DEEP LEARNING FROM NATURE AND MACHINES: FRACTURE AND FATIGUE OF ENGINEERED AND BIOLOGICAL MATERIALS

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Abstract
This plenary lecture will provide an overview of recent research illustrating how biomimetics, experiments, computational modeling and physics-informed machine learning algorithms synergistically provide unique insights into the deformation, fracture and fatigue characteristics of diverse classes of engineered and biological materials. Specific examples and applications considered here include: fracture and fatigue of compositionally graded nanostructured metals; metallization of diamond by engineering its elastic strain and fracture at nanoscale for applications in microelectronics and energy storage; deformation, failure and fatigue characteristics of human red blood cells with implications for clinical manifestations and human diseases; and design of plant-based materials for self-actuating soft robotics and as substrates for flexible electronics.

1. Introduction
Many approaches to the design and development of materials with unprecedented properties and performance characteristics have been demonstrated in recent years through advances in nanotechnology, multi-scale mechanical testing, computational simulations, biomimetics and machine learning. These advances offer unique and new avenues for mechanistic understanding of the mechanics of deformation and fracture, design of materials for industrial applications, and improving clinical outcomes in the treatment of human diseases. This work integrates experimental studies of mechanical properties, microfluidics, large-scale computational simulations, and multi-fidelity analyses of neural networks to develop mechanistic insights into deformation, fracture and fatigue of materials. The presentation will focus on a variety of examples of how multi-disciplinary perspectives from materials science, engineering, computer science, physics, plant science, and medical science can be combined to design and produce materials with unprecedented properties and performance newer of interest and relevance in structural, functional, and biomedical applications. Specifically, the topics covered include: tailoring the fracture and fatigue responses of nanostructured metals through compositional gradation; partial to complete metallization of nanoscale diamond through elastic strain engineering and fracture suppression to modulate its bandgap and potentially enhance its performance in microelectronics and energy applications; fabrication of plant-based natural materials for applications in soft robotics and environmentally sustainable consumer products; and biorheology, deformation, failure and fatigue of human blood cells and their connections to clinical data in the context of disease diagnostics and treatment.

2. Results
Through a combination of nanomechanical to macro-scale mechanical experiments, microfluidics, computational simulations, as well as structural, functional and biological characterization of materials, and/or multi-fidelity machine learning algorithms predicated on physics-informed neural networks, the following observations have been made:

a. Employing a multifidelity approach to train deep-learning algorithms (1), a general framework has been developed to extract the elastoplastic stress-strain response of metals and alloys from instrumented indentation to achieve improved accuracy in mechanical characterization, especially for thin films and 3D-printed structures.
b. Mechanical deformation experiments (2) conducted on nanoscale monocrystalline and polycrystalline diamond needles inside a nanoindenter have led to the discovery of ultralarge reversible elastic deformation with maximum local tensile strains of about 9% prior to the onset of fracture. By recourse to first principles calculations, finite-element analyses and machine learning, it has been established (3) that metallization and indirect-to-direct bandgap transitions can be activated without phonon instability.

c. Using a process similar to that employed for soap-making, hard plant pollen can be transformed into a soft microgel which can then serve as a building block for the fabrication of plant-based materials for a variety of eco-friendly applications (4). With this plant-based material as a substrate, a wide variety of geometrical features can be purposely designed using digital printing techniques to customize hygrophobicity and complex shapes (5). Such digital printing of shape-morphing natural materials provides a flexible means to create soft robots and substrates for flexible electronics (5).
d. Combining microfluidic experiments with physics-informed neural networks, a general platform for microaneurysm-on-a-chip and artificial intelligence velocimetry has been developed to quantify the three-dimensional fields for blood flow in physiology and for diabetic retinopathy (6).
e. The biomechanics of the human spleen and its implications for hereditary blood disorders have been studied using a variety of experimental and computational tools (7). Specifically, how human red blood cells navigate through the most stringest mechanical deformation in the spleen is linked to clinical observations in different hereditary blood disorders.
f. With a general microfluidics platform in which amplitude-modulated electrodeformation induces static and cyclic deformation, mechanical fatigue of human red blood cells has been investigated (8). Fatigue of RBCs leads to significantly greater loss of membrane deformability, compared to static deformation under the same maximum load and maximum-load duration. This study has identified unique effects of cyclic mechanical deformation on the properties and function of biological cells, and provides a pathway to quantify the mechanical integrity and damage arising from repeated stretching of RBCs in blood circulation (8).

3. Conclusions

The case studies and examples presented in this lecture illustrate how biomimetics, experiments, computational modeling and machine learning can be combined to elucidate the deformation, fracture and fatigue characteristics of a wide variety of engineered and biological materials with applications in materials and structural engineering, plant science and biomedicine.

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