2.0 New Comprehensive Materials Policy and Infrastructure

2.1 Introduction

The Technological Importance of New Materials

Many materials have emerged during the 20th century, enabling technologies that impact directly on our defense systems. In the context of the Air Force, the discovery of a synthetic route to aluminum metal and other materials with high strength to density ratios for airframes, synthetic rubber for tires, and large silicon single crystals for computers have all been key discoveries of this century. The potent technology-enabling power of new materials is obvious if one considers a hypothetical 1995 world in which these three materials and the processes for their large-scale synthesis were not known but are to be discovered during the next 50 years. Fifty years is, in fact, the historical time span over which these three materials emerged during this century. There are many other materials discoveries in this century that might be considered in this illustration, including systems such as lightweight organic composites, high-temperature titanium and nickel alloys, piezoelectric materials, capacitors, high-temperature ceramics, synthetic diamonds, and many others.

Our capabilities in chemical synthesis, characterization of structure and properties of materials, and computation are rising exponentially. Thus, there is virtual certainty of successfully discovering even more new materials and process technologies in the next 50 years. However, U.S. capabilities, working independently in the three areas needed for new materials and process discovery (synthesis, characterization, and computation), will not easily lead to success. The key to maximizing the probability of success is for the interested parties, the Air Force being one, to develop a well-thought-out new comprehensive materials policy.

Over the past century, the discovery and invention of new materials occurred largely in synthetic chemistry laboratories. The large-scale synthesis of aluminum and other metallic systems, synthetic rubber, ceramics (silicon nitride with potential for high-performance engines), and the epoxy matrices of composite materials are all obvious examples. More recently, as the field of materials science and engineering has developed, more structural components have entered the field of new materials discovery. These new elements bring an appreciation of the impact that microstructure or nano-structure has on the characteristics of materials systems and of the critical role that materials processing plays in defining these materials systems. Silicon chips are a good case in point. Silicon was known at the dawn of aviation, but the exotic electronic properties of the low-defect density single crystals that led to the information age were not known until more recently.

It is impossible to predict the technical breakthroughs that may emerge in the next 50 years, but it is possible to envisage potential discoveries. It is reasonable to believe that systematic coordinated research by scientists of many disciplines will lead to many if not most of those discoveries. Furthermore, the high-risk nature of investment in new materials research and the current industrial climate in the U.S. will require greater amounts of federal funding for basic research and exploratory development (i.e., 6.1 and 6.2) to maintain the critical mass required to successfully invent and transition technology-enabling materials.

There are several reasons to believe that materials science breakthroughs might be more difficult to attain over the next five decades. One is simply the current technological sophistication, which makes the targets much more specific and the required novel properties extremely demanding. Another is the number of requirements that new materials will have to satisfy in order to be acceptable to designers. Two key requirements for all materials will be the environmental impact of their preparation and disposal and the closely coupled requirement of implementation cost. The combination of these two cost factors, with acquisition cost, reflects a new or renewed interest in affordability as a design factor. Before describing what might enhance future mechanisms of new materials discovery, it is useful to consider what could be considered at this time as typical of the "technological gems" the Air Force will find in the arena of new materials and processes.

