# 1 Career 2016

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### 

## 1.2 Tasks

### 1.2.1 T.3 Things to do Haneesh:

1. ~~Email Wenqiang and ask for input to construct the current achievements for the section~~ [~~(iii) Results from Prior NSF Support~~](#h.3pm0x94ma1o7)~~.~~
2. ~~Prepare Task Biographical Sketch for Max.~~
   1. ~~Read Biographical sketch requirements from GPG~~
3. Read the ARO proposal.
   1. Introduction to Phase field modeling.
4. Read previous CAREER proposal.
5. Take images from your own paper.
6. Send email to Douglas asking for the Letter from Larry.
   1. Send last years letters.
7. Send the CMMI program information to Priscilla.
8. Contact Sci-Toons
9. Contact Leadership Alliance

### 

### 1.2.2 T.1 Things to do Kaushik:

*(Strike out completed tasks)*

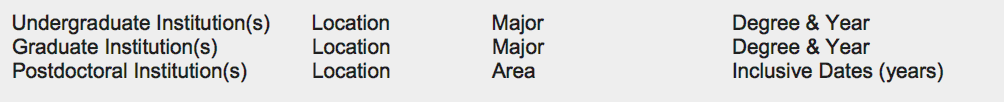
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### 1.2.3 T.2 Things to do Max:

1. Prior NSF Support
   1. ~~Create a new latex file for the Project Description Document (PDD) in~~ [~~ProjectDescriptionFolder~~](https://drive.google.com/open?id=0BzvB0ovUAchRWGlNT05lQUtfLVE) ~~folder in Google drive folder~~ [~~CAREER2016~~](https://drive.google.com/open?id=0BzvB0ovUAchReDBPd2xIMVJZdm8)~~. You can use the latex template from the latest NSF proposal we wrote:~~ [~~SurfaceInstabilities~~](https://drive.google.com/open?id=0BzvB0ovUAchRQ0cwZGxjdXZkQ2M) ~~(also in Google drive).~~
   2. ~~In PDD construct the section “Results from Prior NSF Support”~~[~~.~~](#h.3pm0x94ma1o7) ~~The guidelines for this section can be found in~~ [~~(iii) Results from Prior NSF Support~~](#h.3pm0x94ma1o7) ~~section of this document. These instruction were taken from the~~ [~~gpg document~~](https://drive.google.com/open?id=0BzvB0ovUAchRYUJiTUh2T0luZXM)~~, p. 22.) Some of the info needed for composing can be found~~ [~~here~~](#h.s3rhnkpflgmj)~~. Some example prior support sections from can be found in~~ [~~ExamplePriorSupport~~](https://drive.google.com/open?id=0BzvB0ovUAchRQ0J0NENJNkRUMjg)~~. (Prof. Powers section does not adhere to the guidelines very strictly.)~~
   3. ~~Keep Prior NSF Support less than 1 page~~
2. Biographical sketch.
   1. ~~(The phone number is correct. Address is correct. )~~
   2. ~~Move the post doctoral training information from section “~~**~~(b) Appointments~~** ~~to~~ **~~“(a) Professional Preparation”.~~** ~~The format should be as follows.~~



~~For format should be as shown below.~~

~~Further information about the format can be found on p. 24 of the~~ [~~gpg document~~](https://drive.google.com/open?id=0BzvB0ovUAchRYUJiTUh2T0luZXM)~~.~~

|  |  |  |  |
| --- | --- | --- | --- |
| ~~Indian Institute of Technology Guwahati~~ | ~~Guwahati, India~~ | ~~Mechanical Engineering~~ | ~~B.Tech, 2005~~ |
| ~~Stanford University~~ | ~~Stanford, CA, USA~~ | ~~Mechanical Engineering~~ | ~~M.S., 2007~~ |
| ~~Stanford University~~ | ~~Stanford, CA, USA~~ | ~~Mechanical Engineering~~  ~~(Mechanics and Computation)~~ | ~~Ph.D., 2011~~ |
| ~~Brown University~~ | ~~Providence, RI, USA~~ | ~~Theoretical and Computational Solid Mechanics~~ | ~~2011–12~~ |

* 1. ~~Remove post-doctoral training information from “~~**~~(b)~~****~~Appointments”.~~**
  2. ***~~“(c) Products”~~***
     1. ~~Add in the following paper between current items no. 1 and 2 in “~~***~~(c) Products~~****~~, Products most Closely Related~~***~~”~~**

*~~Stout, David A., et al. "Mean deformation metrics for quantifying 3D cell–matrix interactions without requiring information about matrix material properties." Proceedings of the National Academy of Sciences 113.11 (2016): 2898-2903. (include DOI)~~*

~~This will bring the total no. of “~~*~~Products Most Closely Related” to 5.~~*

* + 1. ~~Add in the following paper between current items no. 1 and 2 in “~~***~~(c) Products~~****~~, other significant products~~***~~”~~**
* ~~Eric Chason, Fei Pei, Cylde L Briant, Haneesh Kesari, and Aallan F Bower. “Significance of Nucleation Kinetics in Sn Whisker Formation”. In:~~ *~~Journal of Electronic Materials~~* ~~43.12 (2014), pp. 4435–4441.~~

~~This will bring the total no. of “~~*~~Other Significant Products”~~* ~~to 5.~~

* + 1. ~~Ensure that the bibliography style for all entries is the same. Some more guidelines: gpg, p.24, “Include names of all authors, date of publication, title, volume, issue, pages, DOI, ”~~
  1. **~~“(d) Synergistic activities”~~**

~~From gpg. p. 24,~~

*~~development of curricular materials and pedagogical methods); contributions to the science of learning; development and/or refinement of research tools; computation methodologies, and algorithms for problem-solving; development of databases to support research and education; broadening the participation of groups underrepresented (Horacio, ) in STEM; and service to the scientific and engineering community outside of the individual’s immediate organization.~~*

