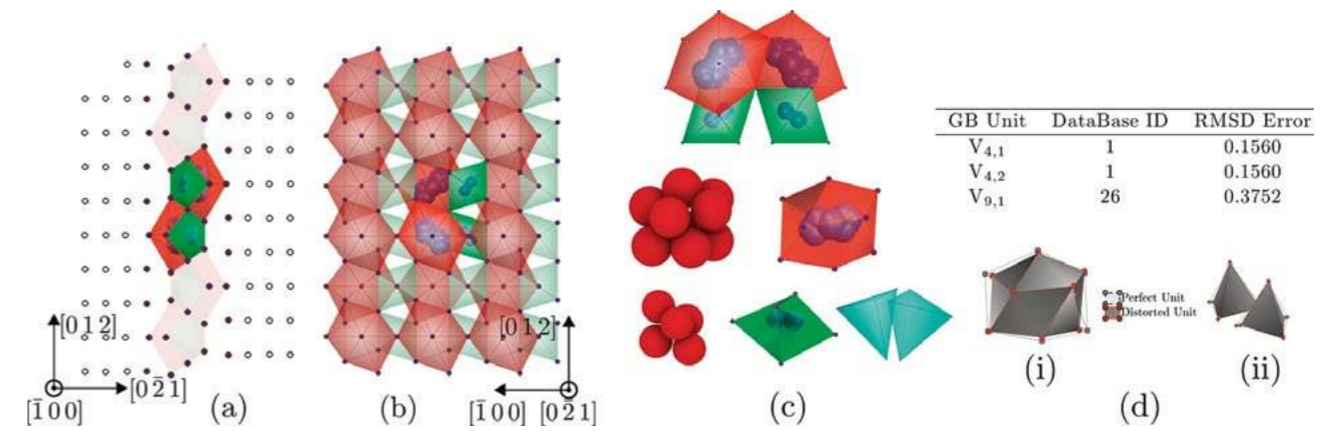
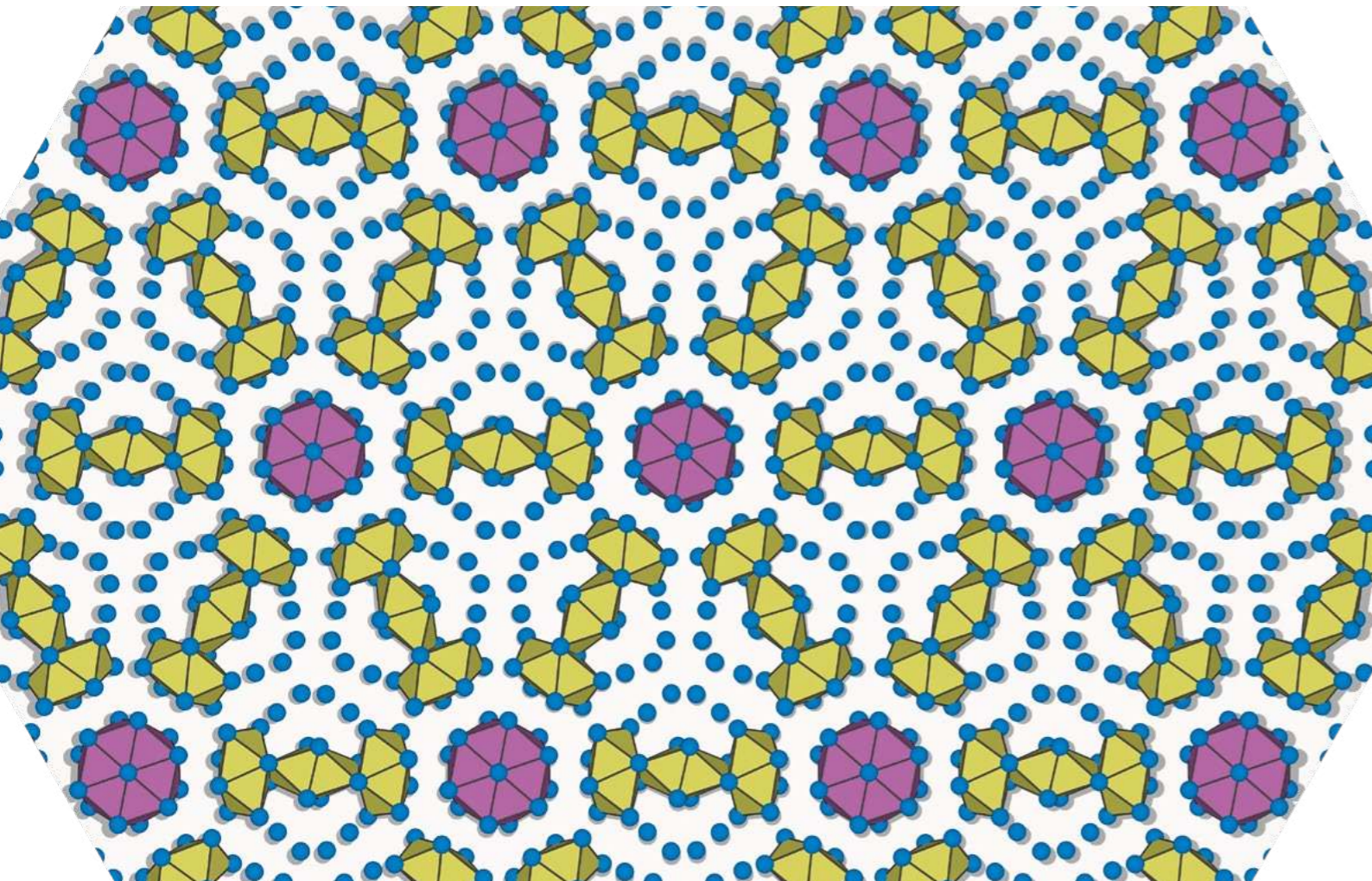