High Aims in New Materials for the Air Force

Consider a new generic class of structural polymers for ultralight airframes that does not require carbon fibers for reinforcement, and is processed by "reversible sintering." This type of processing, presently unknown, would be somewhat analogous to ceramic sintering or powder metallurgy techniques, and would impact greatly on the cost relative to current day composites. More importantly, however, its reversible nature, possible given the molecular nature of the material, would offer the possibility of recycling airframes for other uses if not for aircraft. The basis for this concept is offered in Section 13. Another example would be finding revolutionary photonic materials that utilize photons instead of electrons, and that may increase by orders of magnitude the rate at which we transmit, process, and store information. With such materials, switching speeds can be 10,000 times faster than current electronic silicon-based technologies. Based on current knowledge, these materials are likely to be fully or at least partly organic composite in nature. Thus, they would significantly affect the weight and possibly the size of devices on aircraft, satellites, missiles, or rockets, impacting also on the number of new technologies that could be accessed with these materials. Again, some thoughts are offered on this subject in Section 13. One last example could relate to solid energetic materials that would be molecularly designed to have nanometer- or micron-sized regions of all key ingredients. The vision would be to generate the ability to design single-component solid propellants and explosives with microstructural control and with the capability of being processed as macroscopically ordered structures, for example, nano- or microtubes of oxidizer in fuel matrices oriented in a common direction within a charge. Alternatively, consider layered structures self assembled from a fuel-oxidizer block copolymer. Such materials may bring spatial control of focused energy, homogeneous energy dissipation and safety, as well as enormous increments in specific impulse given their densities and other factors detailed in Section 10 of this report. Self-assembling materials as described by George Whitesides in the September 1995 *Scientific American*, may enable not just materials, but these revolutionary materials systems, and perhaps self-assembled devices and machines. The generic concept here for such new materials could probably also be applied to the fuels area.

2.2 The Evolution of Mechanisms for Materials Discovery

Generic Evolutionary Changes for All Materials

As mentioned previously, some of the Air Force-critical materials of this century, such as aluminum produced in large scale and synthetic rubber, were discovered in chemistry laboratories. In these two cases, and in others as well, a target was being pursued. Aluminum was known in the 19th century as a laboratory curiosity, but because of its low density there was interest in finding a viable methodology for its synthesis in large scale. In the case of synthetic rubber, a material like it, natural rubber, was already known and was determined to be a technologically desirable substance for military purposes during the Second World War. Thus, the transition from polyisoprene to vulcanized polybutadiene was in a sense a biomimetic discovery. This begs the question of whether or not a material like rubber, which is critical for the landing of aircraft, would have been invented in the absence of polyisoprene in nature. The point is how different will be the mechanisms for materials discovery in the future, in that the infinite number of synthetic permutations will have to be guided by at least a rudimentary knowledge of how molecular structure is connected to physical properties. This type of expertise does not exist in the classical chemical laboratory. Also, the expansion of our knowledge base has been such that an exponential rise is occurring in the number of possible permutations for new materials. For example, in the early part of the century, there was little awareness of the potential of engineered composite materials. Also, our organic synthesis capabilities have been increasing steadily over the past few decades, thus increasing the number of possible structures that could be explored. Thus, a permutation explosion will exist for new organic structures, ceramics, metallic alloys, intermetallics, and composites. For this reason, on the experimental side, the future mechanisms of materials discovery will have to include rapid property-screening methodologies with very small laboratory-scale quantities, milligrams to grams, and also will have to be closely coupled to a scaleup resource when a promising new material is identified. On the theoretical side, there is no question that the “dry” search for new materials using computers will aid the exploration, and this will raise the probability of critical discoveries. Both rapid screening of new materials with small quantities and the computational search for new structures are important evolutionary changes in the mechanisms for materials discovery.

Combinatorial Libraries: One Possible Mechanism for Materials Discovery

In the context of the permutational explosion in metals, ceramics, organics, and composites, how will the scientific community proceed to search for technologically important new materials? For example, how should we search through structural space for superconducting solids at temperatures approaching room temperature, highly efficient luminescent materials for displays, nonlinear optical materials for photonics, polymeric structures of high compressive strength and stiffness, powerful adhesives for adverse environments, and for many other technically important materials? It is clear that, at the present time, the theoretical and computational resources, including thermodynamic data and models, to fully predict these structures of technological importance, are not in place anywhere in the world. Over the past decade, chemists and biochemists have developed the so-called combinatorial approach to search for specific molecules, particularly for drug development. This approach generates “combinatorial libraries" consisting of large arrays of specific families of molecules to test for molecular binding characteristics or catalytic activity. The application of this approach to the search of superconducting solids was reported very recently.[1] This work described methodology for parallel synthesis of spatially addressable arrays containing superconducting copper oxide thin films. Libraries containing more than 100 materials were generated by sequential sputtering of various precursors on different substrates, using masks to vary the chemical composition. The final materials were produced by thermal processing and then screened for superconductivity using rapid scanning probes.

