Organic inspiration

Dr Vikas Tomar recounts how a complex combination of modelling systems and quantum mechanics has helped bring about important advances in his field of materials failure

What are interface mechanics and how are multiphysical issues affecting their utility?

A basic premise in structures and materials research is to join two disparate materials/structures to form new and improved ones, and most of the time it works. When it doesn't work, results are often catastrophic.

My research deals with analysing the effect of interfaces on material failure properties. These analyses focus on the effects of interface construction on material and structural failure mechanics as a function of temperature and the chemical environment. Such analyses invariably involve an understanding at the interface of thermal, chemical, electrical and mechanical properties as these issues are invariably coupled with each other. They can be summarised as 'interface multiphysics'. Examples are materials in the core of nuclear reactors, or naval materials affected by stress-corrosion cracking.

Interfaces in nanostructures occupy an order of magnitude higher volume than conventional everyday materials and their influence in determining structure and material response is therefore significant. Overall, measurements focus on interfacial failure and multiphysical properties at a single interface level as well as for collective sets of interfaces in various arrangements at different length scales.

How do these problems feed into your overall objectives?

A material interface is a location where separately orientated crystal lattices join each other. The overall objective of my lab is to understand how the electronic, lattice vibrational and lattice translational (straining) properties of a single crystal are affected by the formation of an interface. The underlying emphasis is on finding common denominators that fundamentally influence the material behaviour in the problems highlighted earlier. Our hope is to use such an understanding to evolve new principles and new interface modifying paradigms for technological advances.

You draw from quantum mechanics, molecular modelling and continuum modelling. How do they factor into your experiments?

Quantum mechanical modelling, especially the use of *ab initio* molecular dynamics methods, has helped me significantly in understanding multiphysical properties of organic and inorganic material interfaces.

Lattice vibrational properties analysed using classical molecular dynamics methods has helped me significantly in understanding nanoscale interfacial interactions and interface arrangement issues that influence material properties.

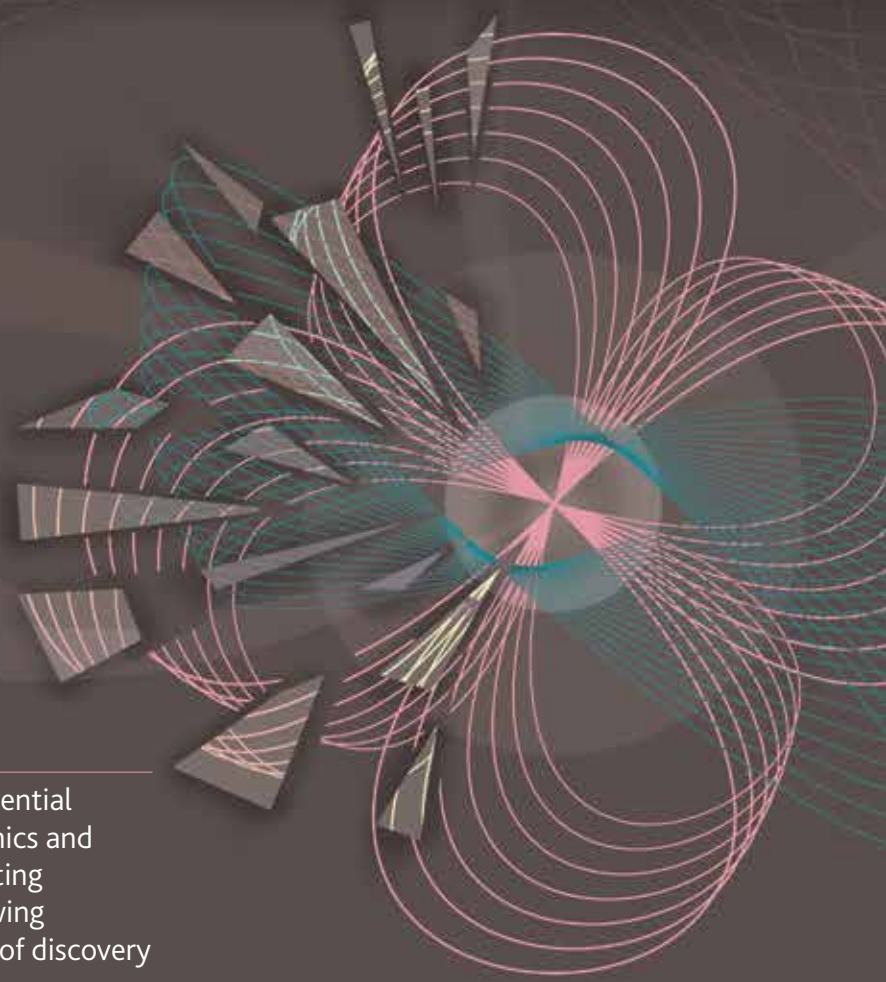
Lattice translational properties which relate to material deformation behaviour and flow of defects across both time and distance involve the use of molecular as well as continuum models.

