Plan for Metal Barrier Selection and Testing for NNWSI

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List of Acronyms

AISI - American Iron and Steel Institute

ASTM - American Society for Testing and Materials

CDA - Copper Development Association

CFR - Code of Federal Regulations

DOE - Department of Energy

ESCA - Electron scattering for chemical analysis

EIS - Environmental Impact Statement

FY - Fiscal Year

IN - Information Need

LLNL - Lawrence Livermore National Laboratory

NACE - National Association of Corrosion Engineers

NNWSI - Nevada Nuclear Waste Storage Investigations

NRC - Nuclear Regulatory Commission

NWMP - Nuclear Waste Management Program

OCRWM - Office of Civilian Radioactive Waste Management

QA - Quality assurance

QAPP - Quality Assurance Program Plan

SCC - Stress corrosion cracking

SCP - Site Characterization Plan

SIP - Scientific Investigation Plan

WBS - Work breakdown structure

Preface

The Department of Energy's Nevada Nuclear Waste Storage Investigations (NNWSI) Project is evaluating a site at Yucca Mountain in Nevada as a geological repository for the storage of high-level nuclear waste. The Nuclear Waste Management Projects (NWMP) at Lawrence Livermore National Laboratory (LLNL) has the responsibility for design, testing, and performance analysis of the NNWSI waste packages. One portion of this work is the selection and testing of the material for container construction. The anticipated container design is for this material to be a corrosion resistant metal called the metal barrier.

This document is the publication version of the Scientific Investigation Plan (SIP) for the Metal Barrier Selection and Testing Task. The SIP serves as a formal planning document for the investigation and is used to assign quality assurance levels to the activities of the task. This document is an informal version for information distribution and has the sections on 'Schedule and Milestones' and the 'Quality Assurance Level Assignment Sheets' removed.

Plan for Metal Barrier Selection and Testing for NNWSI

1.0 Purpose and Objectives

1.1 Regulatory Requirements

The purpose of the work outlined in this plan is to determine the rate at which the metal barrier will be degraded by its interaction with the repository environment and to project these determinations over the time scale of interest in demonstrating first, the containment of the waste, and second, the controlled release of radioisotopes. Several degradation mechanisms of the metal barrier are possible, and a significant effort in this plan is directed toward providing information which will be used in determining which of the several degradation mechanisms will operate in the repository environment. In addition, several candidate metal barrier materials are presently under consideration, and a large effort in this plan is directed toward providing information that will be used as the basis in selecting the material for the license application waste package design. A brief discussion of how the current list of candidate materials developed can be found in Section 6.0.

The information generated in this plan will be used to show that the waste package meets the containment requirements of 10 CFR 60.113. In addition, the information is used, in part, to demonstrate the waste package retrievability requirements in 10 CFR 60.111 (b). Along with information generated in the plans for waste form testing (both spent fuel and glass waste forms), the information from this plan will serve as a component in determining the source term for repository performance assessment modeling. Results from this work will provide the waste package environment task with information describing critical environmental parameters and how they affect the container material performance, thus indicating areas to be examined during the exploratory shaft investigations. Furthermore, the information will contribute, in part, toward estimating the source term in the calculation of long term cumulative releases. These calculations form part of the estimates of releases to the accessible environment required for 40 CFR 191.13 (cumulative releases after 10,000 years) and for completion of the site evaluation process required for 10 CFR 960.3-1-5 (cumulative releases after 100,000 years).

The Metal Barrier Selection and Testing Scientific Investigation Plan addresses the following SCP information needs:

Issue 1.4: Will the waste package meet the performance objective for containment as required by 10 CFR 60.113?

- IN 1.4.1 Waste package design features that affect the performance of the container.
- IN 1.4.2 Material properties of the container.
- IN 1.4.3 Scenarios and models needed to predict the rate of degradation of the container material

Through input to the above information needs, the work covered by this plan will also provide data used to address information needs 1.4.4 and 1.4.5 (Performance assessment for containment objectives); 1.5.4 and 1.5.5 (Performance assessment for controlled release objectives); 1.10.1 and 1.10.2

(Waste package design), 2.6.1 (Preclosure design criteria concerned with materials, handling, and identification), 4.3.1 (Waste package production technology), and 4.5.1 (Waste package costs).

1.2 Metal Barrier Selection and Testing Activities Grouped by SCP Investigations

The investigations and activities of the three 1.4 Information Needs (IN) from the Site Characterization Plan (SCP) are grouped as follows: (1) IN 1.4.1 is concerned with characterization of the as-fabricated and as-emplaced waste package container; (2) IN 1.4.2 is concerned with characterization of the waste package container after emplacement (hence the emphasis on different degradation modes); and (3) IN 1.4.3 is concerned with modeling to predict the rates of these different degradation modes.