Understanding why materials fail

After receiving a Young Investigator Program award from the US Air Force Office of Scientific Research, **Dr Srikanth Patala** and his research team at North Carolina State University have studied the impact of 'grain boundaries' on the structural integrity of many materials used in critical applications. This includes materials commonly found in jet engine turbine blades, nuclear power stations and internal combustion engines.

Society's reliance on the properties of key components in critical structures – made up of metal alloys and ceramic materials – is without question. Of course, many of these materials perform well but require scheduled maintenance to detect defects, such as cracks or heat damage, before they become serious or create a situation where a failure would threaten life.

Materials used are often polycrystalline, meaning they comprise a structure made up of joining many regularly shaped crystals. For example, metals used in aircraft engine turbine



blades rely on a polycrystalline Nickel alloy. Cracks in these components can form at high temperature but their rate of formation remains unclear. Evidence suggests that the interfaces between crystals of the material – the grain boundaries – influence how materials will fail. This area has been the subject of Dr Srikanth Patala's research.

Above: The polyhedral unit model of the $\Sigma 3(1\ 0\ \bar{1})$ asymmetric tilt grain boundary is illustrated. (a, b) The atomistic structure and the polyhedral units, along two different views (the tilt axis and the plane normal), are shown. The polyhedral units corresponding to the smallest asymmetric unit (the unit-cell) are highlighted. (c) The unit-cell polyhedral units, along with the overlapping voids and the clusters of atoms that correspond to the polyhedral units, are shown. (d) The unique GB units are the 9-atom unit and the 5-atom dual-tetrahedron. The dual-tetrahedron is split further into two seed tetrahedra. The 9-atom GB unit best fits a 9-atom seed cluster in the data-base with RMSD error of ~ 0.38. The error is calculated using the point-pattern matching algorithm.

Metals used in aircraft engine turbine blades rely on a polycrystalline Nickel alloy. Cracks in these components can form at high temperature but their rate of formation remains unclear

CRYSTALLOGRAPHIES

Dr Patala and his team investigated how crystals come together to form a material and how its structure influences properties like rate of diffusion, corrosion resistance, conductivity, inter-granular cracking, resistance to failure and the impact of extreme environments. The geometry, or crystallography, of the interfaces between the crystals is complex – it must describe three parameters called misorientation and two additional parameters for the orientation of interface. This makes a total of five dimensions to define the structure of each grain boundary rigorously. Dr Patala's team developed tools to visualise the grain boundary misorientations and to represent the variations of the properties of interfaces as the geometrical parameters are varied in the five-dimensional space.

UNDERSTANDING STRUCTURE-PROPERTY RELATIONSHIPS

In materials science, to predict how a material behaves requires an understanding of the underlying structure – i.e., how atoms pack together to form the material. Computing the

atomistic structure of grain boundaries represents a significant challenge but one that would, if achieved, show how the influence of a collection of grain boundaries would affect the properties of a material.

This was the challenge that Dr Patala set himself and his team: to create a reduced-order mathematical model that predicted how polycrystalline materials would perform and discover how grain boundaries would impact their ultimate strength, toughness and performance. To overcome the complexity of grain boundary structures, Dr Patala's team plans to adopt machine-learning algorithms that make use of pre-existing and large databases of grain boundary structure-property relationships.

