MULTISCALE MODELING OF BONE FRACTURE AND STRENGTH

Allocation: Illinois/50.0 Knh
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EXECUTIVE SUMMARY

In this project, nonlinear finite element models of trabecular bone were used with the aim of building a predictive tool to capture plasticity and strength of this biological material. The complex, random, and irregular features of bone were effectively imaged using micro-computed tomography to build three-dimensional finite element models. The complexity of the structure, material and geometric nonlinearities, along with complex contact conditions, make the numerical analysis very challenging even on the latest high-performance computing (HPC) platforms. Our results closely match experimentally measured stiffness and strength and capture experimentally observed plasticity of the trabecular bone, demonstrating the potential of the model to predict the mechanical behavior of bone. This model provides a crucial step in creating a multiscale model of whole bone based on patient-specific data. Such a model will serve as a novel tool for more accurate prediction of osteoporosis, a bone disease characterized by bone's susceptibility to fracture.

INTRODUCTION

Osteoporosis, which is a growing clinical problem in aging societies, is a bone disease characterized by low bone density and deterioration of bone's structure leading to bone fragility and increased risk of fractures [1]. It is a silent disease with no symptoms prior to fractures and no cure, but treatments can slow its progress. Thus, its early and accurate diagnosis is crucial. Currently, bone quality is assessed clinically by measuring the bone mineral density while other factors such as bone's complex hierarchical structure also contribute to bone's properties. Thus, a new approach is needed for more accurate diagnosis of osteoporosis. Computational mechanics modeling can provide an effective new tool for the clinical assessment of bone.

Bone is a multifunctional biological tissue. One function is to serve as a structural support for soft tissues in the body. As a structural material bone has an ideal combination of properties when healthy: high stiffness, strength, and fracture toughness, and light weight. Bone is made of a compact cortical bone forming an outer core and a spongy trabecular bone filling an inside space and ends of long bones (Fig. 1). Such geometry is optimal as it minimizes weight, reduces bearing stresses at joints, and allows the body to withstand high functional loads. These superior properties are due to the hierarchical structure of bone spanning from molecular to macroscopic levels [2].

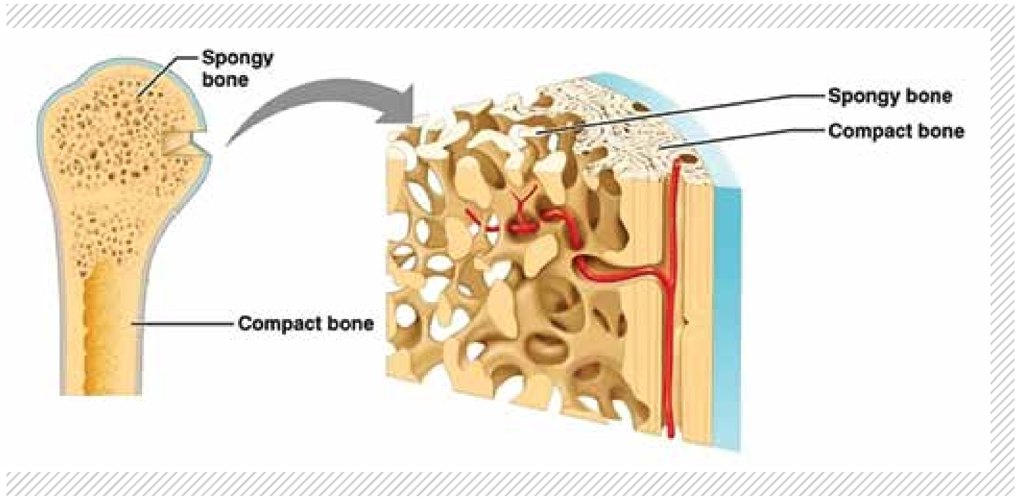


FIGURE 1: Structure of bone showing cortical (compact) and trabecular (spongy) bone.