Figure 2.1 A Combinatorial Library Design to Search for High-Temperature Superconducting Materials

It is reasonable to assume that this type of empirical search for new materials could be extended to other types of solids considered to be critical for Air Force technologies. These

1. *Science*, Vol. 268, p. 1738 (1995).

would include nonlinear optical materials for sensors and rapid information processing, advanced magnetic materials for the more electric aircraft, luminescent materials for aircraft panel displays, energetic materials, conducting polymers, intermetallic alloys, or even single or multicomponent composite structural materials. However, each different physical property will require the development of different rapid scanning probes, which may have to be new technologies in their own right. Furthermore, the three-dimensional hardware required to search for new materials in large arrays containing hundreds or thousands of compartments may be quite challenging. It will also be necessary to find methodologies that will allow in situ organic chemistry to be performed in materials libraries. Such reactions would include polymerization schemes, as well as the chemical synthesis of monomers or oligomers. Finally, the simulation of materials processing in the microenvironment of the combinatorial library is not a trivial objective but should be explored. This is, of course, necessary in order to access microstructural factors and not simply chemical composition in a new materials library.

It is unlikely that combinatorial libraries alone will lead to the successful search of new Air Force-critical materials. However, it may be useful to couple empirical combinatorial efforts with computation in order to select the correct homologous sets of materials that should be investigated. Another approach involving computers coupled to combinatorial libraries would be to use genetic algorithms to optimize the property being searched and in this way guide the experimental array to be investigated. When promising materials are identified through combinatorial libraries, it will be critical for investigators to have access to a scaleup infrastructure. In fact, this coupling should be considered a critical issue in any Air Force decision to fund exploratory work for new materials and must be an integral part of a new materials policy.

2.3 Scaleup of New Materials and U.S. Industrial Capabilities

Scaleup Procedures

The full potential of a new material for technological implementation cannot be assessed without scaleup of mass by at least three orders of magnitude relative to the amount typically produced by the original discoverers. In research dealing with organic materials, which tend to be the most synthesis-intensive, once a synthetic pathway has been identified, researchers will produce less than one gram of the substance. Even though a materials target might have been identified, the driving force of the investigation is often the development of new chemistry. A similar situation is encountered in inorganic synthesis targeting the discovery of new chemical precursors for ceramic materials.

Conventional characterization of structure and sometimes physical properties, which does not require large quantities, is often done in-house or through external collaborations and quite frequently is the end of the loop for that particular material. The infrastructure to pursue scaleup of what appears to be a promising material as defined by the original target is in most cases nonexistent. This particular situation is very common in both academic and government laboratories, and sometimes even in industrial laboratories. Traditionally, however, U.S. chemical industries have had scaleup capabilities for their own internal explorations.

Scaleup efforts are not trivial to undertake, since they most likely will involve not only chemists but also chemical engineers, materials scientists, and mechanical engineers. In a scaleup effort, chemists and engineers need to work closely because often the synthetic pathway that works for laboratory-scale synthesis cannot be implemented in large scale. A redesign of the pathway, often suggested by the specific problems faced in scaleup, needs to be implemented. The number of chemical reactions required to reach the final product must be minimized, and the yield of each reaction has to be optimized. This is clearly necessary, since the final of the yields for the new material is given by the product of yield in the six various reactions of the pathway.

The U.S. Industrial Problem for New Materials Exploration

At the present time the United States faces a major problem with regard to exploration of new materials. R&D efforts are being downsized substantially in all areas, but the exploration for new materials followed by in-house scaleup is possibly affected even more than other technical areas. For example, software and silicon device industries seem to be in a relatively healthy state with regard to R&D, and, of course, computer-based service industries are extremely popular. The sector that transforms raw materials into high value-added materials is definitely weakened in our country. Over the past decade, chemical industries such as Celanese Corporation, and engine companies such as Allison, and others, have been sold to foreign multinationals. Those chemical industries that still retain new materials interest will only pursue systems that can be produced in the billion-pound scale needed for consumer goods. On the other hand, the sizing materials that bond fibers and matrices in composites, and make up hardly a few percent by weight of a structural composite, do not justify a serious exploratory effort for a large chemical company. Yet molecular explorations for sizing materials could improve significantly the performance and reliability of composites used in advanced airplanes; novel sizing materials could also be used to improve fire retardancy of composite vehicles, develop self-monitoring composites for microstructural damage, and perhaps even self-healing of damage. To summarize, in the context of new materials, our infrastructure for discovery in all classes of materials is eroding rapidly.

