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Strategic Thinking in Chemistry and Materials

Office of Defense Programs
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REVISION OF THE TREATMENT PLAN

10/1/77

Inter-laboratory Report for DOE-DP-11: Strategic Thinking in Chemistry and Materials

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The material in this report is a compilation of contributions from many authors and represents a Strategic Focus document to integrate and guide Chemistry and Materials research at the three DP design laboratories. Responsibility for generating this report was assigned to a tri-laboratory working group comprised of the editors.

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EXECUTIVE SUMMARY

The Department of Energy nuclear weapons program during the Cold War required an expansive base of chemistry and materials expertise, facilities support and technological capability. Following the end of the Cold War, this competency base has experienced a rapid erosion due to significantly reduced production requirements with associated declining budgets, and a shrinking integrated contractor network. At the same time, the science and technology challenges and opportunities have expanded significantly due to the loss of underground nuclear testing, the extended life expectations of our stockpile, and an increasing likelihood of common-mode vulnerabilities within the stockpile. The essence of this dichotomy is addressed within the strategic thinking of the chemistry and materials contributions to Science-based Stockpile Stewardship (SBSS).

Science and technology challenges facing the Chemistry and Materials program relate to the fundamental problem of addressing the critical needs to improve our understanding of how nuclear weapons function and age, while experiencing increased pressures to compensate for a decreasing technology base. Chemistry and Materials expertise is an enabling capability embedded within every aspect of nuclear weapons design, testing, production, surveillance and dismantlement. Requirements to capture an enduring chemistry and materials technology base from throughout the integrated contractor complex have promoted a highly visible obligation on the weapons research and development program. The only successful response to this challenge must come from direct improvements in effectiveness and efficiency accomplished through improved understanding. Strategic thinking has generated the following three overarching focus areas for the chemistry and materials competency:

As-built Materials Characterization and Performance directed at developing a modern baseline understanding of how the stockpile was produced and a fundamental understanding of quantitative materials performance metrics to create a bridge between our underground testing knowledge and the emerging aboveground testing requirements.

Materials Aging knowledge that allows predictive extension of performance metrics to include age-related reliability determinations for the enduring stockpile.

Materials Synthesis and Processing knowledge that will enable the certification of reliable replacement materials and remanufacturing sources needed to address future stockpile improvement requirements.

An investment strategy is also described to illustrate the competing requirements between maintaining the enduring chemistry and materials competency base while making science and technology investments for the future. Significant investment leverage is realized by the expanded Chemistry and Materials Technologies mission which includes working with industry to conduct research of mutual interest, DoD conventional munitions, environmental cleanup and energy research. Each of these leverage initiatives helps to maintain chemistry and materials expertise by establishing the multi-program diversity needed to attract a quality work force to the Laboratories. But the leverage activities are not specifically beneficial to expanding the

knowledge needed for SBSS. Therefore additional research and development investment is needed to enhance this specific knowledge base. The underpinning assumption is that as current efforts related to stockpile maintenance and SBSS require an extensive chemistry and materials technology base, investments in science and technology can vastly improve this competency's effectiveness and efficiency.

II Chemistry and Materials Vision

Chemistry and Materials Science expertise at the DOE weapons laboratories will enable Science-based Stockpile Stewardship by the development and application of a competency base to address issues associated with stockpile aging, reliability and surety. We will develop a competent predictive understanding of materials performance within a very wide range of time scales, encompassing the slow dynamic rates associated with real-time materials aging up to the very high rate dynamics associated with explosive and radiation driven events. We will achieve an understanding of materials synthesis, processing and fabrication sufficient to create realistic models and simulations. This understanding will provide a knowledge base for concurrent engineering, rapid prototyping and agile manufacturing schemes that are necessary for reliable, economical stockpile component replacement.