There is not a one-to-one correspondence between the full set of investigations and activities listed under the above INs and the activities described in this Scientific Investigation Plan (SIP) for the Metal Barrier Selection and Testing Task (WBS 1.2.2.3.2). This situation occurs because the 1.4 Issue and subsumed Information Needs exist to resolve containment issues, while the content of this SIP is addressed specifically to the metal barrier, which is not the only engineered containment barrier. Thus, the investigations and activities associated with the properties of a ceramic liner in IN 1.4.1, 1.4.2 and 1.4.3 as an alternative waste package design are discussed in the SIP for "other materials" (WBS 1.2.2.3.3). The Metal Barrier SIP is centered around laboratory testing, development of models to predict resistance to various degradation modes, and characterizing the properties of the candidate metals and alloys as materials of construction. The characteristics of the processes for actually fabricating the container and constructing the waste package are, therefore, discussed in the SIP for "Design, Fabrication, and Prototype Testing" (WBS 1.2.2.4). Thus, some of the activities discussed in IN 1.4.1 more logically fall into that SIP. There is the obvious need for close co-operation between the activities for these different WBS element SIPs, hence the identification of integration activities between the appropriate plans.

Although the Metal Barrier SIP has several features analogous to those found in the SIPs for characterizing the spent fuel and the borosilicate glass waste forms (WBS 1.2.2.3.1), there are two unique features of the Metal Barrier SIP that distinguish it and influence the course of the planned activities. These features are:

(1) the process for specifying which of the several candidate materials will be selected for the license application design. In order to arrive at a defensible selection process, many of the activities must be conducted in parallel for the different candidate materials. This means that a number of activities will be carried out to a level to provide needed information for the selection process, but that the full suite of activities will be completed only for the candidate material that is selected for the license application design.

(2) much information on characterizing the candidate metals comes from the open literature and from various commercial sources, including potential vendors for the container material. The information often derives from non-nuclear applications. Unlike information on other materials that are part of the waste package (e.g. borosilicate glass or uranium dioxide fuel elements), these sources of information are largely outside the control of the DOE, NRC, or other governmental agencies.

This has important quality assurance implications with regard to the number of possible sources of information and the completeness of the documentation. Because a strong argument for the selected container material will be built on previous and successful uses of the material in other engineering applications, it is vital to use available information on performance of the candidate materials. Therefore, a considerable effort is involved in determining what previously published information in the technical literature is relevant and applicable to the present work.

METAL BARRIER WORK OUTLINE FROM SCP

Note: The asterisked (*, **) investigations and activities from the SCP (as listed below) are not discussed in the Metal Barrier Selection and Testing SIP. Discussions of these will be found in the SIP for Design, Fabrication and Prototype Testing (items marked *), and in the SIP for Other Materials (items marked **).

Info Need	Investigation	Activity	
1.4.1	Waste package design features that affect the performance of the container		
	1.4.1.1	Integrate design and materials information (metal container)	
		1.4.1.1.1	Mechanical properties
		1.4.1.1.2	Microstructural properties
		*1.4.1.1.3	Physical properties
		*1.4.1.1.4	State of stress in the container
		*1.4.1.1.5	Characterization and inspection of weld integrity
		*1.4.1.1.6	Characterization of the container surface
	**1.4.1.2	Integrate design and materials information (metal container with a ceramic liner)	
		**1.4.1.2.1	Feasibility evaluation of fabricating a ceramic-lined waste package
1.4.2	Material properties of the container		
	1.4.2.1	Selection of the container material for the license application design	
		1.4.2.1.1	Establishment of selection criteria and their weighting factors
		1.4.2.1.2	Material selection

Info Need	Investigation	Activity

1.4.2.2 Degradation modes affecting candidate copper-base container materials

- 1.4.2.2.1 Assessment of degradation modes in copper-base materials
- 1.4.2.2.2 Metallurgical aging and phase stability
- 1.4.2.2.3 Low temperature oxidation
- 1.4.2.2.4 General aqueous corrosion
- 1.4.2.2.5 Hydrogen entry and embrittlement
- 1.4.2.2.6 Pitting, crevice, and other localized attack
- 1.4.2.2.7 Stress corrosion cracking
- 1.4.2.2.8 Other potential degradation modes

1.4.2.3 Degradation modes affecting candidate austenitic container materials

- 1.4.2.3.1 Assessment of degradation modes in austenitic materials
- 1.4.2.3.2 Metallurgical aging and phase transformations
- 1.4.2.3.3 Low temperature oxidation
- 1.4.2.3.4 General aqueous corrosion
- 1.4.2.3.5 Intergranular attack and intergranular stress corrosion cracking
- 1.4.2.3.6 Hydrogen entry and embrittlement
- 1.4.2.3.7 Pitting, crevice, and other localized attack
- 1.4.2.3.8 Transgranular stress corrosion cracking
- 1.4.2.3.9 Other potential degradation modes

**1.4.2.4 Degradation modes affecting the ceramic liner

- **1.4.2.4.1 Assessment of the degradation modes affecting the ceramic liner
- **1.4.2.4.2 Laboratory test plan for ceramic liner materials