* + 1. ~~In “1. Journal article reviewer for” add the following three journals~~
       1. *~~Annals of Biomedical Engineering~~*
       2. *~~International Journal of Fracture~~*
       3. *~~Scripta Materialia~~*
    2. ~~Include new item in Synergistic activity:~~ *~~Faculty research mentor/advisor of students who belong to (African American (Brian Williams, Summer 2015 ) and Hispanic (Horacio Ferrandiz,~~* ~~Fall 2014~~*~~), Vineeth (2015, Summer)) underrepresented groups in STEM fields.~~ ~~Specifically the PI’s has participated in the following activities:~~*
       1. *~~Faculty advisor for the Undergraduate Teaching and Research Awards program at Brown (2013–16).~~*
       2. *~~SPIRA, annual four week summer camp hosted at Brown for high-school age girls on STEM topics (2015–16).~~*
       3. ~~Faculty observer for the Reginald D. Archambault Award for Teaching Excellence, Brown University, (2015). This award program aims to train graduate students in teaching high school age students in STEM subjects.~~
    3. ~~Include new item in Synergistic activity:~~ *~~Extra curricular teaching activities~~*
       1. ~~Faculty instructor for the course:~~ *~~Material Science and Engineering: where would the world be without it, (2015). This course is aimed at high school age students.~~*
       2. *~~Instructor for Summer Institute for Middle School Teachers, Stanford, 2007, 2008~~*
       3. *~~Instructor for National Hispanic University Workshop, Stanford, 2007~~*
    4. ~~Include new item in Synergistic activity:~~ *~~Organization of the Society of Engineering Science, Annual Technical Conference, 2013~~*
       1. *~~Judge for the student paper competition in the Structures/Solids track that was organized as part of the SES Annual Technical Meeting 2013.~~*
       2. *~~Member of local organizing committee, SES Annual Technical Meeting 2013.~~*
  1. **~~Graduate thesis Advisees.~~** 
     1. ~~Change~~ *~~Total~~* ~~from 1 to 2.~~
     2. ~~Add in Jarod’s Name after Tianyang Zhang’s name.~~

***Stopped Here***

1. Budget.

a. ~~Cover Sheet~~: ~~(~~priscilla and Douglas will handle this~~)~~

b. Project Summary

c. ~~Table of Contents~~ (automatically generated)

d. Project Description

Broader Impacts

e. References

~~f. Biographical Sketches~~

g. Budget and Budget Justification

h. ~~Current and Pending Support~~ (priscilla and Douglas will handle this)

i. Facilities, Equipment, and Other Resources

j. Special Information and Supplementary Documentation

#### 

Data Management Plan

~~Postdoctoral Mentoring Plan.~~ (Let’s not ask for a postdoctoral scholar)

**d. Project Description**

### 1.2.4 Biographical Sketch-Guidelines

* + – Two pages
  + – Senior personnel – *Haneesh Kesari*

### 1.2.5 Results from Prior NSF Support-Guidelines.

~~The following information should be provided.:~~

1. ~~The NSF award number, amount and period of support;~~
2. ~~The title of the project;~~
3. ~~A summary of the results of the completed work, including accomplishments, supported by the award. The results must be separately described under two distinct headings: Intellectual Merit and Broader Impacts; (ask Wenqiang to prepare the~~ *~~Intellectual Merit~~* ~~part of this,~~~~)~~
4. ~~A listing of the publications resulting from the NSF award (a complete bibliographic citation for each publication must be provided either in this section or in the references cited section of the proposal);~~ if none, state “No publications were produced under this award”
5. ~~Evidence of research products and their availability, including, but not limited to: data, publications, samples, physical collections, software, and models, as described in any Data Management Plan; and~~
6. ~~If the proposal is for renewed support, a description of the relation of the completed work to the proposed work~~

~~Reviewers will be asked to comment on the quality of the prior work described in this section of the proposal. Note that the proposal may contain upto five pages ti describe the results. Results may be summarized in fewer than five pages, which would give the balance of the 15 pages for the Project description.~~

#### ~~1.2.5.1 Results from Prior NSF Support: Info~~

~~Title: "~~*~~Emergence of New Properties at the Large-Scale on Elastic Surfaces due to Small-Scale Adhesion and Waviness~~*~~"~~

~~Sponsor: NSF~~

~~Award No. (FAIN): CMMI-1562656~~

~~Award Date: March 3, 2016~~

~~Managing Division Abbreviation CMMI~~

~~Grant amount: $375,000~~

~~Start date: March 1 , 2016~~

~~End date: February 28, 2019.~~

# 

Theoretical mechanics and phase field computational tools for the 3D architectural design of tough, bio-inspired, interface dense materials.

1. ***Research objective***

***Research objective***: To derive new knowledge (theoretical and experimental) and develop the computational capability to discover, and understand new toughening and strengthening mechanisms in interface dense materials and to model them through the formulation of new, predictive micromechanics theories.

## *1.3 Introduction*

As we continue to build higher, travel faster, and live more sustainably, we also must search for new materials that are lighter, stronger, and tougher. While strength–or the ability to bear the largest load–may appear to be the most crucial property, in many cases, toughness is actually more desirable. Specifically, in applications in which safety or reliability is paramount (e.g., bridges, turbine engines in aircrafts, or XXX), the best material is the one whose ability to carry loads is minimally affected by damage or wear-and-tear accumulated through use. For example, no matter how strong a bridge is, it would not be reliable if it were to fail catastrophically without any warning signs. Rather, small amounts of cracking or deformation of its components should not drastically reduce the bridge’s load carrying capacity. Consequently, the damaged components can be identified, and either be replaced or repaired before they lose complete functionality.

A material’s ability to impede the growth of cracks or defects is captured by its toughness properties. When a crack is created in a tough material, such as ductile steel, that material’s ability to carry loads is not drastically reduced. Furthermore when the crack does propagate through the material is does so in a steady, controlled manner. On the other hand, the load carrying capacity of brittle materials, like glass, is highly affected by the presence of defects or flaws. While these materials tend to be strong, they typically fail through abrupt, catastrophic fracture during which cracks propagate in an uncontrolled manner.

In most engineering materials, from steels to ceramics, strength and toughness are mutually exclusive. That is, there are few materials that are both strong and tough. Recently, however, it has been shown that some structural biomaterials (SBs) possess both high strength and high toughness. In many cases, SBs are heterogeneous, and consist of a ceramic and an organic phase mixed together in intricate 3D patterns at the micrometer scale. The way that these two phases are interlaced–what is known as the SB’s architecture–is extremely complex compared to architectures typically seen in engineering composites, such as XXX. Some examples of architectures seen in SBs are the brick-and-mortar arrangement of ceramic tablets in shells, and the interlocking helices in the club-like appendage of the mantis shrimp (see Figure XXX). Since these SBs are characterized by the numerous, intricately arranged interfaces between the ceramic phases, we refer to them as interface dense SBs, or *id*-SBs.