III. Background

As the Cold War ended, it became apparent that chemistry and materials expertise at the Department of Energy Defense Program laboratories would of necessity be required to change from a knowledge base focused on material synthesis, fabrication and production to one of very careful experimentation and planning, coupled with predictive modeling with the ultimate goal of precise predictive materials models for future weapon designs. Chemistry and materials efforts were also destined to suffer as budgets declined; reliance on nuclear defense as a cornerstone of United States National Security decreased proportionally. The materials community's ability to carry out the ultimate materials and engineering test - the underground nuclear experiment in Nevada - had disappeared as a proof test for new materials and engineering designs. Additionally, we had previously been able to rely on a wealth of material data gathered from weapon production programs, weapon engineering design tests of which weapon materials - nuclear and non-nuclear played a central role. The existing weapons complex (and the requisite materials capability) was designed to meet the requirements of the Weapons Programs mandated by the President's annual Nuclear Weapons Stockpile Memorandum (NWSM). These requirements led to development and application of many new materials required for the nuclear weapons program. It has also made possible materials production in whatever quantities and in whatever percent yield - no matter how minuscule - was deemed adequate to meet production requirements based on national security needs. We no longer need that massive production capability.

Instead, faced with a necessity of selecting very carefully what materials properties could and should be tested, from where that data might be taken and how reliable that data would be in providing a path to new materials and new physics designs in the future, a future where the assemblage of large amounts of data through experiments was gone, we realized that our past reliance on nuclear testing and an inefficient production complex has lead to technological shortcomings in predictive materials capability. To be succinct, materials currently used in weapons will not be available in the future. Real material variations significantly impact our ability to replace "in kind" the materials we currently employ. A continuous surveillance effort on current materials and the development of sources for or routes to alternative materials is essential if we are to maintain required levels of reliability, performance, and safety. Careful material surveillance and prediction were not part of the past DOE materials agenda. We performed in a "reactive" rather than "proactive" mode when confronted with surveillance data.

Not to be minimized or taken lightly is the fact that more restrictive environmental requirements have eliminated and will most certainly continue to eliminate many materials currently in use in the stockpile. Many of the processes used to manufacture current products in the stockpile are no longer employable because of an increased emphasis on pollution prevention and the environment. As we develop new processes for existing materials or improved replacement materials, the drive to feature environmentally friendly technologies in these processes and as progenitors to environmentally benign materials will be the norm. Our ability to predict the aging, performance and response of new materials that result from environmentally-dictated

alterations to "the way things were" will be crucial to a rational effort to sustain and steward the stockpile well into the next millennia.

A move from these previous phenomenological recognition of material changes on aging to a comprehension of the basic science underlying safety and performance and then to prediction of future performance is required. At this point, the main DOE projects upon which chemistry and materials science must be husbanded are weapon dismantlement, and stockpile stewardship. Indeed, the question of how well materials age and in what type of synergistic relation with other materials in proximity becomes key to what is needed to guide DOE requirements in the future. Performing state-of-the-art science in this area of predictive model development virtually guarantees that these efforts will be of additional use to the private sector as their materials needs and concerns coalesce with the needs with which we are faced. This integration with a national science and industrial base will allow information and models to flow in both directions and assures a vital DOE effort in chemistry and materials for the future.

With the above facts in mind, it became apparent that a strategic plan for the DOE Defense Program Laboratories' chemistry and materials science technologies would be necessary to provide a vision for future chemistry and materials science efforts at the national laboratories. This Strategic Plan on Chemistry and Materials was not created in a vacuum. The overarching Department of Energy Strategic Plan has the recently completed National Security Strategic Plan (NSSP) as an intersection point for the Science & Technology, Environment and Industrial Competitiveness Plans. The Chemistry and Material Strategic Plan concurrently flows into and springs from a recently completed plan on SBSS and is closely allied with the NSSP. While the prime focus of the NSSP was on Reducing the Nuclear Danger and was clearly more global than any goal we recognize in this plan, in essence our goal is the same but is as a major cog in the overall NSSP wheel. The NSSP recognized and highlighted five focus areas: 1) Nonproliferation and Arms Control; 2) Stockpile Stewardship; 3) Drawdown and Disposition; 4) Technology Infrastructure and Core Competencies and; 5) Restructuring of the National Security Enterprise. Without exaggeration or expansive detail, it may be seen that Chemistry and Materials Science plays a central, if not lead, role in each of these focus areas. It cuts across them all and provides the unifying science base needed to further the efforts on national security. We have however chosen to highlight and expand what we believe to be the germane focus areas unique for chemistry and materials (*vide infra*).