Info Need	Investigation	Activity

1.4.3 Scenarios and models needed to predict the rate of degradation of the container material

1.4.3.1 Models for copper and copper alloy degradation

1.4.3.1.1 Metallurgical aging and phase stability

1.4.3.1.2 Low temperature oxidation

1.4.3.1.3 General aqueous corrosion

1.4.3.1.4 Hydrogen entry and embrittlement

1.4.3.1.5 Pitting, crevice and other localized attack

1.4.3.1.6 Stress corrosion cracking

1.4.3.1.7 Other potential degradation modes

1.4.3.2 Models for austenitic material degradation

1.4.3.2.1 Metallurgical aging and phase transformations

1.4.3.2.2 Low temperature oxidation

1.4.3.2.3 General aqueous corrosion

1.4.3.2.4 Intergranular attack and intergranular stress corrosion cracking

1.4.3.2.5 Hydrogen entry and embrittlement

1.4.3.2.6 Pitting, crevice, and other localized attack

1.4.3.2.7 Transgranular stress corrosion cracking

1.4.3.2.8 Other potential degradation modes

**1.4.3.3 Models for ceramic material degradation

**1.4.3.3.1 Dissolution of alumina

**1.4.3.3.2 Loss of fracture toughness

At the present time, the NNWSI Project is considering the technological feasibility of producing a ceramic-lined metal container as a waste package design option. In such a case, the long-term container performance function would largely be taken by the ceramic material with the function of the metal to be largely limited to the handling and emplacement operations. If the Project were to choose this option, then much of the work discussed in this SIP would be truncated.

1.3 Activity Groupings for the Metal Barrier Selection and Testing SIP

For this plan, certain of the above activities group together naturally because of parallel efforts (e.g. model development for the various degradation modes in each alloy system; laboratory test plans corresponding to each degradation mode) and because these grouped activities have the same determined quality assurance levels. These groupings define the activities of the Metal Barrier Selection and Testing task as described in this SIP.

Metal Barrier Selection Process (see sections 2.2 and 3.2)

- E-20-13 Degradation mode surveys
- E-20-15 Establishment of criteria for metal barrier selection
- E-20-19 Metal barrier selection

Metal Barrier Performance Modeling (see sections 2.3 and 3.3)

- E-20-16 Development of models for degradation modes, mechanical properties, and microstructure
- E-20-20 Integration of models for selected material
- E-20-21 Performance parameter studies
- E-20-25 Validation of model

Metal Barrier Performance Testing (see sections 2.4 and 3.4)

- E-20-17 Experimental technique development
- E-20-18 Parametric studies of metal degradation and microstructure
- E-20-22 Development of plans for license application support tests
- E-20-23 License application support tests

Design Properties of the Metal Barrier (see sections 2.5 and 3.5)

- E-20-14 Coordination with package design
- E-20-24 Determination of mechanical and microstructural properties of metal

The numbers assigned to these thirteen activities are in approximate chronological sequence of occurance.

The following list is a cross reference between the activities from the SCP Information Needs of Issue 1.4 and the activities described in this plan. The titles of the activities are given in the preceding lists. There is not a one-to-one correspondence, and not all of the activities from this plan are included, because E-20-13 is a precurssor to other work in this plan and does not directly correspond to activities in the Information Needs.

SIP Sections	SIP Activity Number	SCP Activity Number
2.5 and 3.5	E-20-24	1.4.1.1.1, 1.4.1.1.2
	E-20-14	1.4.1.1.3, 1.4.1.1.4, 1.4.1.1.5, 1.4.1.1.6
2.2 and 3.2	E-20-15	1.4.2.1.1
	E-20-19	1.4.2.1.2
2.4 and 3.4	E-20-17, E-20-18, E-20-22, E-20-23	1.4.2.2.1, 1.4.2.2.2, 1.4.2.2.3, 1.4.2.2.4, 1.4.2.2.5, 1.4.2.2.6, 1.4.2.2.7, 1.4.2.2.8, 1.4.2.3.1, 1.4.2.3.2, 1.4.2.3.3, 1.4.2.3.4, 1.4.2.3.5, 1.4.2.3.6, 1.4.2.3.7, 1.4.2.3.8, 1.4.2.3.9
2.3 and 3.3	E-20-16, E-20-20, E-20-21, E-20-25	1.4.3.1.1, 1.4.3.1.2, 1.4.3.1.3, 1.4.3.1.4, 1.4.3.1.5, 1.4.3.1.6, 1.4.3.1.7, 1.4.3.2.1, 1.4.3.2.2, 1.4.3.2.3, 1.4.3.2.4, 1.4.3.2.5, 1.4.3.2.6, 1.4.3.2.7, 1.4.3.2.8

1.4 Information Flow

The goals of metal barrier selection and testing are to select one (or two) material(s) from the present list of six candidates that will be used for advanced waste package design work and to test the selected material(s) to provide adequate data for models concerning the long-term chemical and metallurgical stability of the material(s) under anticipated conditions and a reasonable number of credible but unanticipated conditions. The present list of candidates are AISI 304L, AISI 316L, and Alloy 825 in the "austenitic" family and CDA 102, CDA 613, and CDA 715 as copper-base materials.

As illustrated in Figure 1, information from sources outside this plan is required for several of the activities of this plan. These outside sources, labeled as 'Information Input', include previously published information in the technical literature on the degradation modes of the candidate materials, previous results from NNWSI-sponsored work on metal barrier investigations, NNWSI-sponsored work on the near-package environment, work on other material components of the waste package and engineered barriers (including borehole liners, cements, and grouts), performance assessment scenarios, and geochemical modeling (to derive the physical and chemical environment surrounding the waste package container). Another input will be the use of the EQ3/6 code in the selection process.

