

# Modeling, simulation and experiments related to biological and polymeric materials

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## 1.) Introduction

The sessions on biological and polymeric materials covered the areas of fabrication, characterization and modeling. The talks covered questions related to fabrication methods such as imprinting approaches, fluidic control, organic-inorganic composites/structures at nanoscale (e.g. DNA-CNT complexes), mechanical properties of cells (e.g. diseases change properties), scale effects in biomaterials (length scale reduction for robustness), mechanics of single biomolecules, characterization, modeling (e.g. nano-indentation and fracture at nanoscale and in biomaterials), as well as sensing (MEMS, micro fluidics and biochip, or fluorescence microscopy using quantum dots). We outline some of the fields in more detail in the next sections.

## 2.) Specific research topics

### 2.1 Fabrication and manufacturing

The workshop participants reported several techniques to create small-scale structures. Examples included nano-imprinting; LIGA (a German acronym for lithography, electroforming, and molding), classical techniques such as electron beam lithography and focused ion beam lithography; and self-assembly. Despite significant past progress in this area, tremendous opportunities and challenges still remain. In particular, even the most advanced nanofabrication techniques cannot yet emulate the widespread ability of biological systems to self-assemble. Advances in nanofabrication would enable a wide range of small-scale structures and materials to be created. Examples are include DNA-CNT complex, neuroprobes, bio-molecular sensors, as well as integrated of micro- and nano devices in complex apparatus such as lab-on-a-chip.

MEMS and NEMS technologies are an important gateway to nanotechnology, as they may be used to combine top-down and bottom-up approaches. However, there is still significant need for further research in techniques to fabricate micro- and nano-structures. For example, it is still difficult to mass-produce many MEMS devices on scales that are routinely used to manufacture integrated circuits. Another issue discussed was reliability of the devices, which still poses a problem, particularly in designs that use sliding contacts. In the future, we envision that micron and submicron size MEMS / NEMS devices will play an increasing role to integrate nanomaterials and nanostructures for testing and applications.

## 2.2 Characterization techniques

Techniques such as SEM, (HR)TEM, X-ray scattering and AFM, confocal microscopy, as well as optical tweezers still play an important role in characterizing micro/nano scale materials. Other methods that were utilized are nano-indentation for characterization of polymers, and specially designed micro-channels for studying nano-/micro fluidic systems. In the future, MEMS devices could take over some part of the testing by serving as sensors and actuators. At the important interface of biology and materials science, bio-sensors based on functionalized surfaces may be the key to a number of promising applications. These methods are examples where concepts of mechanics, physics and chemistry are combined. Similar considerations apply for fluorescence microscopy using quantum dots.

## 2.3 Modeling of polymers and biomaterials

Available methods for modeling and simulation in the area of small-scale materials are atomistic methods (e.g. *ab initio* and MD), FEM/BEM based numerical tools, analytical continuum theory, as well as mesoscopic approaches. The workshop highlighted the importance of multi-physics and multi-scale simulations in treating biological and MEMS problems. An important goal for the future is thus the development of reliable, generally applicable multiscale and multi-physics simulation methods. Coupling of different length and time scales, along with development of software tools, is a critical and timely issue. Biology intrinsically operates on multiple scales.

Specific topics covered at the workshop included: fracture at nanoscale (organic versus/and inorganic); adhesion at nanoscale; size effects in biomaterials, and addressing the common “design objectives” in biomaterials. In this particular field, design for robustness was identified as a critical objective of nature’s evolution over millions of years, and it was found for example in bulk and surface materials. Another important area is calculating material properties based on a fundamental perspective (e.g. at the quantum level), polymer properties based on atomistic calculations, and structural properties-functional relationship. It is critical to note that nature does not distinguish between formal scientific disciplines, and therefore, the numerical studies that describe biological materials usually must be multi-disciplinary.

## 3.) Discussion and conclusions

The session on biological and polymeric materials brought together a group of researchers who work in very diverse fields, including fabrication methods; nanoscale testing methods; nano- and multiscale computations; and observations and modeling of biological systems. Studying biological materials is a challenging, timely research opportunity. Investigations of such materials should involve a joint theory-simulation-experimental approach, combining scientists from various fields. We believe that understanding biology, and learning from nature could change engineering and science in the coming decades.