While *id*-SBs are often composed of >95% brittle ceramic material by volume, they have been shown to possess extraordinary toughness properties while being able to maintain both strength and stiffness. For example, the total energy dissipated during the fracture of nacre has been shown to exceed that of its constituent ceramic material, aragonite, by three orders of magnitude. Synthetic variants of *id*-SBs have been produced in an attempt to further investigate the connection between architecture and toughness. New fabrication methods, such as ice templating and slip casting, have been developed in order to produce these synthetic *id*-materials. Recently, a parametric study of toughness properties was performed on a synthetic nacre. This *id*-material consisted of alumina tablets arranged in a brick-and-mortar architecture separated by thin layers of poly(methyl methacrylate); a weak, compliant polymer. The aspect ratio of the tablets and extent to which adjacent tablets overlapped (see Figure XXX) were varied and the material’s toughness properties were measured. It was found that the energy dissipated during fracture (i.e., the work of fracture) could be changed by tuning these architectural parameters. Specifically, with the right choice of aspect ratio and tablet overlap, the work of fracture could be enhanced by up to XXX% over that of monolithic alumina.

The incredible toughness of *id*-materials arises from the large number of weak interfaces and intricate architecture of these interfaces within the material. It is believed that the tremendous amount of interfacial area and the interfaces’ 3D geometry is the key to an *id*-material’s incredible toughness. However, the question of how the architecture and toughness are connected still remains open. Some of the enhancements to the *id*-materials’ toughness properties have been explained using classical toughening mechanisms such as crack bridging, frictional pull-out of fibers or lamellae, or plastic dissipation at the interfaces caused by failure of sacrificial bonds (REF artful interfaces in biological materials, Fratzl 2011). These mechanisms reduce the stress concentration at the tip of a crack and also dissipate energy during crack growth, making it more difficult to propagate cracks. Theoretical mechanics models for *id*-SBs that incorporate these toughening mechanisms predict enhancements to toughness properties (e.g., work of fracture) of up to several hundred percent (REF barthelat vincent, currey, Kamat/ballarini 2000). However, they often do not amount to the toughness enhancements that are observed experimentally (REF currey). One explanation for this is that there could be a large number of toughening mechanisms operating in SBs that are not included in the models. However, it is also possible that what is being witnessed is not a myriad of well-understood mechanisms operating in concert, but rather a completely new mechanism.

Subsequently, molecular dynamics simulations (REF buehler) and large-scale computational micromechanics simulations (REF begley) have been used to identify new toughening mechanisms operating in *id*-SBs. However, these newly identified toughening mechanisms are often very specific to a particular *id*-SB architecture. For example, there are nano-scale asperities on the surface of aragonite tablets in nacre. It has been shown that these asperities cause frictional dissipation when adjacent tablets slide relative to one another. This frictional interaction can reduce the amount of energy available to propagate cracks. This mechanism would obviously not exist in *id*-SBs that do not possess either a layered tablet architecture or asperities between tablets. It is surprising that a toughening mechanism, which accounts for the majority of the observed toughness enhancement, is not shared among a broader class of *id*-SBs. While it is true that each *id*-SB architecture is unique, they share many common features, such as XXX. Therefore, it seems only natural to presume that there must exist some general toughening mechanism that would be shared amongst many different *id*-SBs. This kind of common mechanism would be similar to how dislocation motion is a common failure mechanism in metals. For this reason, the PI believes that there are important toughening mechanisms that are common to most *id*-materials that are still undiscovered.

Discovering new toughening mechanisms or determining which of the previously proposed mechanisms are the most important is quite challenging to do experimentally. This is because quantifying the extent to which different mechanisms are operating in an *id*-SBs requires information about the deformation and damage behavior of the interfaces. Since these interfaces are 3D, complex and internal to the material, it is difficult to directly visualize them. In the past, information about the interfaces’ geometry was obtained by taking multiple cross-sections of an *id*-SB and making inferences about the 3D geometry from these 2D slices (REF). While this method can be used to obtain geometric information, it cannot be used to obtain information about the deformation or failure behavior of the interfaces during mechanical tests. This is because cross-sectioning an id-material could change the extent to which certain toughening mechanisms can operate. Recently, micro-CT scanners have been used to visualize the interfaces of *id*-SB while mechanical tests were being performed. While this method appears promising, for researchers without direct access to a micro-CT scanner, investigating toughening mechanisms in *id*-SBs this way would be prohibitively expensive. Furthermore, some studies have revealed that the high energy x-rays emitted by CT scanners can embrittle the proteinaceous interfaces of *id*-SBs. This embrittlement may affect the extent to which some toughening mechanisms can operate in the material. This makes it difficult to determine which mechanisms are most important to an *id*-SB in its natural state. However, the fact that such expensive resources are being used to visualize the deformation and failure of interfaces in *id*-SBs highlights the importance of this information to the material-mechanics community.

We propose to develop and use a computational tool based on the phase field method (see Section XXX) to investigate toughening mechanisms in *id*-materials. Since the computational tool is still only a model for the real material, the spectrum of toughening mechanisms that it can capture is in some way limited. However, by comparing results generated using a preliminary version of this tool to experiments on *id*-SBs (see Section XXX), the PI believes that the proposed method has sufficient generality to serve as an investigative tool. Compared to existing computational tools (e.g., XXX), the assumptions underlying the proposed method are very basic and therefore it is able to capture a greater diversity of mechanisms. In the proposed computational tool the constituent materials fail in a brittle manner. Therefore failure events are restricted to two categories: 1) brittle failure of the ceramic phase, or 2) brittle failure of the interface. However, prior knowledge of crack trajectories is not assumed, and cracks within the material are allowed to evolve freely. This is a stark contrast to methods like XXX in which both the constituents’ failure behaviors and the anticipated crack paths are required as inputs. Hence, the proposed computational tool can be used to predict the direction of crack growth based on a material’s mechanical properties, architecture and loading (see Section XXX).