Another source of "information" from outside the Metal Barrier Selection and Testing task is in the box labeled 'Working Constraints' in Figure 1. These include the performance requirements established by the various Federal regulations, the assessment of the repository environment before and after emplacement of the waste packages (including the DOE-NRC approved definitions of anticipated and unanticipated processes and events), and the preliminary design requirements (Conceptual Design Level). A unique feature of the Yucca Mountain site is that the repository will be located in the unsaturated zone, above the permanent water table. An important advantage of this location is that some of the environmental features can be "engineered" to create more favorable conditions to prolong the container lifetime. A good example of engineering the environment is to maintain the temperature at the container surface above the unrestrained boiling point of water for as long as possible on a large majority of the waste packages. This is done by considering the heat load per package and configuring the repository with a suitable heat load per unit area. As part of the NNWSI strategy to demonstrate the containment objectives, the waste package container (metal barrier), the waste form, and the engineered environment are jointly considered as the "containment barrier". This strategy is more fully explained in the discussion of the resolution of Issue 1.4 in Chapter 8 of the SCP. The regulatory requirements, the waste package design requirements and the repository environment assessment (including ways to engineer the environment to enhance the waste package performance) are viewed as constraints, because they establish some limits on what must be accomplished in the activities in this plan.

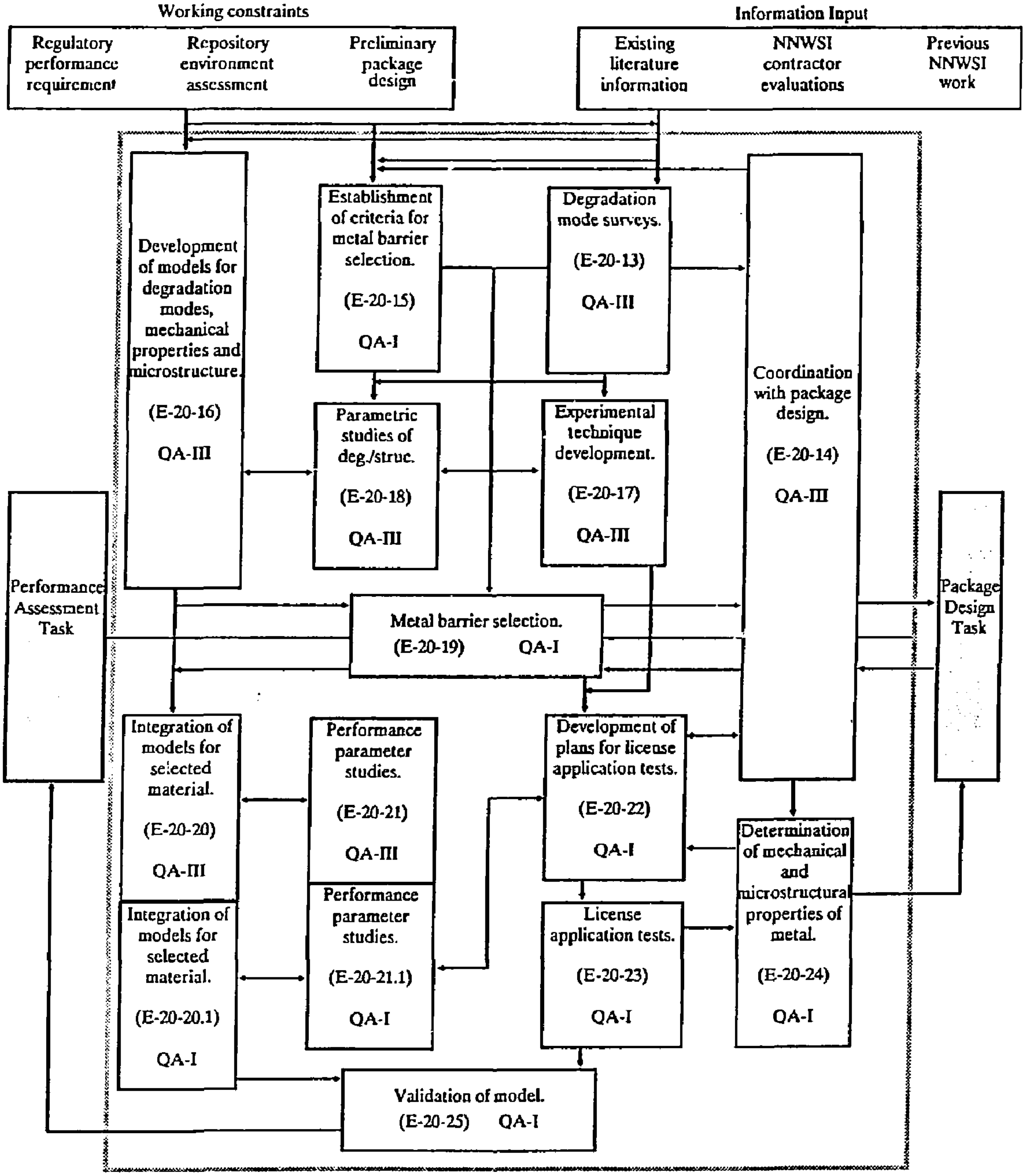
As seen in Figure 1, the activities in this plan are naturally divided into two parts, separated by the selection step. Up until this selection the work covers all six initial candidate metals, including three austenitic alloys and three copper-base alloys. The three austenitic alloys are iron-base (stainless steels) and nickel-base (alloy 825) with the primary phase (austenite) being a face-centered cubic structure in all alloys. The copper-base alloys are also face-centered cubic in structure. All of these materials are hardened by solute additions or by cold work; all of the materials possess considerable ductility over a wide range of temperatures. These materials are widely used in industrial and structural applications; a major reason for their use is good corrosion resistance in many different kinds of environments, although the candidate materials differ on the limits of environmental conditions in which they can be successfully used. In the most general considerations of materials, all of the candidate materials are reasonably simple in microstructure (no intentional secondary phases for hardening), although there are important differences among the candidates on this point. While a high-purity copper is one of the candidate materials, this material, too, can be regarded as a dilute alloy. In fact, it may be desirable to add or retain some deoxidizing elements (in the 100's to 1000's ppm range) to make the material more readily weldable and to prevent formation of internal copper oxides. Thus the words "alloy" and "material" are used interchangeably and synonymously in this SIP.