The global picture in the United States for the discovery of new materials, which would impact directly on the technological superiority and effectiveness of the Air Force on the battlefield over the next fifty years, does not appear to be encouraging, in 1995. A new materials policy in the scientific establishment of the Air Force is therefore of critical importance. To design this policy, the declining interest in this area within U.S. industry must be accepted as a reality, and the origin of the problem must be understood. Without pursuing a detailed economic analysis of the problem, it is probably safe to assume that the slowing innovation in new materials from industry is simply an issue of high-risk capital investment. For the sake of technological lead, the Air Force and other DoD agencies must therefore invest funds in this area.

2.4 The New Materials Exploration Loop: A 6.1 Funding Model for the Air Force

The model proposed is to fund new materials research at Air Force laboratories, research establishments, and academic institutions that would be scrutinized carefully for in-house or external network capabilities for closing the new materials exploration loop. The first step is conventional, and should be a serious evaluation to determine if the proposed exploration is highly innovative and targeted for Air Force-specific needs. However, the new elements in the policy should include requirements that demonstrate real, budget-committed connections to a structure-property screening capability and, most importantly, a second connection to a scaleup capability. The scaleup effort should probably be funded with 6.2 funds, but the basic premise in the proposed loop is to establish an early coupling of 6.1 and 6.2 funding that seems to be critical for the area of new materials to be successful. A final requirement before the 6.1 investment is made should be a vision by investigators, bearing evidence of reality, of identifying an industrial establishment that could implement the production of proposed concepts. The connections for structure-property screening and scaleup could exist in-house or be established externally in industry, other government laboratories, or academic institutions. The importance of a connection to a scaleup capability is, of course, the fact that many properties of new materials remain undiscovered because of limited availability of the novel material.

The basic philosophy of the new materials loop is the fact that proof of concept and application appear to be the necessary driving forces at present for industry to consider investing in the development of new materials. It is in this context that the concept could be regenerative to the national new materials infrastructure. It is also clear that coordination with other DoD agencies is of key importance in this particular area. A part of the overall vision for the Air Force is also to create an internal mechanism to accelerate the acquisition of the many forms of data needed once a new material with technological advantage is clearly visible. A diagram of the new materials exploration loop is shown in Figure 2.2.

