New Materials Development / crystal growth:

*Without the discovery and development of new materials CMMP would simply not exist.*

But often the presence of new materials / single crystals is taken for granted: it is like the air we breath, we assume it is there.

This is a dangerous assumption!!
This presentation is an amalgam of several workshops and talks.

I am presenting an overview of the field of new materials design, discovery and growth based largely on (i) my own experience, (ii) the October, 2003, Ames Workshop “Future Directions of Design, Discovery and Growth of Single Crystals for Basic Research”, and (iii) a recent round of comments (Fall/Winter 2006) solicited from workshop participants for the NAS CMMP 2010 workshop on facilities.

It should be noted that there is an emphasis on DOE sponsored research because (i) and (ii) are based on DOE sponsored efforts.

It should also be noted that industrial, applied crystal growth, e.g. growth of 100 – 1000 kg crystals of Si, has not been well represented in these studies.
New Materials Development / crystal growth:

---This field is about people, not machines. This field is fundamentally person, not machine, limited.

---New Materials development requires an intimate coupling between synthesis and basic characterization. This requires scientists with very broad backgrounds and deep appreciations for the physics and chemistry of novel states of matter.

--New Materials research requires long term funding with a commitment to staffing and a built-in flexibility to pursue the physics of the compounds discovered.

--Without renewed emphasis on support and training of scientists engaging in New Materials Development / crystal growth, the major facilities run the risk of measuring poor samples, over measuring a limited set of known samples, and / or ceding the ability to pursue interesting science to foreign sample growers.
I was asked:

What does a new materials / crystal growth facility look like?

(How many people do we have to hire to cut the grass and do landscaping?)
When people say, “Facility” we usually think BIG.
Facilities usually have massive machines, vast halls, science-fiction-like sterility
New Materials development / single crystal growth is often done with very modest equipment
The spaces are small, and there can be a delivery room-like atmosphere. Crystal growth, like birth, can be messy. It is a fantastic, exciting, and addictive experience, *(spontaneous symmetry breaking at its best)* but it is very different in its nature from being at a large facility.
Some growth equipment can be expensive, and higher tech, but even mirror furnaces or high pressure / high temperature furnaces cost about ¼ million. This is a different scale from SNS, APS, NHMFL, etc.

But this misses the point---completely
If we are going to discuss the Design, Discovery, and Characterization of novel materials (as well as crystal growth) we need to focus on the researchers. (chemists, physicist, metallurgists, ceramicists, etc.)
These are researchers who try to pose and answer questions with the materials they create and develop.

These are scientists for whom crystal growth is a tool that allows access to physical insight.

Each group has its own ideas, criteria, techniques....It is important to have a Darwinian competition between as many different new materials searches as possible....

This keeps the “idea-gene pool” viable.
It’s about the people

New materials design, discovery, and characterization (as well as crystal growth) depends upon having a diverse cadre of skilled scientists practicing and teaching the science and the art.

One of the most important factors in keeping this field alive is to insure mechanisms for the funding of its practitioners. This requires a much greater appreciation of what is involved in the development of a new material or growth technique (time, expenditure, creativity).

A few places have been bastions for such scientists: National and Industrial Labs being the two most obvious historical safe havens. National Labs are now the primary home for such researchers. It can be difficult for these scientist to do well as junior faculty since they fall between traditional boundaries. This problem can extend to hiring, promotion, funding, publishing, etc. and it has kept numbers of such scientists out of academics. (Perhaps this is changing.)

Most of today’s practitioners received part or all of their formative training in the multi-disciplinary (or non-disciplinary) environment of the National / Industrial labs. Ready access to such training is vital to future efforts to grow this field.
The development of a new material is often a long term exploration that involves a combination of scientific interest, growth capabilities, instinct, and (yes) luck (albeit, self-made in many cases). Such campaigns require long term support, and require a diverse set of growth and characterization techniques.

When a significant new material discovery is made, its impact can be immense.