Dense cortical bone and porous trabecular bone work together to provide excellent load-bearing properties. Osteoporosis-related fractures mostly occur in trabeculae-rich areas of bone. Trabecular bone is also the primary site for insertion of orthopedic implant systems. Thus, mechanical properties of trabecular bones are of high clinical and research interest for prediction of age- and disease-related bone fractures, optimizing treatments to reduce fracture risks, as well as designing improved implant systems [3-4].

In this project, trabecular bone was simulated using non-linear finite element (FE) models to gain a better understanding of its mechanical behavior. Such models have the potential to build a structure-based predictive tool to assess strength and damage locations in patient-specific bones. It can also serve as a guide to engineers for design of **novel** synthetic bio-mimetic and bio-inspired materials for a wide range of engineering applications.

METHODS & RESULTS

In this project, nonlinear micro-computed tomography (micro-CT) FE model of trabecular bone was built as a cost-effective compliment to experiments and conventional methods that are expensive, time-consuming and prone to artifacts. In this model, the complex, random, and irregular features of microstructure were captured with microstructure data from the micro-CT imaging. The model was then meshed and analyzed under loading with numerical simulations on trabecular bone samples with complex random microstructures.

An example of our trabecular bone FE model along with stress distribution is shown in Figure 2. Figure 3 shows a sample stress-strain response of a trabecular bone sample under compression obtained from our model and compared to experiments. Our results indicate a close match with experimentally measured stiffness and strength. Plasticity of trabecular bone is also well captured in our simulations, showing the model's potential to predict the mechanical behavior of bone.

The effectiveness of micro-CT FE models as predictive tools for mechanical properties of trabecular bone is directly dependent on proper calibration and validation. As such, this project investigates the influence of using different constitutive laws and parameters at the tissue level on apparent response through a systematic study to serve as a guide for modeling bone.