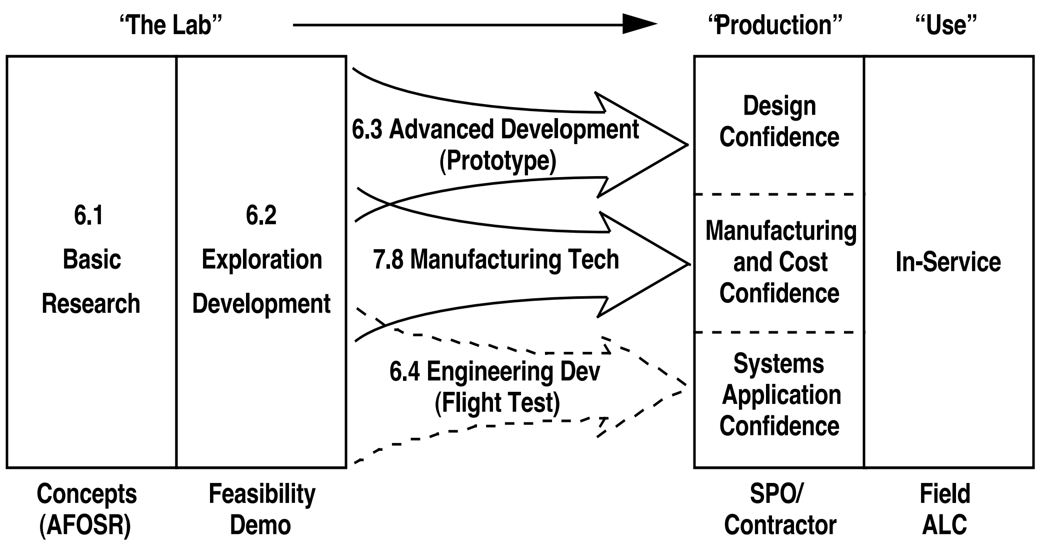

Figure 2.2 New Materials Exploration Loop

2.5 Scaleup Stations for New Materials

From an R&D standpoint, scaleup of new materials is a unique activity for the following reasons. At academic institutions, and even at private research institutions, and government laboratories involved in basic research, scaleup of materials is not regarded as an intellectually challenging, creative activity. In academic institutions, for example, it is difficult to involve creative graduate students in scaleup work. In fact, it is often difficult to integrate with current degree programs research on scaleup of new materials. This is particularly true in chemistry programs. At the same time, in chemical engineering programs, where there used to be some emphasis on scaleup research, there has been a declining interest in the subject. The situation in industry has already been described; therefore, serious consideration must be given to the establishment of scaleup stations at either Air Force or academic laboratories. In these stations, promising new materials would be scaled-up by two or three orders of magnitude relative to basic research laboratory scale. The advantage of establishing these stations in laboratories, where the truly exploratory synthesis and characterization work is being conducted, is fairly obvious. The colocation would offer the possibility of a very beneficial synergistic interaction for the final outcome. At academic institutions, these stations should employ primarily professionals and technicians to address the incompatibility issue between scaleup efforts and academic materials synthesis research leading to a degree. The downsizing of industrial R&D efforts has created a surplus of highly trained personnel with technical degrees that could be employed for this important effort.

2.6 Commercial Payoff in Materials Innovation

There is great potential for commercial payoff in new materials discovery, since they seldom have unique applications. In contrast to specific devices, the potential commercial payoff is almost guaranteed, since new structural and functional materials permeate automatically into many other sectors of the world's economy. Among many examples, one could cite two that demonstrate this principle: the use of aerospace metals in orthopedic surgery and the use of advanced composites in sporting goods.

2.7 Conclusions and Recommendations

- A strong program of 6.1/6.2 funding for Air Force-relevant new materials exploration needs to be established. This program should be established under the guidelines of a new materials exploration loop described above with the objective of inducing some regeneration of a new materials infrastructure.

- We need scaleup stations that will support synthetic and characterization activities in, and the capability of, academic and government laboratories in new materials research.

- While the next 50 years might be totally infertile worldwide with respect to technological implementation of new materials, or may produce revolutionary discoveries, an important policy question to address is whether or not U.S. government institutions, the Air Force in particular, will take the risk of <u>not</u> investing in the exploration for new materials. The risk is to be assessed considering that other important countries, and potential adversaries, are investing in new materials exploration, especially Japan, Germany, France, Korea, China, and several emerging countries in the Third World, as well.

- The absence of a U.S. government-supported effort in new materials augments the risk to technological lead, since U.S. industry is only weakly involved in this exploration at present, and is unlikely to be strongly involved in the foreseeable future.

- There is great potential commercial payoff in new materials discovery, since they seldom have military-unique applications. In contrast to specific devices, the potential commercial payoff is almost guaranteed, since new structural and functional materials permeate automatically into many other sectors of the world's economy (e.g. composites in aircraft, sporting goods, and orthopedics). However, advanced materials of specific interest to the Air Force frequently represent a market that is too small to interest commercial suppliers. Accordingly, it would be foolish and inappropriate for the Air Force to rely solely on commercial suppliers for its advanced materials needs. This argues strongly for a robust in-house materials R&D program and possibly even production capability.