The most dramatic example of this was the discovery of Hi-T\textsubscript{C} superconductivity in the cuprates. This curve is fairly generic in shape.
There are many examples of such progressions. Here are three from the field of intermetallic superconductors.

There are three basic stages to a materials research trajectory:

(i) its basic synthesis and properties are understood,

(ii) more complex properties are measured and it evolves into a model system,

(iii) specialized (often facility based) experiments are made, often on specialized samples.

The sum of these discoveries is what keeps the field of CMMP vital and active.
The Design, Discovery and Growth of new materials directly impacts all forms of research. It acts as the center of CMMP research efforts.
Over the past decades DOE has created and maintained a *distributed facility* of new materials / crystal growth scientists throughout its labs and also supported university based research in this field.

This is one of the world’s *largest new-materials resources*.

Recently there has been an appreciation that new materials development / crystal growth research has suffered in comparison to large facility pushes and there has been a commitment to rebuilt / strengthening this vital effort.

Some of these issues were addressed in a recent DOE/BES workshop

**Design, Discovery and Growth of Novel Materials**

For Basic Research:

An Urgent U.S. Need

Report on the DOE/BES Workshop:

“Ifruture Directions of Design, Discovery and Growth of Single Crystals for Basic Research”

Ames Laboratory, Iowa State University
(October, 10-12, 2003)

“Future Directions of Design, Discovery and Growth of Single Crystals for Basic Research”

Ames Laboratory, Iowa State University
(October, 10-12, 2003)

Over 50 participants from National Labs, Industrial Labs and Research Universities

Organizing Committee:

Lynn Boatner, Oak Ridge National Laboratory
Mac Beasley, Stanford University
Paul Canfield, Chair Iowa State University and Ames Laboratory
Robert Cava, Princeton University
Doon Gibbs, Brookhaven National Laboratory
Thomas Lograsso, Iowa State University and Ames Laboratory
David Mandrus, Oak Ridge National Laboratory
John Mitchell, Argonne National Laboratory

Plus
Art Ramirez, Lucent / Bell Labs (on the writing committee)
Smaller number of specific Labs / groups that can work with extremes in size, purity, toxicity, radiations, pressure, temperature, etc.

Large number of University and Lab based groups pursuing diverse and sometimes high risk ideas.
The main finding of this workshop can be summarized briefly:

*Current infrastructure and personnel levels are insufficient to discover novel materials and to grow high quality, specialized samples at a level commensurate with demand by facilities and experimental groups so as to maintain international competitiveness in materials-driven research. The linkage among existing synthesis groups is not optimal, contributing to bottlenecks in the creation and dissemination of research specimens to the condensed matter community.*
Three broad recommendations to DOE-BES were identified to address this finding:

Increase the level of funding for research activities in the design, discovery and growth of novel materials for basic research. This would include appropriate funding increases in existing programs as well as the creation of new programs at universities, national laboratories, and select industrial labs.

Establish a novel materials design, discovery, and growth network to enhance the links among the various existing and future BES research efforts through meetings, personnel exchange, and materials databases. A more tightly interacting research community will more effectively leverage DOE’s investment and reduce duplication, dead-ends, etc., and better integrate the materials synthesis community with the condensed matter science community.

Create a set of multi-investigator materials preparation facilities. In addition to their existing research efforts, PIs at these centers would provide high quality materials for users, advance specialized techniques, and train new crystal growth scientists.
These recommendations tried to address problems at each level of the research pyramid, removing bottlenecks and redundancies while, at the same time balancing the need for broad access to samples with the need to train, grow and support new-materials research efforts.

At this point there are more sophisticated and higher impact methods of refining the community’s message about this need:

A DOE/BES, Basic Research Needs workshop. This is a more formal method of conveying important needs to Congress.

The NAS CMMP 2010 report

A full NAS study such as this one.