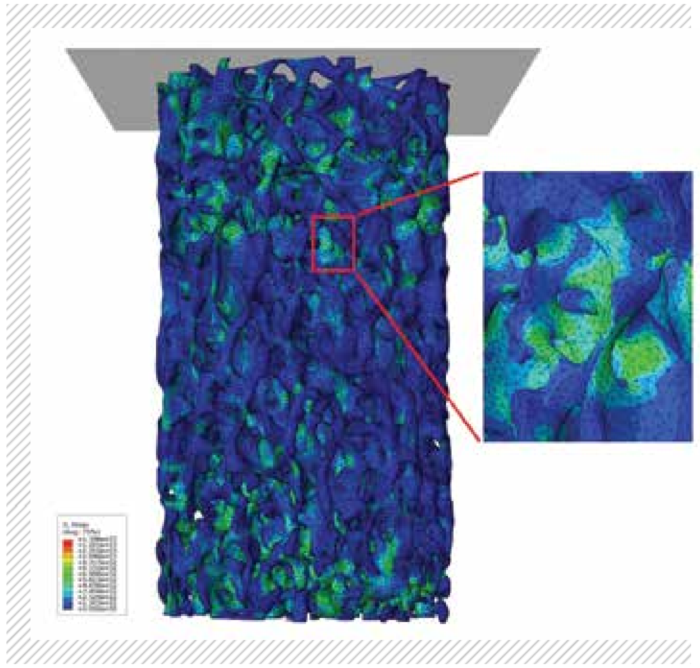


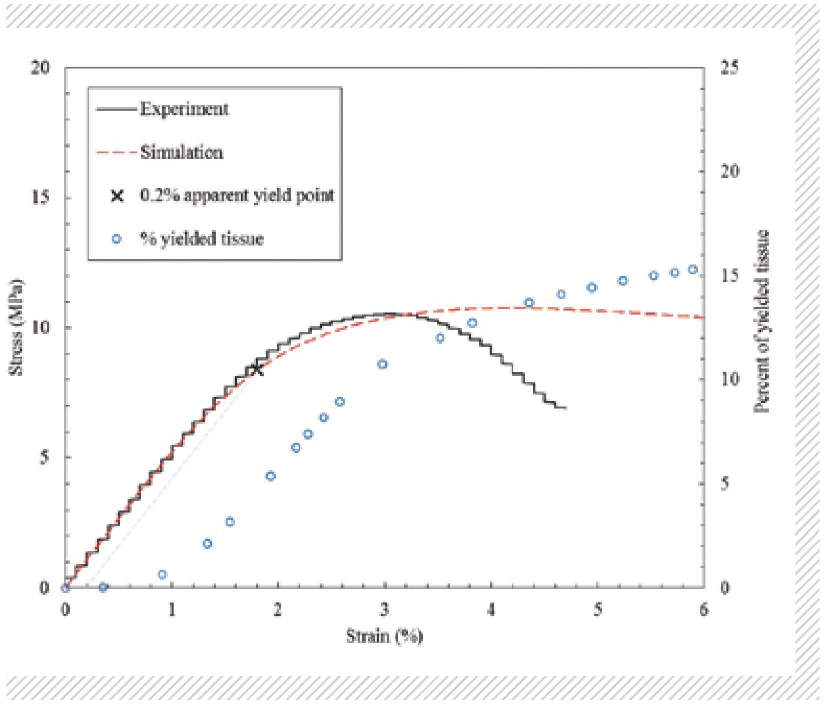
FIGURE 2: Distribution of stress in a trabecular bone sample under compression.

WHY BLUE WATERS

Our simulations involved a large number of finite elements, material, and geometric nonlinearities, along with complex contact conditions which made the numerical analysis challenging, even on the latest HPC platforms. The model analysis was performed utilizing up to 256 CPU cores and the large memory capabilities of Blue Waters. It has been recently shown that the similar multifrontal solver had enough scalability and robustness to perform computations on large ill-conditioned FE analysis problems on many thousands of CPU cores [5], thus potentially opening the door for future higher fidelity and complexity simulation studies in biomechanics.

NEXT GENERATION WORK

We plan to extend our modeling to a whole-bone level with the aim of building a patient-specific predictive tool for clinical use capable of assessing bone quality and bone response under loading. Once the model is established for healthy bone, bones



affected by diseases like osteoporosis, or diabetes and also aged bone will be modeled to better understand how the properties of bone are affected by various factors, assess effects of medications and to predict risk of bone fracture for patients.

PUBLICATIONS AND DATA SETS

Koric, S., F.A. Sabet, O. Jin, I. Jasiuk, Direct numerical simulation of bone plasticity and strength. *International Symposium on Plasticity*, Keauhou, Hawaii (2016).

Sabet, F., et al., Hierarchical modeling of plasticity and strength of trabecular bone, *XXIV ICTAM*, 21-26 August (2016) Montreal, Canada.

FIGURE 3: Prediction of stress-strain behavior of trabecular bone under compression along with percent of yielded tissue.

NANOSCALE ELECTRONIC DEVICES WITH NEMO5

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EXECUTIVE SUMMARY

Relentless downscaling of transistor size has continued according to Moore's Law for the past 50 years. According to the International Technology Roadmap for Semiconductors (ITRS), transistor size will continue to decrease in the next 10 years, but foundational issues with currently unknown technology approaches must be pursued. The number of atoms in critical dimensions is now countable. As the materials and designs become more dependent on atomic details, the overall geometry constitutes a new material that cannot be found as such in nature. NEMO5, the software package developed by the Institute for Nanoelectronic Modeling (iNEMO), is designed to comprehend the critical multi-scale, multi-physics phenomena through efficient computational approaches and to quantitatively model new generations of nanoelectronic devices including transistors and quantum dots, as well as to predict novel device architectures and phenomena [1,2].