MODELLING USING THREE-DIMENSIONAL GEOMETRY

An important step in quantifying and understanding how atoms pack

at grain boundaries has been made with an algorithm recently developed by Dr Patala's team. The algorithm describes the structure as a packing of three-dimensional polyhedra (a many-sided three-dimensional shape with flat sides – a cube is a polyhedron but they can have many more sides).

The creation of arrangements of 3D polyhedra to model grain boundaries from a disordered set of atoms that form a material is complex. Dr Patala chose to use the mathematical properties of the well-established Voronoi network, a method of partitioning space, to automatically identify the network of three-dimensional polyhedra (whose vertices or corners represent the atoms) that are present in the structure of a grain boundary.

Dr Patala's team also developed a pattern-matching technique that allows the comparison of the polyhedra

found in the grain boundaries to a pre-existing database of hard-sphere packings (the way that atoms arrange themselves in a model material system). This allows for the classification of the type of polyhedra observed in grain boundaries and comparison of their structure.

While Dr Patala's research has focused on the analysis of grain boundaries in aluminium, his findings are applicable to most metals, ionic solids and some ceramics. However, they are not applicable to organic materials, which have directional bonds that define their material structure. This is a focus of future research in Dr Patala's research group.

VOIDS MATTER

Using the polyhedral geometries allows for the identification of voids – the space that is unoccupied by atoms – in the grain boundary region. Evidence suggests that the structure of voids, or the free-volume, at grain boundaries influences material properties. This is similar to observations in amorphous or metallic glass metals – those with a more disorganised structure at the atomic scale. Grain boundaries are disordered and Dr Patala anticipated that modelling a polyhedral unit structure that analysed the void content of a material at grain boundaries would prove beneficial, offering practical applications. For example, identifying the voids in the grain boundary would help understand how small solute atoms

Dr Patala and his team were then able to analyse the voids in the grain boundaries using the three-dimensional polyhedral geometries

interpose themselves within the grain boundary, influencing the ultimate strength and toughness of structural materials (e.g., through hydrogen embrittlement).

WHY THE RESEARCH MATTERS

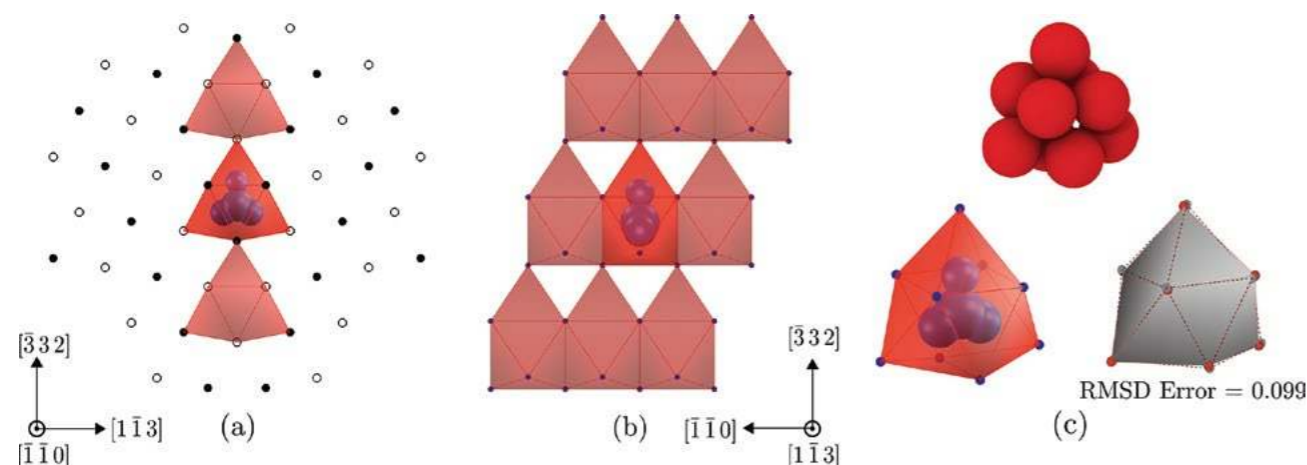
Dr Patala's research has shown that it is possible to generate a coarse-grained geometric description of the structure at grain boundaries, and especially the atomic packing. They expect their model to replace the traditional structural unit model currently in use. Grain boundaries that are similar in terms of their crystallography can now be compared.

The rigorous mathematical approach and comparison of the results obtained with a database of rigid hard-sphere packings provided a robust basis for

classifying grain boundary structures. It will be possible to use the results in autonomous learning algorithms to discover a fundamental set of polyhedral units at grain boundaries, improving understanding and allowing prediction of properties – such as resistance to failure.