Criteria for selecting the material(s) or alloy(s) for use in the final design must be decided upon, and an information base prepared to support these criteria. This information base includes corrosion models, corrosion data, existing literature, and evaluations from authoritative sources in the metals industry. After the selection of the alloy(s), the activities concentrate on generating a validated model for the material(s) performance in the repository environment. This model will be confirmed by laboratory tests. In effect, those elements of the plan above the "selection" activity in Figure 1 are directed toward making that selection. Those activities below the "selection" are directed toward validation of the long term performance model of the metal selected. When this task is completed, the validated model will become a portion of the overall repository performance assessment model used to support advanced designs and the license application.

Two other waste package tasks that have substantial interaction with the Metal Barrier Selection and Testing Task are shown in Figure 1: the Waste Package Design, Fabrication and Prototype Testing Task and the Waste Package Performance Assessment Task. There must be interaction between the Metal Barrier Selection and Testing work and the work in these two tasks to provide coordination as the work evolves. This is to insure that the metal barrier selected will be compatible with the design and fabrication features being researched (and vice versa), and that the degradation models developed in this task will mesh when needed with the overall performance model. The output from this task will be: 1) the selection of one (or two) alloys, a description of mechanical and microstructural properties, and performance confirming tests, provided to the Design Task; 2) validated models to describe the behavior of the material under repository conditions provided to the Performance Assessment Task.

Information from some additional waste package tasks (not shown explicity in Figure 1) influences the course of activities in the Metal Barrier Selection and Testing Task. To a lesser extent, information from the Metal Barrier Selection and Testing Task is used in these tasks but does not have a primary influence on the course of work planned in them. Information about the environment near the container surface comes from the Environment Task and is shown in Figure 1 as one of the "Information Inputs" and one of the "Working Constraints". The primary concern is the environment outside the container, but in a few instances there is concern about the environment inside the container. This information is important in analyzing the degradation modes for the candidate materials. Information derived in the Metal Barrier Task on corrosion of candidate materials influences the Environment Task and also the Waste Form Testing Task. Corrosion products formed during the long-term degradation of the container will influence the waste package environment (particularly if the products are somewhat soluble and can be transported) and may degrade the performance of the waste form. The "compatibility" of the package container and the waste form is proposed as one of the factors in selecting the container material. Output from the Metal Barrier Selection and Testing Task on corrosion product formation is one of many factors that goes into the EQ3/6 geochemical code, shown in Figure 1 as the Performance Assessment Task.

Figure 1
Metal Barrier Selection and Testing Information Flow



2.0 Rationale for Selected Activities and Quality Assurance Level Assignments

The rationale for the four work areas and thirteen activities listed in Section 1.2, and their QA level assignments are discussed in this section.

2.1 Introduction

The work in this plan is the content of WBS element 1.2.2.3.2 (Metal Barrier Selection and Testing) and is concerned with the long-term models to predict the mechanical and microstructural properties of the container material, and the rates of occurrence and rates of propagation for the different possible degradation modes. In most cases, the environmental, mechanical, and metallurgical factors that cause the different degradation modes are known from previous experience with the candidate materials, so that the starting point for model development comes from observation, measurement and understanding of those environmental, mechanical, and metallurgical factors that influence these degradation modes in the context of the repository setting. Laboratory work is centered around quantifying these degradation modes in the time periods generally available for laboratory testing (periods ranging from several hours to a few years). The general purpose of this laboratory work is to determine the rates of the different degradation modes as they relate to the physical, chemical, and mechanical properties of the container material and its surroundings. Confidence is gained in the model development by predicting to progressively longer time periods what is expected to occur and then actually conducting experiments or tests over those time periods to confirm the prediction. The rationale of this approach is to begin the laboratory activities in more highly aggressive conditions than expected (where the phenomenon under investigation is accelerated to occur in a short period of time) and then to reduce the aggressiveness of the conditions in order to approach the anticipated environmental conditions as a limit (where the same phenomenon occurs in progressively longer time periods). As needed, the models are modified in accordance with the results from the laboratory work.