Let me end by returning to some of the points from the Ames-Workshop report in the context of the NAS Facilities workshop.
Explicit concerns for (photon, neutron, field) Facilities… (as well as for other researchers who do not make samples).

The lack of abundant, readily available, physically interesting samples that are well characterized and meet stringent needs on size, perfection, purity, mosaic, stoichiometry, etc., leads to a national loss in scientific productivity and impact.

Facilities want to avoid under-utilizing the precious beam (field) time by measuring less than ideal samples or over-measuring a limited set of “available” samples.

Researchers need to have the freedom to measure what they want with a minimum of restrictions placed on them (e.g. the Japanese/German/French sample grower only will let me measure this quantity over this limited parameter range).

All of these concerns can be addressed by strengthening the U.S. commitment to the discovery, development, and growth of new materials.
Possible Solution:  A Facility, but not the usual type.

The U.S. New Materials Development and Growth effort is fundamentally a distributed facility: fund it as such---at the funding level of a traditional facility. This would address all of the recommendations of the 2003 Ames Workshop.

---Augmented funding from such a facility will leverage existing expertise and equipment with more staff.

---A facility framework will allow for the creation of “New Materials Network” to enhance interaction between researchers and facilitate distribution of existing samples / classes of materials.

---Facility framework will allow for enhanced capabilities for growth of extreme materials (size, perfection, composition) and will allow for users as well as training of new scientists skilled in the art.
Questions from 11/22 e-mail from Natalia Melcer

NOTE: “NEW MATERIALS DEVELOPMENT / CRYSTAL GROWTH” REPLACES “crystal growth” THROUGHOUT QUESTIONS.

What future challenges in CMMP are new materials development / crystal growth facilities well-suited to address?

The ultimate challenge: developing materials that will define the physics to be studied over the next decade.

In the past 10 years, what science opportunities have arrived or are looming that are addressed through the use of new materials development / crystal growth facilities?

Scores and scores: Superconductivity in oxides, borides, intermetallics; quantum critical materials; magnetoreistance; multiferroics; thermoelectrics; half-band ferromagnets; magnetostrictive; magnetocaloric; .... *New materials gave birth to these fields*

How is the US doing in the area of new materials development / crystal growth?

Mixed. In some areas we lead the world, in others we lag. The concern is that we are loosing ground and, given time lags, may end up being a service provider (measure your stuff at our facilities) rather than agenda setter.

Is there new or other technology that could compete with or complement traditional new materials development / crystal growth facilities over the next decade?

Hopefully band-structure will continue to improve to the point it becomes truly useful as a predictive tool to identify new materials.
Questions from 11/22 e-mail from Natalia Melcer

How can we increase the scientific impact of new materials development / crystal growth facilities?

There needs to be an increased appreciation of the immense impact that new materials design and discovery does have on the CMMP community and then funding has to be commensurate.

What is the current status or need for R&D funds for future facilities?

There is a clear dearth of staffing / person power. This field is much more person limited than machine limited. Almost every group I have talked to bemoans the lack of person power to (i) pursue the ideas that might lead to new discoveries and (ii) make enough research samples to feed the number of collaborators who would like samples.

Modest increases in funding (percentage of a big facility budgets) would yield immense payoffs, not just in new discoveries but in much better use of facility resources.

**THIS IS A SIMPLE FIX THAT CAN YIELD HUGE, MULTIPLICATIVE PAYOFFS.**
CMMP is a field defined by new materials.

Design, discovery and growth of new materials has import far beyond just feeding the facilities. This is often a reason given for the need for new materials, but it is, at best, a partial reason.

Designing, discovering, growing novel materials is the heart of CMMP. Those who control the new materials set the direction for CMMP.
Broad Concerns for consideration and discussion:

Many scientists involved in the design, discovery and growth of novel materials do not view themselves simply as crystal growers.

Cultural problems often faced by new materials scientists

Funding specifically for searches for new materials (currently it is hard to fund an exploration of phase space, be it physical, chemical, or technique-based).

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