The role of materials as a central cross cutting technology in the NSSP focus areas delineated above extends as well to the other Strategic Plans which are currently being contemplated, authored or recently completed. The Nuclear and non-Nuclear Components, System Integration, Manufacturing and Materials Technology, Advanced Surveillance, Computations and Test Plans all rely, as a major component of their strategies, on the incorporation of chemistry and materials as featured enabling sciences for their measurable milestones. The inclusion of a fundamental understanding of aging processes in each of these areas coupled with an increased predictive capability in materials models resulting from enhanced surveillance of in-service materials provides an underpinning technology base which each of these plans may use as a foundation to attain their strategic ends.

IV The Strategic Planning Process

The process for writing this plan began with the assembly of representatives of the three weapons design laboratories under the auspices of DOE DP-11 in September 1994. The charter was to create strategic plans for research and development in Chemistry and Materials and in Manufacturing which directly supported the strategic plan on Science Based Stockpile Surveillance. Two small tri-laboratory groups were formed, and they met several times jointly and separately to identify issues, linked visions, and synergistic strategies. During the month of December a series of workshops were held at the laboratories to present the draft plan and solicit comments from a wider, knowledgeable group.

1. Tri-Lab Working Groups;
2. Local Internal Workshops (12/94 Meeting);
3. Final iteration of DP Laboratories with DOE DP-10;
4. Combining Materials Strategic Plan with Advanced Manufacturing Strategic Plan;
5. Publication of the final Chemistry and Materials Science Strategic Plan.
6. Development of a Tri-Lab Implementation Plan

V. Chemistry and Materials Focus Areas

A. As-Built Materials Characterization and Performance

Strategic Goal: Understand the materials properties needed to meet key performance requirements in weapons components and subsystems sufficiently to certify replacement materials.

Priority Objective: Determine what materials properties, and their range of values, are required to meet designed performance specifications.

Issues:

- Previously materials could be demonstrated to be adequate through successful underground testing without a detailed knowledge of their key properties.
- Neither components nor subsystems can be proof tested by nuclear explosion testing.
- Current above ground explosive test results cannot be reliably scaled to underground test results of the past.
- The materials processing capabilities for manufacturing many nuclear and non-nuclear have been lost or changed so identical replacement materials are not available.
- Past characterization data are frequently not as informative as modern tools can produce.

Strategic Approach

- Develop characterization techniques and instrumentation to measure the performance of materials in tests which closely simulate nuclear weapon detonation and abnormal safety environments.
- Fabricate replicas of existing components using materials with a range of properties, and experimentally test their performance with techniques as realistic as possible.
- Develop models of materials properties to predict their performance in both nuclear explosive and abnormal safety conditions.

Success Indicators

- Critical components will have pertinent materials properties documented through experimental validation and computer simulations.

B. Materials Aging

Strategic Goal: Maintain the materials-related component performance and system surety at the designed level, independent of time in the stockpile.

Priority Objective: Develop the capability to accurately predict materials age-related reliability problems in the stockpile.

Issues

- The stockpile is required to function beyond its original certified design lifetime.
- The probability of common mode failures increases as the number of separate weapons systems in the stockpile decreases through dismantlement.
- Over time materials can change composition and microstructure, particularly at interfaces of dissimilar materials and in reactive environments.
- The reliability, safety, and performance of the stockpile degrades as materials age.
- The current surveillance programs are focused on identifying subsystem functionality and engineering or manufacturing defects rather than materials performance.
- The dismantlement program is not currently focused on capturing materials aging data. This is deemed appropriate because the data obtained from this source would not directly benefit the needed quantitative understanding.
- Replacement materials will need a reliability assessment in the component design phase.

Strategic Approach

- Develop and experimentally validate predictive aging models of materials.
- Develop analytical and characterization techniques for accelerated aging and instrumentation sensitive enough to detect aging changes in short times.
- Enhance the surveillance and dismantlement programs to incorporate quantitative materials characterization.

Success Indicators

- No stockpile failure surprises.
- Verified prediction of materials aging in a destructive test of weapons components.

C. Materials Synthesis and Processing

Strategic Goal: Have predictable and environmentally acceptable materials and processes available for manufacturing and recertification of new or replacement nuclear weapon components.

Primary Objective: Develop the knowledge and demonstrate the ability to synthesize and process materials with properties which meet design performance specifications by means with no adverse environmental impact and compatible with rapid prototyping and agile manufacturing.