The proposed computational tool will first be used to investigate toughening mechanisms in *id*-SBs (see Section XXX). Consequently, based on the knowledge gained through this investigation, the computational tool will be used to develop new designs for engineering composites that possess similar toughening mechanisms as those observed in the *id*-SBs. In both cases, the interfaces in the material are both densely distributed and have complex geometries. Therefore, describing the configuration of the interfaces will likely require many parameters. When developing the new, *id*-SB inspired designs, we want to determine the values for these parameters that correspond to the material with the greatest toughness. Due to the sheer number of parameters, however, performing a full parametric study of the effects they have on the material’s toughness would be impossible. Furthermore, due to the size and dimensionality of this parameter space, it could be difficult to even determine sets of parameters that produce even modest enhancements to toughness. Therefore, it would be valuable to have reduced-order analytical theories that, although coarse, could model the toughening mechanisms in *id*-materials. While these theories would be less precise the computational tool, they could be used to quickly identify a region in the parameter space in which significant toughness enhancements can be attained. After using a reduced-order model to identify the region in the parameter space over which to search for beneficial architectures, the computational tool could be used to arrive at near-optimal designs with high precision (see Figure XXX). The PI proposes to use continuum mechanics theories and asymptotic analysis to derive suitable micromechanics theories to provide a rough characterization of the parameters’ effects on toughness. Preliminary efforts toward developing a micromechanics theory of toughness are presented in Section XXX.

1. ~~SBs are composites,or heterogeneous. Composites is an old word and does not do justice to the incredible complexity seen in SBs. They are best described as architectured materials.~~
   1. ~~Perhaps we need a figure showing the different types of biological materials systems. (shrimp, nacre, spicules, etc.). Point out that in all of them there is a brittle phase and a weak interface.~~
2. ~~We focus on the sub-class of materials in which the stiff phase is a mineral and there are exceedingly filled with weak-brittle interfaces . We term these materials id-materials.~~
   1. ~~We can give both synthetic and biological examples.~~
3. ~~Need to make the case that there is strong potential that these materials systems hide some incredibly ingenious, new physical mechanisms of toughening and strengthening.~~
   1. ~~Start with giving numbers showing that the toughness of SBs is much higher than that of their constituents (at least their brittle constituent). Nacre, bone, etc.~~
   2. ~~This is believed to be due to small-scale architecture. This is best highlighted by the experiments conducted on synthetic materials made by Ritchie’s group. Here we should give the examples of the materials made by Rob Ritchie’s group. They made different types of synthetic nacre (I think using freeze casting method) and show that small-scale architecture has an incredible impact on the large-scale toughness and strength of these materials.~~
   3. ~~These results are in violation of the rule of mixtures.~~
   4. ~~So, now we know that architecture is giving rise to the property enhancements. But the question remains as how? That is what are the mechanisms?~~
4. ~~Several researchers has investigated this question, starting with Curry, barthelot. Nacre and bone have been the most investigated materials. People have used molecular dynamics (Buehler, large scale computational micromechanics simulations (Matt begley)). A plethora of mechanisms have been put forward explaining the enhancement of toughness in SBs. However, in most cases there is no clear consensus as to which of those mechanism is the most important, or whether there even exists an important set as such. Furthermore, most of the proposed mechanisms are very specific to a particular SB. This is quite surprising to the PI. It is true that every SB is unique in its own way. However, based on the vast commonality in the underlying mechanical and architectural design of id-materials one would have presumed that there would exist at least some general mechanisms that would be common to most of the~~ *~~id~~*~~-materials. Such as dislocation motion being the general failure mechanism common to most metals. For this reason the PI believes that some important mechanisms that are common to most~~ *~~id~~*~~-materials are as of yet still unknown.~~
5. ~~Discovering new mechanisms or scrutinizing which of the proposed mechanisms are the most important is quite challenging to do experimentally. Scrutinizing the different mechanisms requires information about the deformation and damage behavior of the interfaces. Due to the highly intricate and 3D internal nature of the interfaces it is quite difficult to directly visualize the deformation or damage behavior of these interfaces. If the SBs are cross-sectioned then the mechanisms itself may change. Owing to this reason significant efforts has been directed in using~~ *~~in-situ~~* ~~mechanical testing of SBs inside a micro-CT scanner. However, this method is still under development and for most researchers would be prohibitively expensive. Furthermore, some studies reveal that the high energy x-rays cause artificial embrittlement of the SBs. The embrittlement would move the material’s deformation and damage mechanisms even further aways from those operating in the material’s native state. The fact that such expensive resources as micro-ct scanner, are being explored to visualize the internal deformation and damage in SBs highlights the importance of the material-mechanics community’s need for a method through which to visualize the SBs internal deformation. And it also highlights the fact that a considerable section of material-mechanics community still believes that some imp. failure mechanisms in SBs have still not been discovered.~~
6. ~~We propose to develop and use a computational strategy based on the phase field method (see XX for details. ) to investigate the imp. toughness enhancement mechanisms in id-materials. The computational tools we propose, fairly sophisticated though they might be, are still models of the real material. Therefore, it is natural to be skeptical about the investigative potential of the tool. However, based on the results that we generated using a preliminary version of the computational tool and their comparison with known experimental results we believe that the the proposed computational method has sufficient generality to serve as an investigative and discovery tool when supported with some basic information that can be generated through straightforward experiments.~~
7. ~~However, the computational model is based some very basic assumptions, and therefore are very general and allow for the possibility of different mechanisms to operate. The material and the interface failure is modeled to fail in brittle fashion. So, there can be essentially be two types of failure events, brittle failure of the mineral phase or that of the mineral-protein-mineral interface. The protein phase is not explicitly modeled. This leads to a phenomenal gain in computational efficiency. However, the model allows for unlimited freedom for evolution of the cracks networks.~~
8. ~~There is tremendous interest in discovering the origin of the SBs’ remarkable properties. This is despite the fact that traditional structural materials, such as steels, far outperform SBs mechanically. Because it is believed that combining the new mechanisms from SBs with modern synthetic materials and chemistry would lead to a new generation of structural materials whose qualities far exceed those of today’s state of the art. Even with the power of the proppsed computational tool, owing to the incredible number of degrees of freedom afforded by the complexity of the 3D weak interfaces, it is challenging to arrive at the optimal, or even satisfactory, material design using the computational tools alone. Therefore, it would be highly valuable to have reduced-order analytical theories that are coarsely, yet accurately, model the toughening mechanisms in id-materials.~~
9. ~~The mechanics theories, which will be quite imprecise compared to the computational tool, would yet, due to small number of parameters, quickly able to point roughly our the region in the parameter space where significant enhancement in enhancement can be attained. With the rom reducing the size of the parameter space over to perform the search, the computational tool can then be used to arrive at the final design with high precision (see Fig. xx). The PI would use continuum mechanics theories and asymptotic analysis to derive the micromechanics theories/reduced order models. Preliminary efforts in this direction are presented in section XX.~~