We have seen great progress in developing techniques to fabricate nanostructures, but this remains a rapidly evolving field, and much progress remains to be made before we can even begin to rival nanoscale structures observed in nature. This is clearly an area that will continue to require significant long term investment. Manipulating discrete elements of a nanosystem is a particular challenge. Progress in this area could be accelerated by providing mechanisms experimentalists to obtain access to novel fabrication tools. More could be done to establish shared facilities that can be used at low cost; and also to accelerate

commercialization of promising techniques. Mechanisms to permit postdocs and students to visit facilities and learn techniques would also be valuable.

Advances have also been made in developing methods to study material behavior at the nanoscale. Ex-situ microscopy is highly advanced and widely available; in-situ testing is more difficult, but advances continue to be made in this area. Quantitative measurements are very difficult, and other than nano-indentation, there are virtually no commercially available tools to measure material behavior at nanometer length scales.

Our ability to model systems at nanoscale has improved greatly with advances in computer power, and with the development of widely available codes such as VASP, DYNAMO for ab-initio and molecular dynamic simulations, and many commercial and free finite element codes. Wide gaps remain in the length and time scales that can be resolved by *ab initio*, MD, and continuum simulations, however. Methods to simulate nanostructures with atomic or meso-scale resolution for realistic time scales, without undue reliance on phenomenological constitutive equations, are a particular problem. Even the most advanced atomic scale simulations of polymers, for example, can only simulate behavior of short chain molecules (500 atoms or so) over a few nanoseconds. An enormous challenge in this field, which would have particular applications to biological systems, is to connect chemistry to mechanics. Multi-scale simulations are one promising approach, but much more work needs to be done before this become more than an exploratory research tool. In addition, there is a critical need to develop experimental methods that can be used to validate nanoscale simulations. This means we need to develop techniques to measure atomic scale phenomena quantitatively. In this regard, two interesting, and very different, approaches were presented in the workshop: one was K.S. Kim's field projection method, which can be used to extract quantitative measures of stress and strain around defects from high resolution TEM images. The other was F. Spaepen's innovative use of a colloidal system to mimic the behavior of a hard-sphere simple liquid.

Studies of biological systems are extremely helpful to identify physical phenomena that can be exploited to design materials and systems at nanometer length-scales; and also to identify processes that are beyond our current understanding. Traditionally, biology, and also bio-mechanics, have aimed to provide a descriptive understanding of natural phenomena and living systems. We have learned a great deal from these studies, and we shall undoubtedly continue to do so. But to fully exploit the power of mechanics, we need to develop the ability to predict, rather than describe, the behavior of nano-scale systems. In this regard it may be advantageous to design experiments and simulations that enable us to study phenomena of interest in isolation and under controlled conditions, rather than in the natural state. Four specific examples of specific phenomena that are observed in nature and could be studied in this way were presented in the symposium:

- (i) Crystal growth mediated by organic molecules;
- (ii) Nanoscale mechanisms of adhesion;
- (iii) Deformation mechanisms in biological bone-like materials;
- (iv) Nanoscale composites based on organic molecules trapped in a crystal.

We envision that international collaboration could help to address some of the described issues and to achieve the long-term goals of utilizing the concepts of biology or biomaterials itself in technological applications. There are already numerous funding agencies that, for instance, offer specific programs for funding US-Taiwan collaboration, such as NSC agreements with NSF, NIST and AFOSR. The next step could be to identify strategies,

develop key projects, and establish joint research and education programs. We believe there is necessity for a greater modeling effort for biomechanics problems, for instance in atomistic understanding. An example is the role of biomolecules trapped in single crystals (challenging because of time and length scale, and the interaction potential between different atom species). Also, we envision that combining MEMS devices with bio-problems may lead to development efficient sensors (e.g. “lab on a chip” technologies). Linking simulation-experiment-theory, for example by joint studies carried out between different groups should also be a key aspect in future research, as for example in projects focusing on a fundamental problem such as functioning of muscles. Today, an important experimental limitation is how to handle small size samples for instance in clamping CNTs, handling biomolecules, or dealing with nanofluidics.

In summary, there is lots of room to find interesting materials, experimental techniques and phenomena in nature: Nature had taken millions of years to develop very powerful concepts in building wonderful materials and eventually intriguing “machines” that we refer to as “life”. We believe that future research at the bio-nano interface needs to focus on learning the fundamental principles that are exploited by nature in the design of living systems, rather than simply copying or describing natural systems themselves.. This may eventually enable us to use them in manmade technology that would have similar superior features. Biology is nanotechnology by nature, and nano-mechanics is the key yet to be understood!