Issues

- Limited Lifetime Components, remediation of known performance and surety deficiencies, and degradation of performance through the aging of materials will require a continuous program of component re-manufacture.
- ES&H issues will eliminate many synthesis, processing, and materials choices for re-manufactured components.
- Some synthesis and processing techniques used for original manufacture are now technologically obsolete and not available.
- Small lot fabrication due to cost, facilities limitations, and demand for only small numbers will challenge quality control and assurance.

Strategic Approach

- Develop environmentally conscious synthesis and processing techniques for component replacement materials that incorporate all elements and features required from a performance standpoint.
- Develop a knowledge of materials and processes adequate to design and build quality performance into components rather than inspect for quality after fabrication.
- Develop experimentally validated models and computer simulations of materials syntheses and processes sufficient to guarantee manufacturability, performance, and reliability of components.

Success Indicators

- Proven materials and processes are available to re-manufacture and re-certify stockpile components.

VI. Investment Strategy

Strategic Goal: Leverage DOE-DP research through strategic partnerships with industry, universities, and other federally funded programs.

Primary Objective: Develop a core DOE/DP program which will attract collaborative synergistic programs.

Issues:

- Funding for current DOE/DP programs has been and will probably continue to decrease.
- The level of funding currently available for stockpile surveillance is not sufficient for a comprehensive science based program.
- The materials related reliability of weapons components is not decreasing uniformly with time for all materials.
- The consequences of materials aging and reliability loss are more severe for some components than others.
- Valuable materials aging data from the current surveillance and dismantlement programs is being lost for lack of small incremental funding to obtain.
- Requirements for high product reliability and safety are not unique to nuclear weapons systems.

Strategic Approach

- Invest in a chemistry and materials program which is designed to yield a fundamental scientific understanding of materials and processes which will form the base for weapons and non-weapons technologies.
- Utilize synergistic programs in non-DP offices of DOE and other federal agencies.
- Establish partnerships with private industry to implement computer based modeling and simulation of materials synthesis and processing, validate process models, and develop a mutually beneficial knowledge base to improve product reliability.
- Develop collaborations among the DP weapons labs to take maximum advantage of established strengths and avoid duplication.
- Team with universities to expand the science basis of synthesis and processing and materials aging.

- Develop a prioritization methodology to identify and fund the most critical chemistry and materials problems associated with stockpile surveillance.

Success Indicators

- DOE/DP programs in the three focus areas will have non-DP collaborators and funding.
- Critical chemistry and materials programs for stockpile surveillance will be identified and funded.

Appendix: **Chemistry and Materials Definitions**

- Agile Manufacturing - Small-lot manufacturing environment with sufficient flexibility to promote rapid response to product design.
- Aging - The evolution of a material's composition and structure towards equilibrium. The evolution may be intrinsic, driven by internal gradients of intensive variables (chemical potentials, stress) or extrinsic, driven by environmentally imposed gradients and chemical reactions.
- Chemistry and Materials - A DOE/DP program element which, for purposes of this plan, specifically excludes energetic materials and actinides.
- Components - Functional sub-assemblies for designed weapon.
- Composition and Structure - The atomic and molecular description of what a material is. This encompasses multiple length scales and morphologies and includes chemical and structural defects.
- Dismantlement - The program of removing nuclear weapons from the enduring stockpile, disassembling them, functionally destroying components, and disposal of most materials as waste.
- Fabrication - Materials processing leading to functional weapon components.
- Performance - The utility of a material to a class of applications and its ability to function at the specified level.
- Production - Fabrication or procurement of components, sub-assemblies, or assemblies suitable for long term deployment in the nuclear weapons stockpile.
- Properties - How a material responds to changes in intensive thermodynamic variables such as temperature, pressure, and electric field.
- Rapid Prototyping - Fabrication of components, sub-assemblies, or assemblies suitable for demonstrating product performance and production process capabilities at the development level.
- Recertification - Experimentally validated performance determination of previously certified components or systems.
- Reliability - The component or system-specific ability to perform within design specifications and tolerances.

Chemistry & Materials Strategic Plan

- Remanufacturing - Fabrication of components, sub-assemblies, or assemblies using methods, materials, processes, or resources different from the original quality baseline.
- Science-based - The use of the scientific method and a fundamental physics and chemistry based understanding to determine the performance characteristics of components and systems.
- Surety - Safety and security doctrine applied to the protection of nuclear weapons.
- Surveillance - The current, routine process of destructively evaluating stockpile assets to substantiate continued reliable performance.
- Synthesis & Processing - How materials are made.

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