Specific research objectives

## 1.4 Motivation.

*As long as a branch of knowledge offers an abundance of problems, it is full of vitality.*

–David Hilbert

The goal of the proposed project is to generate new knowledge (experimental and theoretical) and computational capabilities for the discovery, understanding, and modeling of new toughening and strengthening mechanisms in *id*-brittle materials. As elaborated in section~\cite{NewMechanicsinIdMaterials}, experimental investigations on biological and bioinspired *id*-brittle materials show that there is high probability that these materials hide some very ingenious, hitherto unknown, mechanisms. The discovering of such mechanisms would in itself constitute valuable new scientific knowledge. However, the new mechanisms would also create plentiful new opportunities for the development of new mechanics theories. The PI himself plans to dedicate as part of his career in development such new mechanics theories. However, the new knowledge generated by this project is expected to be sufficiently broad and rich to stimulate/galvanize and aid/facilitate the generation of new knowledge by the wider mechanics community.

At his most optimistic, the PI hopes that these new opportunities to model new mechanisms/phenomena will re-vitalize and re-invigorate the theoretical mechanics community. The development, study, refinement, and expansion of the modeling and the mathematical aspects of such theories is expected to be an expansive and an enriching scientific endeavor.

However, it is likely that the reader might wonder as why the PI has selected to focus his career on *interface dense brittle materials. Surely, there must be other materials classes with similar or even greater potential for the discovery of new mechanisms, and consequent development of new mechanics theories.*

Well

it is might be useful to discuss as to why the PI plans to focus on the particular class

1. Technological progress strongly depends on our ability to meet humanity’s ever growing need for energy. Recently, this has led us to explore a number of new and innovative directions both in the production and the storage of energy. For example, solar energy production capacity in the United States has grown by nearly 700% in the last five years alone (REF SEIA). However, a number of energy production technologies, such as hydroelectric, natural gas, and coal implicitly rely on turbine engines. This is likely to hold true even for some of the next generation of energy production technologies, such as nuclear fusion, concentrating solar power, and ocean thermal energy conversion (OTEC).
2. The thermodynamic efficiency of gas turbine engines (GTEs) is increased with increasing turbine inlet temperatures. Therefore, in the case of GTEs it is important to use materials that are capable of withstanding high temperatures yet still have high strength, stiffness and toughness. Traditionally, Nickel-based superalloys have been used to fabricate the hot components (such as the turbine blades and combustion chamber) of the GTEs, as they are some of the most lightweight and tough materials capable of withstanding very high temperatures (up to 1500 degrees). However, in order to further enhance the GTE’s efficiency the temperatures in the hottest parts of the engines are being raised even further. This is made possible by applying ceramic-based thermal barrier coatings (TBCs) to the surfaces of the superalloys. While ongoing research continues to raise the temperature capability of TBCs, the temperature capability of the Ni-based alloys has mostly remained flat. To compensate for this discrepancy between temperature capabilities, currently the superalloy components are cooled using air circulation systems to allow them to operate alongside the higher temperature capable TBCs. However, adding the cooling systems significantly reduces the specific power produced by the GTEs.
3. XXX STOPPED HERE XXX Therefore, there is a search for a new class of materials that can replace the Ni-based superalloys. Such materials should be capable of operating at higher temperatures than Ni-based superalloys without the need for any additional cooling, and have equal or better specific mechanical strength and toughness. Research into finding a replacement for Ni-based superalloys has been going on for decades, primarily along two lines: (i) Mo-based and Nb- based alloys and (ii) ceramic matrix composites (CMCs). It appears that CMCs are winning that race, as is evidenced by the significant investments made into CMCs by a major engine manufacturer, and the recent demonstration of engines that use both stationary and rotating CMC components in the hot-section.
4. Ceramics are as strong as superalloys while being lighter and being able to withstand higher temperatures and corrosive environments. However, they are brittle and are prone to fracture during thermal or mechanical shock loading. Therefore, to increase the toughness, the ceramic materials are made into composites (e.g., CMCs) ~~heterogeneous~~. ~~Traditionally, this was done by making ceramic materials into composites~~. However, there are still many hurdles that stop us from taking advantage of the tremendous potential of CMCs.
5. The first generation of CMCs simply involved dispersing one ceramic phase in the form of particles or fibers in another ~~different or same~~ ceramic phase ~~that acted as the matrix~~. It was found that only when the dispersed phase was in the form of very long fibers was there a substantial increase in the toughness of the CMC. Leading from that, currently, CMC parts are created additively. First, ceramic fibers are laid flat or woven together to form sheets/plies. Then a preform~~/mold/scaffolding~~ in the shape of the final part is created by stacking the plies one on top of another. ~~Among several other processing steps~~ The preform is then infiltrated with the ceramic matrix phase to get the final part. The primary architectural design in such cases is within the plane of each ply. Since, in the stacking direction, at the most, the plies can be simply rotated in-plane with respect to each other. Due to this reason, these CMCs are typically termed 2D CMCs. One of the primary hurdles that is stopping us from taking advantage of CMC is that 2D CMC parts are invariably weaker–by almost an order of magnitude–in the out-of-plane direction and are prone to delamination failure. There are currently attempts to circumvent this problem through the use of sophisticated 3D architectures. These architectures are constructed using a variety of new fabrication techniques such as slip casting, ice templating, robo-casting, and weaving techniques adapted from the textile industry. For example, consider the case of integral ceramic textile structures (ICTSs). The fiber preforms of these CMCs are created using 3D textile weaving methods that produce interlaced in-plane and through-thickness fibers. The fibers in ICTSs that bridge multiple plies enhance out-of-plane toughness properties and alleviate the delamination problems characteristic of 2D CMCs.~~For example consider the case of ICTS.~~
6. The new 3D architectures are highly complex and are radically different from the 2D CMC designs. Many of them are inspired from architectures seen in structural biomaterials (SBs), which also in many cases are composites consisting of ceramic tablets, fibers or layers glued together using an organic/polymeric phase. Some examples of SBs with these types of 3D architectures are bone, the nacreous layer in abalone shell, and the club-like appendage of the mantis shrimp. While these SBs are often composed of >95% ceramic material by volume, they have been shown to possess extraordinary toughness properties while being able to maintain both the strength and stiffness of the constituent ceramic material. For example, the total energy dissipated during the fracture of nacre has been shown to exceed that of its constituent ceramic material, aragonite, by three orders of magnitude. The incredible toughness in SBs arise from the large number of interfaces and intricate architecture of these interfaces. . It is believed that the tremendous amount of interfacial area and the interfaces’ intricate 3D geometry is the key to the structural biomaterials’ incredible toughness, damage tolerance, and energy dissipation. Some of the enhancements to the SBs’ toughness properties have been explained using classical toughening mechanisms such as crack bridging, frictional pull-out of fibers or lamellae, or plastic dissipation at the interfaces caused by failure of sacrificial bonds (REF artful interfaces in biological materials, Fratzl 2011). All of these mechanisms reduce the stress concentration at the tip of a crack in the material, and consequently make it more difficult to propagate cracks. Models for SBs that incorporate these toughening mechanisms predict enhancements to toughness properties (e.g., work of fracture) of up to several hundred percent (REF bathelat and Kamat 2000). However, they do not account for the toughness enhancements that are observed experimentally. One explanation for this is that there could be a large number of other toughening mechanisms operating in SBs that are not included in the models. It is also possible that what is being witnessed is not a myriad of well-understood mechanisms operating in concert, but rather a completely new mechanism. While these mechanisms can be used to explain the observed enhancements of toughness properties, they cannot be used to predict the anticipated toughness of a new design based on the architecture alone. This is because, in general the link between architecture and toughness is not well-understood. This type of predictive power would allow the deliberate design of CMCs as opposed to merely mimicking the architectures of SBs with enhanced toughness properties. In this case the architectures of the SBs could serve as a starting point from which the architecture is tuned to give rise to even greater toughness enhancements.
7. The large amount of interfacial area and its intricate 3D nature provide a large amount of design freedom. The SBs intelligently take advantage of this design freedom by coupling old toughening mechanisms or precipitating completely new ones to substantially enhance their toughness, compared to the toughness of their constituents. When creating the next generation of interface dense CMCs (id-CMCs), this large amount of design freedom provides us with not only an incredible opportunity but also a daunting challenge. Because, the large design freedom makes it prohibitively time consuming and expensive to to figure out the optimal, or even satisfactory, small-scale architecture design by simply performing a large number of experimental parametric studies. Therefore, to leverage the power of 3D id-CMCs we must develop a better way to predict toughness from information about a CMC’s small-scale architecture and constituent material properties alone.
8. The PI plans to take up this challenge as his long term career objective. In order to intelligently take advantage of the design freedom afforded by the 3D, interface dense designs, it is necessary to first understand the mechanisms through which interfaces and their geometry enhance the large scale toughness. Then it is necessary to consolidate that knowledge to create a computational tool that will enable one to connect small-scale architecture parameters and the large-scale toughness in *id*-materials. In line with this long term objective, the specific research objective of the proposed project is as follows:  
     
