1.0 EXECUTIVE SUMMARY

The Brown University Materials Research Science and Engineering Center (MRSEC) is entitled Micro- and Nano-Mechanics of Materials. It is organized into two interdisciplinary research groups (IRGs) and one seed project, with 18 faculty, 12 graduate students and 2 post-doctoral associates currently participating. The MRSEC supports not only scientific research but also an infrastructure of central research facilities and a wide range of educational and technological outreach activities consistent with the broader impact goals of the National Science Foundation and U.S. science policy. The following report documents the achievements of the MRSEC in the period 4/1/2008 – 3/31/2009.

The goals of the center are to 1) perform field-leading research in the area of mechanics of materials on multiple length scales down to the nano-scale with applications some of the most difficult and fundamental issues in the field, and to apply principles of solid mechanics to cell adhesion and other biological problems; 2) use the faculty and university resources to achieve broader impact in the areas of science education, technology transfer, human resource development and creation of a more diverse scientific community. The MRSEC is administered through the Institute for Molecular and Nanoscale Innovation (IMNI) and the Center for Advanced Materials Research (CAMR) at Brown University. The Director of the MRSEC is **W.A. Curtin** and he is advised by an executive committee that contains a representative from each IRG (**E. Chason, A. Bower**) and the seed project (**L.B. Freund**).

Scientific Accomplishments: Research in the current MRSEC is organized into the following topical areas: IRG1 - Stress in Thin Film and Small Scale Structures; IRG2 - Multiscale Mechanics of Complex Microstructures; Seed project: Micromechanics of Cell Adhesion. Each project area consists of linked program of experimental and theoretical investigations. The Center aims for strong synergy between theory and experiment, with new theoretical insights suggesting new experimental studies and new experimental results driving advances in modeling; this is a hallmark of the Center at Brown. The IRGs and Seed are complementary and interactive, with faculty often participating in projects in more than one area or IRG.

During the current reporting period, MRSEC researchers published 30 scientific papers with full or partial MRSEC support, and numerous others using shared facilities or in connection with industrial collaborations. Some research highlights for the past year include:

- New mechanistic insight into the problem of Sn whisker formation in Pb-free solders for electronics manufacturing has been gained through identifying, quantifying, and modeling the fundamental mechanisms controlling the whisker formation in Sn coatings on Cu. Experiments reveal a complex interaction between the formation of Cu-Sn intermetallic compounds, stress generation in the Sn layer, and the nucleation/growth of whiskers in Sn and Sn-Pb systems. Using insights from the quantitative experiments, finite element simulations are able to calculate the rate of whisker growth due to intermetallic formation in a Sn film with columnar grain structure containing plastically “soft” grains on a Cu substrate, accommodating the volumetric strain of intermetallic growth by a combination of dislocation motion and grain boundary diffusion.

- Modeling of heteroepitaxial growth of strained multilayers, of interest for optoelectronic devices and photovoltaic cells, as been used to predict morphologies of these structures. Experiments show the strained islands adopt highly-correlated patterns resulting in periodic

lateral composition modulations in the multilayer structure, and the model captures these features through a phase field model that captures the complex interplay between the elastic relaxation and growth rate. A key feature of this model is use of an iterative higher order Fourier convergence method to compute the elastic fields without imposing any geometric restrictions on the shapes of patterns.

- Crack growth across twist-misoriented boundaries in elastic brittle materials has been studied using 3D finite elements to understand prior experimental results performed in this MRSEC. The simulations predicted that cracks will only propagate into the second grain if the toughness of the grain boundary exceeds a critical magnitude and have shown the influence of GB toughness and twist misorientation on the effective toughness of the solid. Both simulations and experiments show that twist boundaries give rise to very substantial increases in toughness, and that the strength of the grain boundary is a critical parameter in controlling the crack path and crack geometry in the second grain.

- A novel micro-molded axially symmetric conical pillar has been used to study cell aggregation phenomena associated with tissue growth. Cell restructuring leads to climb of a toroidal cell aggregate up the pillar against gravity, a process monitored by time lapse photography, providing a history of the motion, size, and shape of the aggregate. A theoretical model of the process has been developed to extract values of the parameters characterizing the evolution behavior. Comparison of the model to the experiments has shown a definite relationship between the unknown surface energy of the cluster and the unknown dissipation in the surface diffusion mechanism.

Education and Outreach: The MRSEC organizes and executes several dynamic outreach programs in the areas of education and technology. These programs have reached over 3500 students since 2005 as well as influencing the undergrads performing the program, some of whom have gone on to careers in K-12 science education. Specifically, our BrownOut classroom visits program brings Science, Technology, Engineering and Math topics to local schools, using fun and interesting presentations to demonstrate science principles, technological advances, or using mathematics to solve problems. Our Research Experience for Teachers program provides local educators with a summer experience to develop new curricular materials or perform research in collaboration with faculty. A summer Research Experience for Undergraduates program attracts excellent undergraduate students from a range of national universities including students from under-represented minorities, and through a varied cohort experience teaches them about research and research careers, providing encouragement for the pursuit of careers in science. We work with our partner at Florida A&M University to increase participation of women and minority students at both undergraduate and graduate levels. Collaborative activities with industrial partners remain a valuable component of the Center. A centerpiece of this effort is the Collaborative Research Lab with General Motors, where we continue to make important new advances in advanced metals and surfaces. Additional industrial interactions maintain links between the Center's fundamental scientific research and the technological applications of that research.

Broader Impacts: The Center's activities have both scientific and educational impact. The results of our research are widely disseminated in the scientific community and are recognized as being innovative and valuable. Our research is developing new experimental techniques for observing nanoscale and biological phenomena, and new theoretical and simulation methods that advance our

fundamental understanding of material behavior and that can be used to guide design and optimization of new classes of materials for electronic and structural applications. With our industrial partners, these advances are applied to issues of technological importance, such as the development of stronger or more-easily-processed structural materials and the processing of electronics without the use of environmentally hazardous materials. The educational activities of the Center impact the Rhode Island community by bringing our faculty and students in contact with students and teachers in the local schools, particularly in Providence and in schools with high minority enrollment. Our summer programs bring in students from a wider area, with emphasis on recruitment and retention of groups that are under-represented in the sciences and engineering. Finally, the training of graduate students within our research programs is instrumental in creating the next generation of leaders in the area of mechanics of materials.