

W.K. Liu, E.G. Karpov, S. Zhang, H.S. Park. An Introduction to Computational Nano Mechanics and Materials Computer Method in Applied Mechanics and Engineering 193, 1529-1578, 2004.

C. McVeigh, F. Vernerey, W.K. Liu, L. Cate Brinson. Multiresolution analysis for material design. Computer Methods in Applied Mechanics and Engineering, 195, 5053-5076, 2006.

G.J. Wagner, W.K. Liu. Coupling of Atomistic and Continuum Simulations using a Bridging Scale Decomposition. Journal of Computational Physics, 190, 249–274, 2003.

Corresponding author contact information

Wing Kam Liu, w-liu@northwestern.edu