   (i) Understand the mechanisms underlying how the small-scale interface architecture can enhance large scale toughness, and (ii) develop a computational mechanics method that captures such mechanics and can be used for designing the next generation of *id*-materials.

Proposed

### As evidenced by structural biomaterials, intelligently taking advantage of the the almost unlimited degrees of freedom in -architectures is the key to creating CMCs with incredibly high damage tolerance and notch-insensitivity. The additional design free in the With the introduction of this micro-architecture design comes the problem of being able to reliably connect the large-scale mechanical properties to those of the constituent phase and the micro-architecture parameters.

For example consider the case of

The properties of the CMC critically of course depend on the properties of the constituent phases, but what is very in very interesting is that the depend in a nonlinear fashion on the small-scale geometry of the architectures of phases.

***Previous and related work***

*Experimental–(Max)*

1. *Barthelot.*
2. *Christine Ortiz*
3. *Espinosa*
4. *Ravichandran wood*

*Theoretical–(Haneesh, Wenqiang)*

1. Shuman Xia
2. Huagian Gao
3. Kaushik Bhattachary
4. Zhigang Suo
5. Askan Vaziri

*Computational–(Kaushik, Welin)*

1. XFEM, Cohesive zone methods.
2. Bourdin
3. Self.
4. Pablo Zaviretti
5. Allan Bower
6. ~~Outline current method for making CMCs (ply layup)~~
7. ~~What are limitations of this method? (limited scope of tuneable design parameters, low toughness when loaded out of plane)~~
8. Are there any examples of people making new 3D architectures already? How did they arrive at their designs?
9. These next generation CMCs are limited by 1) fabrication complexity and 2) lack of design tools
10. Fabrication has been stepped up recently (ice templating, MM 3D printing, etc), however there is no robust design tool to predict the effective toughness of a CMC from its microarchitecture.
11. These were mostly chosen arbitrarily not deliberately because there is no way currently to relate the architecture to the expected toughness
12. We want to develop this tool.
13. However, with such a large design space, where do we start?
    1. A theoretical framework to determine the based places to look
    2. Couple this with looking to tough composites in nature. What do their architectures look like? We have seen that synthetic variants of these composites display the similar enhancements to toughness → not a bad place to start.

**1:23, June 22,** I have everything I need here for Broader impacts. I just need to massage it and get it into shape.

# **2 Broader Impacts**

## 2.1 Integration of Research and Education

### 

### 2.1.1 Educational Outreach

The PI strongly believes that everyone should have an opportunity to experience the excitement of science and has planned a broad range of educational outreach activities. The proposed research has strong links to the subjects of patterns in nature, evolution through natural selection, and bio-inspiration which generally attract wide public and student interest. Thus, the PI will use the research results from the proposed project to reach people from all backgrounds and excite in them an interest and appreciation of science and engineering. This goal will be pursued through a range of outreach activities. The activities (collaborations with LA, SPIRA) are targeted at specific student groups and focus on underrepresented minorities in science and engineering, while others (Sci-Toons) have a more global scope.

#### **2.1.1.1 Collaboration with The Sci-Toons Initiative**

The PI will collaborate with the Sci-Toons initiative at Brown to create scientific cartoons on topics related to bio- and nature-inspired engineering. Please see the attached letter of collaboration from Dr. Oludurotimi O. Adetunji, ‚Ä®Director of Brown's Science Center Outreach. The Sci-Toons initiative is an informal science education program at Brown University's Science Center. Sci-Toon videos combine art, animation, high-quality multimedia and storytelling. In the Sci-Toons collaboration, the PI and his students will work with both STEM and non-STEM students, as well as animators in the development of the script, storyboard and science animation. Sci-Toons videos are a powerful tool for engaging and communicating scientific research and concepts to a broad audience. Through the effective use of “jargon-free” language and engaging storytelling, the Sci-Toons videos aim to get non-STEM majors interested in STEM subjects, STEM majors to appreciate the importance of scientific communication, and the general public to develop a greater understanding and appreciation of science. The Sci-Toons are distributed via a variety of social media platforms.

