"Good Materials Lead to Good Science"

BY BREEHAN GERLEMAN LUCCHESI

Ames Lab interdisciplinary research group seeks to expand materials synthesis capabilities

AMES LABORATORY EXPERTS IN MATERIALS synthesis and characterization have joined forces in a new research group to advance the Lab's ability to grow and study high-purity, high-quality crystal samples.

Materials and Engineering Physics Program Director Thomas Lograsso, senior physicist Paul Canfield and senior metallurgist Bill McCallum have formed the Rational Growth, Control and Modification of Novel Materials research group to close the loop between materials characterization and synthesis and, ultimately, expand the range of techniques for growing and studying materials.

Lograsso sat down with *Inquiry* to discuss the new research team.

Inquiry: **What are the overall goals of the new Rational Growth, Control, and Modification of Novel Materials group?**

Lograsso: Ames Lab was founded on high-purity synthesis, and we've maintained a high level of expertise and experience. Whether it's the rare-earth metals or any other material, we pride ourselves on knowing that we are doing the best science on the best materials. And, if we come to find out that materials can be improved, then we improve them to make sure that high-quality materials continue to be our unique niche. I think the continued focus on producing the best materials is the most important and exciting thing that will come out of this new research group.

So we're bringing together characterization and synthesis so we can more easily make the connection between the best science and the best materials. Good materials lead to good science. But, doing good science on bad samples is just as easy as doing good science on good samples. The difficult part is getting the good samples. That's where the new Rational Growth research group comes in.

It's rare to have all the tools and expertise in one spot like we have here at Ames Lab.

Paul Canfield brings his expertise in solution growth of single crystals and in characterization of thermodynamic, magnetic and transport properties of materials. Bill McCallum also has expertise in those types of characterization methods, and he has experience developing processing techniques. I will focus on enhancing several types of synthesis methods and offer my expertise in single-crystal characterization like X-ray diffraction. We each bring a different set of skills to the table to form this interdisciplinary group.

Our effort combines broad research interests that cover a wide range of physical phenomena and ground states, property mechanisms and methods to manipulate that property. Among the three of us, we also have a diversity of material growth techniques, extensive experience in developing new growth techniques and pushing the limits of the ones we already have, and a broad range of characterization techniques that we can use to inform the material design, growth and discovery process.

With that in mind, we have three main goals for our group. The first is to advance the ability to synthesize and characterize high-purity, high-quality materials, mostly in single crystal form, and the second is to quantify and control the synthesis-structure-property relationships, which are the basic science of how chemical inhomogeneities and structural defects affect the properties of responsive materials. Third, we want to explore promising phase spaces that we see as compelling based on advances in synthesis of novel materials.

Overall, we're focused, as always, on making high-quality crystals. But "high quality" means different things depending on what kind of science you are doing. Sometimes high quality can mean a crystal with minimal defects or a crystal with chemical or phase homogeneity. But, at the heart of the term high quality is the processing-structure-property relationship for any given material. This relationship is always important, but it becomes more important in responsive materials, which are the materials we are going to work with.

In the Rational Growth group, we've closed the loop between the synthesizer and the characterizer here at Ames Lab to help best understand and use the synthesis-structure-property relationships.

Why is bringing together synthesis and characterization important?

The people who make materials must understand how synthesis affects structure and properties, and the ability we have here at Ames Lab to connect each part of the synthesis-structure-property relationship is exceptional. It's not just enough to grow a crystal. Characterization of the crystal is of vital importance for two different reasons. The first and obvious reason is to measure its properties, its structure, perhaps the nature of the defects and their population.

Secondly we need then to utilize this detailed characterization information to improve our control over the synthesis process. Such feedback is important, because, again, if you are trying to study some particular behavior, some particular fundamental question of physics or chemistry, defects in synthesized materials are going to affect that measurement. And as one gains a better understanding of the origin of that behavior, then one begins to ask "how do I control the defect(s) that may be affecting that behavior?" So, materials behavior is elucidated through characterization, and, in turn, characterization has to inform the synthesis methods so that you can control and manipulate the materials' behavior.

What kind of new possibilities does the Rational Growth research effort bring about?

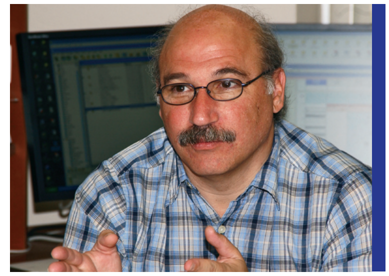
I've been collaborating with a lot of other scientists at the Lab for years, developing crystal-growth protocols and supplying crystals for research. My team could attack specific types of materials, but we were limited somewhat in expanding into other areas or searching for new materials and new types of synthesis due to a limited number of techniques. The particular synthesis method or process often defines the materials on which our group could focus our attention.

But now, in the consolidated research group, we can apply what we learn about growth mechanisms and have the freedom to expand our synthesis methods in a more general way.

The Rational Growth group will expand into new synthesis techniques not typically done in the Materials and Engineering Physics program, such as optical float zoning, vapor transport and solution growth, the latter through a closer working relationship with Paul Canfield.

And forming this team allows us to submit a proposal for advanced crystal growth furnaces that would allow us new flexibility in growth parameters and will, I hope, enhance our capability to work with a broader range of materials.

Likewise, we are pursuing new opportunities by developing those methods required for using reactive materials. Some of the reactive materials can be difficult to work with because they are so air sensitive, and the Rational Growth team wants to have the capabilities which will allow us to do a lot of processing and characterization in an inert environment. Again, that opens up combinations of elements that we, and many others, have not yet been able to consider.



What new synthesis methods do you plan to pursue?

We will advance both the Bridgman and solution growth techniques. In the case of the Bridgman technique, I hope to gain greater dynamic control over nucleation and growth processes that can be optimized to improve uniformity of large single crystals.

We will also be looking to advance solution growth with the aim to understand the limitations of the technique, such as defining growth regimes where proper control of growth can be exercised. The growth regimes are defined in terms of materials and processing parameters, as well as cooling rates and composition. As with the Bridgman technique, the goal is to manipulate the growth processes to achieve single crystals of the desired scientific quality.

We'd also like to expand our repertoire of growth methods to include physical vapor transport. This technique is particularly useful in the synthesis of materials containing volatile constituents, such as arsenic, tellurium, etc. Gaining expertise in handling these components will open up new possibilities in research of superconductors, thermoelectrics and other energy-related materials.

How does the Materials Preparation Center fit in with your effort?

The MPC is a crucial part of our team's research, and we have interacted closely in the past and will continue to do so. The MPC provides the purification processes and other processing to support our research team's goals. The materials and synthesis protocols we discover in the Rational Growth group are then, in turn, transferred into the MPC, where we can make these materials available to the broader DOE community and researchers worldwide.

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