Does a multidiscipline approach present and benefits or potential pitfalls

The use of three different scales in my research programme is quite a challenge. I try to use pre-existing methodologies in quantum mechanical and classical molecular modelling domains unless my work specifically needs a new approach. The bulk of my model development approaches are centered on how classical molecular information can be used to reveal new mechanisms at continuum levels. A lot of research work has gone into showing novel properties at the nanoscale but instances where these actually result in a real mesoscale material property can be counted on my fingers.

Why is there a need to combine quantum mechanics and experimental methods? Could you elaborate on what you have gained from this merger?

Most classical models can be used to interpolate between experimentally known data points but when these are used for extrapolation from experimentally validated behaviour, their predictions are considered untrustworthy. The ability to extrapolate from experimentally known data points therefore gives quantum mechanics a definite edge. Another benefit that quantum mechanical models have over other known approaches is an ability to 'most correctly' model multiphysical behaviour due to their ability to resolve electronic properties, lattice vibrational properties and lattice translational properties in a single setting. Our experiments are costly both in terms of money and time. We therefore need quantum mechanics to extrapolate our data. We then use classical molecular models and continuum mechanical models for interpolation and interpretation.



Material meltdown

Understanding why manmade materials fail is essential to bettering future efforts in engineering, electronics and multiplicity of fields. For **Purdue University**, exciting developments in materials failure analysis is allowing scientists to take bioengineering into new realms of discovery

SINCE THE EARLIEST technological breakthroughs, human beings have looked to nature as a source of inspiration. Today, materials are developed to create structures ranging from the macro- to the nanoscopic with physical properties often derived from the desired qualities found in natural substances. Typically, biomaterial engineering of hard materials looks for organic archetypes of strength and resilience in order to manufacture biomimetic structures capable of withstanding large amounts of stress and strain, while other biomaterials have a wide variety of applications in healthcare. Sometimes, however, they do not perform as expected. Analysing the causes of failure is vitally important for developing new biomaterials and improving those that already exist.

Studying the processes at play between the interfaces of composite layers in biomaterials is integral to understanding the multiphysical properties that determine the formation of a structure as well as its failure. To do this, Dr Vikas Tomar has combined a quantum mechanical and experimental study of interfacial biomaterial mechanics to measure how the properties of single crystals are affected by the formation of an interface.

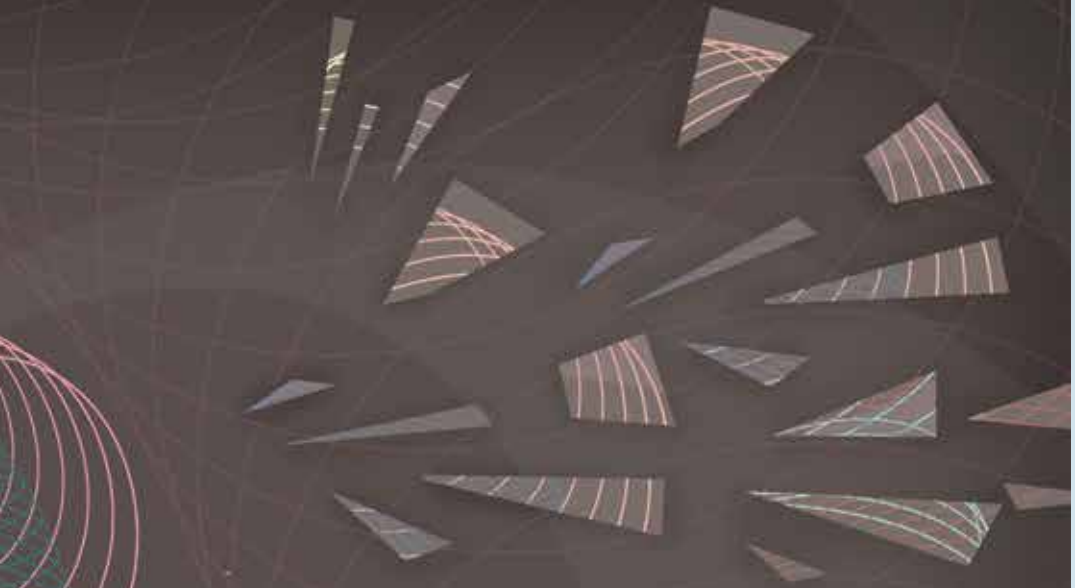
A tenured Associate Professor at Purdue University's School of Aeronautics and Astronautics and Director of the school's Interfacial Multiphysics Lab, Tomar is the recipient of five awards including the American Society of Mechanical Engineers (ASME) Materials Division 'Orr' Family Award for excellence in failure of materials research. Collaborating with Professor Aman Haque of the Department of Mechanical and Nuclear Engineering at Pennsylvania State University and funded by the US Department of Energy (DoE) Basic Energy Sciences, Tomar's lab has developed an exciting new method of measuring multiphysical properties.

MODEL DEVELOPMENT

Energy is created in the vibrations of the crystal lattice which, in turn, dictates the formation of defects in the materials of interest. These 'defects' are also the desired properties that inspire the engineering of biomaterials. Wishing to understand how the interfaces of composite layers contribute toward a material's defects has led Tomar to study the chemomechanics of these biological interfaces and their mechanical behaviour overall. Of particular interest are bone, nacre and more recently, sea-sponge spicules. These hard biomaterials have exactly the qualities that bioengineers are eager to emulate in the lab: rigidity and durability.