In parallel with modeling and laboratory activities, this task will also select one (or two) materials for advanced study from the preliminary list of candidates. This selection process provides a dividing line between broad-based preliminary screening activities and the detailed final activities producing documentation for a license application design metal barrier. As noted above, this task will also interface with two others: waste package design and performance assessment. The intent of these interface activities is to insure that the results of this task are compatible with the results and requirements of these other efforts, and to keep the effort of this Scientific Investigation Plan directed toward the same goals as the other program elements.

2.2 Metal Barrier Selection Process

These activities describe the process for selecting one or two materials for advanced design and performance testing. A set of criteria for material or alloy selection is needed to compare candidate materials with one another. An initial set of 'survey papers', each of which assesses the importance of particular degradation modes to a family of alloys, will provide a framework for evaluating the performance of candidates in the selection process. The selection process includes the documentation and review requirements for metal barrier selection.

Activity E-20-13 Degradation mode surveys

The 'Degradation mode surveys' (E-20-13) are a consolidation of available information related to the expected performance of the two families (copper-base and austenitic) of candidate alloys with respect to each particular mode of degradation (e.g. localized corrosion). The surveys will specifically concentrate on documentation of data needed to compare degradation rates of the container material over long time periods. The degradation modes are defined as chemical or mechanical processes (and sometimes combinations of these) that penetrate the metal structure and ultimately perforate it. The reason for separating the processes into the different modes is that the penetration follows different propagation patterns. These modes are explained more fully in the parts of Chapter 7 and 8 of the SCP dealing with metal barriers and in several texts on corrosion of metals - see Section 7.0 of this SIP.

The rate of perforation of the metal container and the number of containers perforated are important factors in demonstrating the performance of the waste package for containment and of the engineered barrier system for controlled release. The goal is to determine for each candidate alloy which degradation modes are insignificant, which are potentially significant, and which appear to limit an alloy in meeting the performance objectives. The rationale for this activity is that a great deal of information is available on metal performance, but it must be evaluated and applied to the specific case of a metal barrier in a Yucca Mountain waste container to assess the prospects for repository performance. Thirteen combinations of alloy family and degradation modes have been identified for assessment. Completion of these surveys will provide documented statements of potential alloy performance, which will serve as the input to the selection process. The data assessed will also provide input to model development.

This activity (E-20-13) will be conducted at QA Level III. The container material selection criteria (E-20-15) and the selection process itself (E-20-19) will be conducted at Level I. However, the survey information that is used in the selection is not directly tied to the license application data, which will be generated after the container material selection. The purpose of the survey information is to guide the work that will be followed once the selection is made. Much of the basic information to be used in the survey of degradation modes comes from the open technical literature, which does not have a QA level associated with it.

Activity E-20-15 Establishment of Criteria for Metal Barrier Selection

The criteria for selection of a metal barrier alloy(s) for advanced work must be developed, reviewed, and approved. Activity E-20-15 'Establishment of criteria for metal barrier selection' is the process of defining those criteria. The rationale for this work is that a metal barrier material cannot properly be chosen until the criteria for selection are established and accepted by a process of peer review and comment as provided for in the Quality Assurance Program Plan (QAPP) of the Nuclear Waste Management Program (NWMP).

This activity will be conducted at QA Level I. The reason for this level assignment is that the selected material and the defense of its selection are fundamental bases of the license application data base. The container material selection is also an important project milestone, and its delay would cause considerable slip in the project schedule. This fact alone would make the material selection and selection criteria Level II, but the fact that the primary intention of the activity is to provide the reasons for selecting the material for the license application design makes the activity Level I.

Activity E-20-19 Metal barrier selection

'Metal barrier selection' will be performed in activity E-20-19. Input for the selection will come from the performance models developed in this task and described in section 2.3, from the degradation surveys described above, and from the parametric studies described in section 2.4. The selection will be based on the criteria described in activity E-20-15, and will also be subject to peer review and comment. The rationale for selecting the barrier material(s) before the completion of model development and validation testing is that much more time and effort are required for validation of the performance model than for an informed and defensible selection. That is, a variety of candidates can be examined to a level that determines which ones are conservatively sufficient to meet the performance requirements, and to rank them in terms of performance. That is all that is required at this level to narrow the candidate list to one (or two). Much more work is then required to complete the long term performance model and validate it with testing. This larger effort, which is required for repository performance assessment but not for material selection, can then be focused on the selected alloy(s).

This activity is assigned QA Level I. The rationale for this assignment is the same as that given for the previous activity on the selection criteria, because the material selected and the defense of the selection are a fundamental part of the data that will be generated to support the license application. The reasons that the criteria for selection and the selection process itself are split into two activities are (A) to allow the timing sequence of the two activities, (B) to allow a possible change in the composition of the peer review panel for the two activities, and (C) to document the selection criteria and the selection process as separate activities.