Void structures can also be classified using Dr Patala's research outcomes and it is anticipated that this information will be utilised to identify potential segregation sites where there are solute atoms at grain boundaries. The developed mathematical model highlights a link between analysed grain boundary structures and those observed in metallic glasses, paving a way to evaluate grain boundaries using the theories proposed for amorphous materials.

Below: The polyhedral unit model of the $\Sigma 11(1\bar{1}3)$ grain boundary is illustrated. (a, b) The atomistic structure and the polyhedral units (capped trigonal prisms (CTP)) of the symmetric-tilt boundary, along two different views (the tilt axis and the plane normal), are shown. The CTP corresponding to the smallest asymmetric unit (the unit-cell) is highlighted. (c) The CTP and the overlapping voids, along with the clusters of atoms that correspond to the CTP, are shown. Also illustrated is a comparison between the observed and a perfect CTP unit obtained using a point-pattern matching algorithm.



Behind the Bench

Dr Srikanth Patala

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Research Objectives

Dr Patala's research interests include the structure of materials and the analysis of defects, particularly focusing on their interactions in polycrystalline materials, and in design principles that improve the performance of structural and functional materials.

Funding

- National Science Foundation USA (NSF USA), Faculty Early Career Development Program, DMR #1554270
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Collaborators

- Christopher A. Schuh, Danae and Vasilis Salapatas Professor of Metallurgy, Massachusetts Institute of Technology, USA.
- Eric R. Homer, Assistant Professor, Mechanical Engineering, Brigham Young University, Utah, USA.
- Arash D. Banadaki, Postdoctoral Researcher, Materials Science and Engineering, North Carolina State University, North Carolina, USA.

Bio

Dr Patala was awarded his PhD by Massachusetts Institute of Technology (MIT) in 2011 where he studied Materials Science

and Engineering. He was also given awards for an Outstanding PhD Thesis Research by MIT and the James Clerk Maxwell Young Writers Prize by the Philosophical Magazine & Letter, both in the same year.

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Q&A

Your research focuses on the structure of aluminium and you suggest that it is applicable to other metals, ionic solids and some ceramics. Can you explain why this is so and expand on the types of ceramics where your research is applicable?

The current limitation of the technique arises from the nature of the bonding in materials. Primarily, bonding can be metallic (found in metals), ionic (found in most ceramics) or covalent (in covalent ceramics and polymers). Metallic and ionic bonds are non-directional, i.e. the energy does not depend on the direction or the orientation of the bond. In covalent solids, the bond energy depends on the angles between the bonds (directionality) and hence the geometries are constrained. Therefore, a polyhedral model might not work very well for covalent solids (like carbon, silicon etc.). We are currently developing tools for describing such structures.

You mention machine learning as a potential next stage for your research. Could you elaborate on this?

Representing the grain boundary structure as a combination of polyhedra is one step in understanding the properties of materials. The next step is to relate the

structure to properties (such as diffusion, corrosion resistance, conductivity, etc.) of interfaces. To accomplish this, we are building a database of properties using high-throughput simulations of interfacial phenomena. By using the structural features of the grain boundaries and the data generated, robust structure-property relationships can be constructed using machine learning algorithms.

The mathematics of your model is complex, mirroring the complexity of grain boundary types. Can you explain why you selected Voronoi network and Delaunay triangulation, and whether any other approach was considered?

I would actually say that the technique of using Voronoi network for identifying polyhedral units is pretty simple. Voronoi analysis is a technique taught in most undergraduate mathematics classes. We use the property of Voronoi networks to identify which atoms should be joined together to form the polyhedral units. The simplicity of the technique is also what makes it powerful and applicable to many different grain boundary types and material systems.

How do you see the results of your work assisting your main sponsor, the US Air Force?

The Air Force Office of Scientific Research is interested in understanding

the performance of materials under extremely high temperatures. In these environments, it is the grain boundaries that tend to fail first. Therefore, developing quantitative structure-property relationships of interfaces will not only help us understand how materials fail but will also help design materials that can withstand extreme environments that are of interest to the US Air Force.

It seems that you have improved science's understanding of grain boundaries in materials. How do you see the research progressing from here?

As I had mentioned earlier, computing the structure is simply the first step in understanding material properties. We are developing novel ways to describe this structure that can be used as input to machine learning algorithms. These algorithms will then be combined with high-throughput simulations and experimental measurements to develop the relationships between the structure of grain boundaries and their properties.