Through the collaboration, the PI will help create two Sci-Toon videos per academic year for the next five years. The collaboration on the first video will begin in Fall 2014. The first video is tentatively titled ``How Natural Evolution Is Helping Engineers.'' The video will discuss how the idea of ``survival of the fittest'' results in biological structures/materials acquiring better and new properties through the accumulation of beneficial changes in their macro- and micro-scale structure. The video will discuss some of the close to optimal designs found in nature, and will give concrete examples of how those designs have inspired engineers and inventors (e.g. Velcro, Chipper Chain~\cite{deyoung2004discovery}). The video will end by highlighting the fact that the vast majority of nature's designs remain unknown to engineers, and excite the viewers about the immense possibilities that the discovery of such designs would create for science and engineering.

The Sci-Toon creation group consists of both STEM and non-STEM students and faculty. Funds to support the PI's collaboration with the Sci-Toons initiative are requested as part of the budget (see Budget Justification). *Evaluation:* The impact of the Sci-Toon videos will be gauged by monitoring the number and geographic distribution of the views that the videos generate. Sci-Toons has produced 12 videos so far, which have been viewed in over 70 countries.

The PI will also post the Sci-Toons videos on his lab website. The website will be set up such that the viewers can post comments and questions about the videos. The PI and his students will host a monthly virtual discussion group on XXX (Pdcost, virtual discussion platform, etc.,) and address the comments and questions.

# 3 Collaboration with SPIRA

SPIRA is a four week camp hosted by Brown every summer for high school-age girls to explore engineering. The PI and his students have been collaborating with SPIRA in order to encourage young women to pursue education in STEM fields by exposing them to interesting applications of engineering. The camp is free to those who attend and often attracts students from underrepresented minorities. The graduate student who will be involved in the proposed research (Max Monn) has been collaborating with SPIRA for the last three years as an invited speaker. Pictures from some past SPIRA activities that were conducted by the PI’s group in his lab are shown in Fig. 7.

Over the course of the proposed project, the PI will help Max Monn design new talks and tutorials for the SPIRA participants that will highlight the importance of contact mechanics and bio-inspired engineering.

His presentations and discussions have focused on the importance of bio- and nature-inspired materials to the future of mechanical engineering. Over the course of the proposed project, the PI will help Max Monn design new activities for the SPIRA participants that will highlight the important topics of structural optimization and biomaterials. An activity under development is the egg drop competition. In the competition the participants are asked to construct an optimal structure for cushioning the fall of a dropped egg by taking inspiration from nature.

The student teams will be supplied with various materials and given access to the microscope, and the micro-manipulation tools in the PI’s lab. Funds to organize this new competition in collaboration with SPIRA are requested as part of the budget. *Evaluation:* The effectiveness of the planned SPIRA lectures, tutorials, and competitions will be gauged using exit interviews. The students’ feedback will also be solicited by encouraging them to post comments and suggestions on the SPIRA section of the PI’s website. The questions in the exit interviews and the website will be designed to determine which activities, and what aspects of them, the participants found most engaging and useful and to determine how the activities can be further improved in the future.

The BSP's mission is to show public high school students the excitement of science through lessons geared towards real-world phenomenon, applicable learning, hands-on demonstration, and experimentation.

The PI will give at least one lecture to the SPIRA students every year. The lectures are tentatively planned to be on topics that introduce mechanical engineering to high school students. Through the use of some concrete case studies, the PI will highlight how the tools developed by mechanical engineers satisfy critical needs in society. An example case study could be how robots are being used by medical professionals, firefighters, and military personnel to save lives.

The SPIRA students will be invited to visit the PI's lab once every academic year. On the lab excursion day, the PI and his students will show the research being conducted in the lab to the BSP students and explain the operating principles behind the different equipment used in the lab.

#### 3.0.0.1 Research Training and Mentoring

The PI is currently advising four Ph.D. students and one master’s student. The PI recently graduated two master's student (Tianyang Zhang, Jarod Ferreira). All their thesis topics are related to the proposed research. The PI collaborated with a Brown undergraduate student (Jarod Ferriera) last summer. The PI's graduate students, principally Max Monn, generated the preliminary results presented in this proposal. Funds to support Max Monn are requested at part of the budget.

The PI's research training and mentoring style mirrors that of his teaching (see section \ref{teaching}). The PI interacts with his graduate students almost daily through one-on-one discussions. The PI welcomes discussions on all topics related to the graduate students' research and maintains an open door policy. The students are provided rigorous training in the research methodology and in a number of research technical skills. They are also provided training in scientific writing, oral presentation, and teaching techniques. For example, the students are encouraged to give oral presentations in the lab group meetings and to serve as Teaching Assistants in the courses taught by the PI. The students are encouraged to think about the relevance and usefulness of their research for solving societal problems and to appreciate the importance of communicating science to an audience broader than the scientific community. As the students progress in their respective programs, the PI will take active part in their placements and will help them integrate into the wider scientific community by providing them with the necessary guidance and support.

Through his educational and research mentoring program at Brown, the PI plans to train and encourage his students to be not just technically brilliant scientists but also creative thinkers who care about societal problems.

#### 3.0.0.2 Collaboration with Leadership Alliance (LA)

In collaboration with LA, the PI will mentor a college student belonging to a group that is an underrepresented minority in the STEM fields. Please see the attached letter of collaboration from Dr. Medeva Ghee, Executive Director, LA. Leadership Alliance, an over 20-year-old consortium of top national universities and colleges, is dedicated to increasing the participation of underrepresented minorities in STEM related graduate programs. LA is conveniently headquartered at Brown and will provide the infrastructure for attracting and recruiting students. The PI will recruit one student every summer through the LA to work with him on a research project that is related to his proposed CAREER research. The PI's collaboration with the student will be one-on-one. He will impart both theoretical knowledge and practical training in academic research to the student. The PI will also provide the student with the guidance and support needed to prepare competitive applications to graduate schools. The student will make either an oral or a poster presentation of the research conducted in collaboration with the PI at the LA National Symposium. Funds to support the LA student in the PI's lab are requested as part of the budget.