In summary, the three activities for the Metal Barrier Selection Process Area are:

Activity No.	Name	QA Level
E-20-13	Degradation mode surveys	III
E-20-15	Establishment of criteria for metal barrier selection	I
E-20-19	Metal barrier selection	I

2.3 Metal Barrier Performance Modeling

These activities are directed toward producing models of material degradation for use in the selection process, and then integrating these degradation models into a metal barrier performance model of the alloy(s) selected, to be validated by laboratory tests and utilized by the repository performance assessment task. Model development work will be conducted at QA Level III. The models will be validated at Level I and data for parameters central to the model will be collected at Level I.

Activity E-20-16 Development of models for degradation modes, mechanical properties and microstructures

Activity E-20-16 'Development of models for degradation modes, mechanical properties and microstructures' will serve two primary purposes. One purpose of this activity is to provide support for the selection process. Degradation models, primarily related to the corrosion resistance of the materials but occasionally concerned with retention of fracture toughness, are based on established electrochemical and metallurgical principles. These models address those modes deemed important to long term performance as guided by the degradation mode surveys, described in Section 2.2. Data input will include the metallurgical literature (especially that which is related to corrosion), and previous NNWSI experimental work. Closely related to modeling the degradation modes are modeling activities for characterizing the mechanical and microstructural properties of the as-fabricated container and the changes that will occur ('aging phenomena') as a function of time in the repository.

For the second purpose of this activity, those models applicable to the selected alloy will be further developed and integrated into a long-term metal barrier performance assessment model to be validated and used by the repository performance assessment task in the advanced design and licensing phases. The rationale is to develop individual degradation mode models for all of the processess which must be considered in the selection activity, then combine those models which are relevant to produce a unified performance assessment model for the container. Thus, the model development activity begins before container material selection and continues for some time after the selection process.

The models for degradation modes can be broken into 'sub-models'; in some cases this is an advantage because some aspects of the degradation process will be more amenable to modeling than other aspects. One example is that the detection of a sensitized microstructure in austenitic stainless steels and nickel-base materials is more readily modeled than the environmental aspects of intergranular attack and intergranular stress corrosion cracking. Another example is that ammonia formation (such as by radiolysis of atmospheric gases) is more readily modeled than the metallurgical or mechanical aspects of stress corrosion cracking in copper and copper-base alloys. In both cases (sensitization or ammonia formation), the process being modeled is the critical step in the degradation mode and can be modeled with greater confidence because the model is confined to either the container material (sensitization) or to the environment (ammonia formation). This point is discussed further in Section 3.3.1.

This activity on model development is assigned QA Level III. The reason for this level assignment is that the individual models themselves are not directly part of the license data base (Level I), nor is the general 'integration' of the models into a single performance model. QA Level III parametric studies (E-20-18) support development of these models (discussed in Section 2.4). The activity on model development (and model integration) does not have a major impact on project schedules or on design phases to conduct comparisons of alternatives (criteria for Level II assignment). However, preparation of the integrated performance model for use in support of the license application (E-20-20.1), the data to support it (E-20-21.1), and validation of the model (E-20-25) are Level I activities. The validation will be made according to results of key performance parameter studies (E-20-21.1) and with data generated under license application support tests (E-20-23). Both E-20-21.1 and E-20-23 are QA Level I activities.

Activity E-20-20 and E-20-20.1 Integration of models for selected material

The 'Integration of models for selected material' activity (E-20-20 and E-20-20.1) follows the previous development phase and the alloy selection. Those degradation models which apply to the alloy(s) selected must be integrated with the design features and repository environment information to produce a long term performance model for the waste package. The reason for this 'integration' activity is that more than one degradation mode can occur at a time. The model associated with aging effects in the container, including the mechanical and microstructural property changes associated with these, and the model associated with low temperature oxidation of the container are applicable from the time the container is emplaced in the repository, while many of the other models (especially those associated with aqueous corrosion phenomena) are applicable to certain time periods or when certain conditions occur in the repository.

The environment around the container will change with time, and waste packages at different locations in the repository will experience different environmental conditions. The containers themselves will be produced over a 25-30 year period of time, and will conceivably have some variation in composition and microstructure. All of these factors will determine when a given model is 'in effect' and when it is not.

This activity is split into two parts with different QA levels because much of the work to integrate the models does not support license application directly but is the process of getting the performance model working correctly. Thus activity (E-20-20) is assigned QA Level III for the same reasons given for assigning the model development activity (E-20-16) Level III. The primary purpose of the integration is to 'allocate' among the several models over what portion of time and over what portion of container population the individual models are applicable. The portion of this activity which is assigned QA level I (E-20-20.1) involves preparation of the parametric data from E-20-21.1 and predictions of container performance. This will be used to support the license application and other critical programmatic decisions in other tasks such as container design and fabrication where the metal barrier performance is important. The parametric data for this activity comes from E-20-21.1 which is also QA level I.