Nacre, for instance, is 3,000 times tougher than its mineral constituent and therefore an obvious focal point for research. Bone is an exemplar of how these properties are successfully twinned despite their contrary nature. As Tomar explains: "Bones need to be stiff to prevent bending but they must also be tough since they should not break catastrophically even when the load exceeds the normal range". This unusual combination has long piqued the interests of researchers in biomaterials though the high level of damage tolerance in the silica of sea-sponge spicules is a relatively new discovery.

As several dimensions are involved in the overall mechanics of the interfacial effects on a crystal lattice, an approach combining different theoretical formulae is required in order to extrapolate trustworthy information from the datasets. In order to lessen the difficulties involved in performing nano- and microscale experiments that require expensive simulations to elucidate the results, Tomar has taken a novel approach to using the existing models. "I have developed two different variants of classical molecular simulation models referred to as the hybrid Monte Carlo method", he explains, a combination of techniques that couples continuum mechanical and classical molecular models. Using these methods, Tomar's lab has published the first paper demonstrating how mechanical stress and thermal conductivity in silicon



simultaneously varies due to the translational properties of the crystal lattice.

IMPROVING IMAGING

Although previous attempts at using quantum mechanical models to change the interface behaviour in tropocollagen-hydroxyapatite initially proved to be a fruitless exercise it eventually led to the development of an innovative imaging tool. Having proceeded as far as employing quantum simulations, a measuring technique that could validate the calculations and enable trustworthy extrapolation did not present itself; the problem lied in the limited abilities of the vast majority of tools set up for taking nano- and microscale measurements. These measurements restrict the user to examining one property of interest at a time while the overall mechanics of the multiphysical properties are inextricably linked.

The advantages afforded to the field of materials failure by spectral tomography is likely to be huge

Advances have been made elsewhere in imaging technology such as with nanomechanical Fourier transform infrared spectroscopy (FTIR), but developments like these only seek to analyse the structures of a single property in new ways. Along with the multiphysical transmission electron microscopy (TEM) tool developed by Haque, Tomar's lab has created an instrument capable of measuring two properties simultaneously by taking into account the structural details influencing their functions. With its theoretical foundations based in spectroscopy this technique has been dubbed spectral tomography. "Using two complementary and competing methods, we are now able to understand origins of multifunctionality," states Tomar. Currently in the process of submitting patents for this innovative tool, the advantages afforded to the field of materials failure by spectral tomography is likely to be huge.

In 2011 the research group used a classical molecular simulation to predict the state of thermal diffusivity in biomaterials. Whereas inorganic materials generally store more heat the more it is applied, Tomar's simulation found that biomimetic materials responded unusually to increased heat with greater thermal diffusivity, that is, more heat was conducted through the material than trapped inside. Recently, Tomar validated the predictions of this strange behaviour when spectral tomography arrived at the same conclusions.

ROOM FOR INNOVATION

The infancy of this discipline is evident as the potential to take it in pioneering directions is proving strong. Although the results of this work are only now appearing, many of the findings have proved significant. Despite dominant theories among multiscale mechanics taking strength for granted as the driving force behind biomaterial structural evolution, it has recently become apparent that lattice translation has a far greater role to play. As Tomar states: "It may be strain that is guiding everything".

As the field opens up and disciplines like bioinformatics begin to be used in combination with novel methods of modelling and experimentation, a greater degree of accurate predictions to become possible and with them an increase in the chances of making new discoveries. What has become evident after his presentation at this years' Materials Research Society meeting in Boston, Massachusetts, is that the innovations Tomar has brought to materials failure analysis concerns more than just the bioengineers. With nanotechnology making its way into everyday use, issues of interfacial multiphysics could soon be an area that affects us all.

A COMBINED QUANTUM MECHANICAL AND EXPERIMENTAL STUDY OF INTERFACIAL BIOMATERIAL MECHANICS

OBJECTIVES

To measure interface stresses in biomaterials and tailor those using quantum mechanics suggested functional groups.

KEY COLLABORATOR

Aman Haque

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VIKAS TOMAR earned his Bachelor's from the National Institute of Technology (India) and his Master's from the Indian Institute of Technology and the University of Stuttgart (Germany). He later received his PhD from the Georgia Institute of Technology. Tomar came to Purdue from the University of Notre Dame, where he was an Assistant Professor. Tomar is now Associate Professor in the School of Aeronautics and Astronautics and his research focuses on modelling and experimentation development to measure interface stresses and thermal properties as a function of temperature, environment and chemistry in biomaterials, biomimetic materials and complex ceramic as well as metallic composites. Tomar has developed a variety of multiscale methods (hybrid Monte Carlo method for non-equilibrium molecular dynamics, equivalent crystal method, stochastic cohesive finite element method). He has also developed a spectral tomography technique to measure interfaces stresses. Based on such developments, his work has provided new insights into interface dependent mechanical and thermal behaviour of a range of biomaterials and composites.

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