#### 3.0.0.3 Curriculum Development and Teaching

The PI regularly teaches both undergraduate and graduate courses at Brown. The PI draws on his research to construct motivational examples and design end-of-semester projects in his courses. For example, he uses the close to optimal shapes of biologically formed structures, such as beehives and trees, to motivate the topic of \textit{Calculus of Variations} in his courses. As another example, a junior student in the PI's course ``Advanced Engineering Mechanics,'' researched and presented on the topic ``The Optimal Profile of Claws and Talons'' as part of her course project. The PI designs his courses such that the students get ample training in critical thinking and he encourages them to initiate and take part in classroom discussions, with the philosophy that no question is too simple or elementary. As a result, several students have expressed interest in joining the PI's lab as undergraduate student researchers. For example, a student, who took the PI's course on advanced engineering mechanics as a junior, will begin working in the PI's lab in Fall 2014 on a topic related to the proposed research.

The PI will develop a new course at the undergraduate level to attract students to engineering. The course will be titled, ``How Engineers Think: An Introduction to Modeling.'' A segment of the course will involve using back-of-the-envelope mechanics calculations to explore size, form, and function relationships in SBs. Example systems for study will include mammalian bones, eggshells, gecko feet and the venus fly trap. These structure-property connections will then be naturally extended to bring out the advantages of engineering at the micro- and nano-scale, especially for innovating the fields of medicine and the life sciences. The goal of the course is to make the students aware of the wide range of exciting opportunities that are only recently becoming available to engineers, and through this awareness attract a more diverse cohort of students to engineering.

## 3.1 Societal and Technological impacts

Such materials will have a wide impact on society by leading to improvements and innovations in a variety of industrial sectors. For example, they will improve fuel efficiencies and safety standards in the transportation (automobile and aviation) and energy sectors.

Main Goal: Next generation of superior structural materials: *light weight, high strength, high toughness*.

used in: GTE combustion chamber (blades; both rotor and stator are too complex), re entry heat shield and steering panels, brake disks, slide bearings for pumps (must be corrosion resistant and tough), nuclear reactor components

The hurdles is the fabrication direction are slowly being overcome. Eq., ICTM. Freeze casting. Slip casting. Multi-material 3D printing. Laser volume engraving. However, the lack of robust and effective design tools is still lacking.

Possible

1. CMC have traditionally been constrained by fabrication techniques and the lack of robust design tools.
2. So to make the next generation of CMCs we need a robust design tool guided by the understanding of the relationship between the CMCs structure and its mechanical properties

1. Fabrication is stepped up. However, design tools are lacking. Because there is heterogeniety, and failure mechnaics can span multiple length scales and quite difficutlt to correlate to the small-scale design-geometry of the composite.
2. However, the increasing severity of operating conditions in future aerospace transportation renders the menu of available materials vanishingly small, and in many cases limits the choice to a very few high-temperature ceramics.1
3. Since ICTS are heterogeneous at all length scales, and there are multiple failure mechanisms that are often coupled, detailed understanding of the ensemble properties are needed.
4. Potentially, in addition to enhancing the toughness properties, the large design freedom also make it possible to simultaneously tune other properties, such as stiffness and strength (are there examples of this?).

Useful Extra sentences:

Useful Extra sentences for broader impacts

Reducing the weight of engineering materials almost always leads to an increase in fuel efficiency and safety standards. Therefore, there has always been an impetus for developing better structural materials that have greater strength to weight ratios. The proposed research will be focussed on understanding how nature achieves this feat so that we can replicate it in synthetic materials.

3.1.1 Useful Extra sentences for Introduction

*Broader Impacts.*

1. We can mention press coverage if we want more outreach and impact.
2. Through his educational and research mentoring program at Brown, the PI plans to train and encourage his students to be not just technically brilliant scientists but also creative thinkers who care about societal problems.

Structural biomaterials are used in structures, such as shells, antlers, and tusks that have evolved for withstanding intense mechanical loading. SBs are composed of a ceramic and a polymer phase mixed together at the micrometer scale in intricate patterns (see e.g. Fig. 1e). SBs’ capability to withstand damage can be thousands of times larger than that of the ceramic and polymer phases4. This fact along with a number of experimental studies5 4 shows that SBs’ microstructure is the key to their strength. The microstructure can be described as an intricate stacking of layers where the layers are alternatingly composed of a stiff, ceramic phase and a compliant, polymeric phase. There is a rich variation on this theme in the individual biomaterials. A number of models have been put forward connecting SBs’ large-scale damage tolerance properties to their microstructure4 6 7. However, there is no clear consensus on what the key mechanism(s) are. This is an obstacle for creating synthetic analogues of SBs.

Potential challenges

Cracks and other damage features span distances of the order of 10-3 meters where as the microstructures are of course at the 10-6 meter length scales. Therefore, in a computational mechanics investigation using standard techniques, e.g. finite element method, simulating the mechanics of damage in SBs would require at least a million degrees of freedom. It is feasible to perform this calculation on a supercomputer but the simulation times and the size of the data sets involved make it impractical to directly use standard techniques as investigative tools.

Experimental tasks

For performing virtual experiments using the MCT we will additional need information about SBs’ 3D microstructure and the material properties of their constituent phases. We

will collect this information on two biomaterials, the root fibers (basalia spicules) of the deep-sea sponge Euplectella aspergillum10 (see Fig. 1) and the stomatopod dactyl club3. We will use focused ion beam milling to cross-section our SBs in different directions. We will use scanning-electron-microscopy (SEM) imaging to construct a nanometer resolution computational model of our SBs. The plain strain Young’s moduli of the constituent phases will be measured using Atomic Force Microscopy (AFM). By nucleating and propagating cracks using nanoindentation we will estimate the fracture toughness of the constituent phases. The PI has experience with measuring mechanical properties using AFM and nanoindentation11.

And *phase field based computational tools that will predict the effective fracture toughness of heterogeneous materials composed of brittle constituents and interfaces.*

The effective properties (strength toughness, etc) depend on the properties of the constituents AND the micro architecture of the design.

How are researchers trying to circumvent these limitations → 3D architecture since we can just make arbitrarily tough/strong constituents.

Scientifically

Profitable

Enriching

Model

Ingenious

Original

Interesting

Clever

Resourceful

Exciting

Probability

Opportunities

Expansive

Pregnant

Pertiel

Scrutinizing

Perennial

Whetting

Primitive