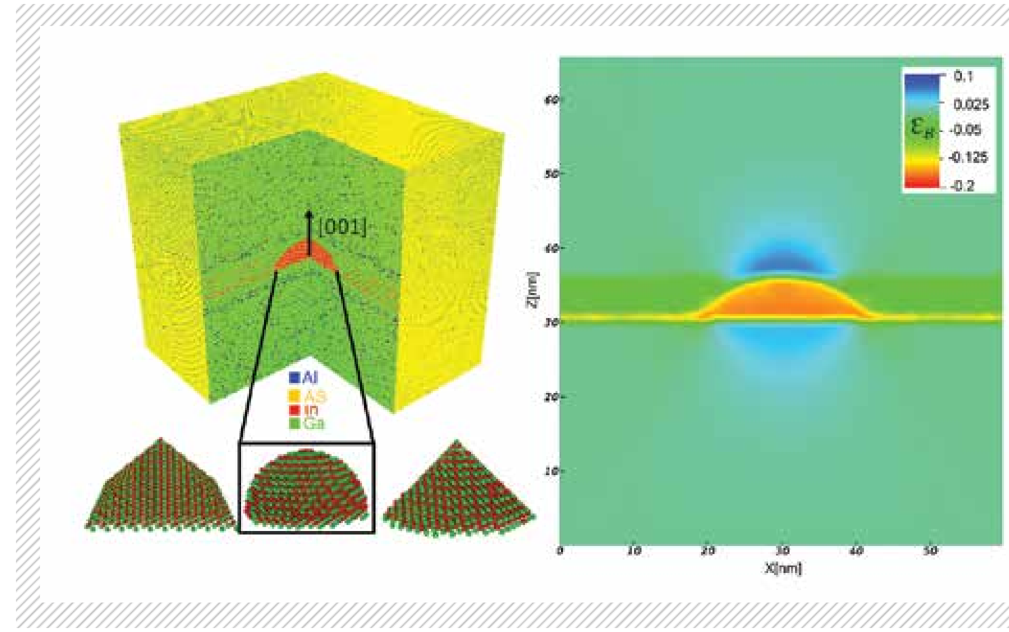

FIGURE 1: NEMO5 can simulate alloys such as this AlGaAs/InGaAs quantum dot system. On the left is the atomistic structure of a simulated 10 million atom system. The right shows the biaxial strain distribution dome-shaped quantum dot of size 20 nm by 5nm. Strain calculations are one of the first steps toward ensuring accurate treatment of the electronic qualities of devices.

INTRODUCTION

The U.S. is a market leader in the semiconductor industry, which produces many high-paying, high-technology jobs. The U.S. semiconductor industry is one of the nation's largest export industries, and the U.S. holds one-third of the global semiconductor device market worth over $300 billion. Simultaneously, the end of Moore's Law scaling as we know it will be reached in 10 years, with devices expected to be about 5 nm long and 1 nm in their critical active region width. Further improvements in shrinking dimensions will come only through the detailed study of device designs, materials, and of quantum effects such as tunneling, state quantization, and atomistic disorder. Fundamental questions remain about the downscaling of the CMOS (complementary metal–oxide–semiconductor) switch and its eventual replacement. What is the influence of atomistic local disorder from alloy, line-edge roughness, dopant placement, and fringe electric fields? How do lattice distortions due to strain affect carrier transport in nanometer-scale semiconductor devices such as nanowires, finFETs, quantum dots, and impurity arrays? Can power consumption be reduced by inserting new materials and device concepts?

NEMO5 is developed and used by the Institute for NanoElectronic Modelling (iNEMO) at Purdue to address these fundamental questions on a variety of semiconductor devices. Besides enabling basic engineering, physics, and materials science research, NEMO5 is used by leading semiconductor firms to design future devices. The source code, binaries and support for academic use are available through nanoHUB.org.

METHODS & RESULTS

iNEMO's research on Blue Waters encompasses simulations of incoherent scattering effects on tunnel FET devices, time-resolved quantum transport, a compact model for self-assembled quantum dot heterostructures, and a multiscale approach for nitride-based light emitting diodes.

The current mechanism of tunneling field effect transistors (TFETs) is through interband tunneling rather than thermionic emission in typical MOSFETs (metal-oxide semiconductor field-effect transistors). Tunneling from the valence to conduction band has the potential to yield significantly improved subthreshold slopes to allow lower supply voltages and better efficiency than MOSFETs. Electron transport through the overall device, including the source and drain, entails significant amounts of computationally demanding scattering, which cannot be ignored in realistic device performance predictions, and these simulations agree well with experimental resistivity data. In an ultra-scaled silicon TFET, simulation also found that incoherent scattering has a significant impact on performance.

Time-resolved quantum transport data allow more accurate calculation of energy/delay device