<u>Activity E-20-21 and E-20-21.1 Performance parameter studies</u>

'Performance parameter studies' (E-20-21 and E-20-21.1) is an activity to interface with the integration of the individual models (E-20-20 and E-20-20.1), described above. This activity involves gathering <u>key</u> parametric input for the integrated metal barrier model, and guaranteeing that the metal barrier model is consistent with the requirements of the repository performance model. It will also provide any additional parametric data needed to complete the individual degradation models. The word 'key' is used here because the parameters that will be studied are those that are identified as being important because of their strong influence on those degradation modes that are determined to be central in predicting container lifetimes in the time periods of concern. Identification of these key parameters comes after container material selection and after the model development work has indicated which parameters have the greatest sensitivity toward the process being modeled (activities E-20-18 and E-20-16). This 'Performance parameter studies' activity may include data collection from outside the project and certification of this data according to the appropriate quality assurance provisions to allow its use to directly support Level I work; this activity may also include laboratory tests. Tests would be performed under this activity if they were not direct performance tests, such as those in activity E-20-23.

This activity is split into two parts with different QA levels because some of the information required for model integration (E-20-20) is of a general nature and does not directly support either the model validation or the license application design, and some of the information does support these Level I activities. The first portion of the activity, E-20-21, which is assigned QA Level III, supplies information on all of the physical, chemical, metallurgical, and mechanical parameters that have some influence on metal performance. It is similar in nature to activity E-20-18 but is focused on the selected material and supports model integration rather than general development. The second portion of this activity is E-20-21.1 and is assigned QA Level I. The rationale for this assignment is that this activity directly supplies input required for completion of the performance model (E-20-20.1 and E-20-25), QA Level I activities that will be used in the license application data base. Activity E-20-21.1 classifies information with regard to its importance and reviews and certifies information needed for QA Level I activities. Documentation of these decisions becomes a central factor in completing the modeling work in the Metal Barrier Selection and Testing Task.

Activity E-20-25 Validation of model

'Validation of model' (E-20-25) will validate the integrated metal barrier degradation model by comparison to QA Level I test data. As described earlier, the model will be based on accepted electrochemical and metallurgical principles. The rationale is to verify that the model is phenomenologically correct by comparison to laboratory tests which map a parameter space in corrosion environment and time. Demonstration that the model accurately predicts the results of these tests will be used to validate the model for use in the Repository Performance Assessment. If suitable natural analogs can be found, they will be used to enhance the validation of the time parameterization. The peer review process may also be used to support model validation.

This activity is assigned QA Level I, because the results of the validation will be a critical part of the data submitted in support of the license application.

In summary, the activities under the Metal Barrier Performance Modeling area are:

Activity No.	Name	QA Level
E-20-16	Development of models for degradation modes, mechanical properties, and microstructure	III
E-20-20 E-20-20.1	Integration of models for selected material	III I
E-20-21	Performance parameter studies	III
E-20-21.1	Performance parameter studies	I
E-20-25	Validation of model	I

It should be noted here that detailed model development and validation plans cannot be provided until after the material selection process is completed.

2.4 Metal Barrier Performance Testing

Laboratory testing of metal barrier performance is required for three reasons. First, in the time leading up to selection of one (or two) alloys, experiments will provide data to the degradation modeling effort and will help guide the selection process. After selection, there will be a need for QA level I input into the degradation models as they are consolidated into a container performance model. Finally, tests will be needed to provide support for validation of the metal barrier model over a range of repository-relevant parameters.

Activity E-20-17 Experimental technique development

Activity E-20-17 is 'Experimental technique development'. Custom laboratory tests are likely to be needed. Standard corrosion test procedures should be adequate for most general material surveys and some of the model development support. However, to precisely conform to the modes of degradation experienced in a repository environment, and to vary the parameters of tests in the same way that the models vary parameters, custom techniques, using recent advances in electrochemical and surface sciences, may be required. To measure the slight degradations experienced in the relatively benign environments expected in experiments and tests performed within reasonable time scale, enhanced sensitivity is required in some experimental techniques. Examples of some techniques that may be employed are discussed in Section 3.4.1.

The work in this activity will be conducted at QA Level III. This is truly experimental work. There is some technological risk involved in undertaking this kind of work in that not all of the promised advances in techniques will necessarily give useful results. On the other hand, there are considerable benefits to be gained if mechanistic arguments can be successfully made about how fundamental electrochemical and metallurgical processes operate, in order to make the unique long-range characterization and performance predictions required for nuclear waste disposal. The bulk of the work undertaken in activity E-20-23 (License application support tests) will likely use standard test procedures and recommended practices developed by professional organizations such as ASTM, NACE, and others. These tests have widespread use and acceptance; however, acceptance of new kinds of tests by professional organizations is a slow process. A good part of the effort in activities E-20-22 and E-20-23 (both QA Level I activities) will be concerned with selection of test methods to use in generating the license application data. The result of work performed in activity E-20-17 is to determine whether some of these advanced techniques should be included in those Level I activities.

Activity E-20-18 Parametric studies of metal degradation and microstructure

During the development of degradation mode models described in Section 2.3 corrosion data will be required that are not available from other sources or are unique to Yucca Mountain repository conditions. These will fall under activity E-20-18 'Parametric degradation studies'. The rationale is to provide the container material selection and model development activities in a timely manner.

The behavior of the container material depends on several physical, chemical, metallurgical, and mechanical parameters; identification of which of these parameters are the central or key ones to predicting the performance under repository conditions is needed to proceed toward generating meaningful data for the license application. This activity begins before selection of container materials for advanced design work and continues until the selection process is completed. After selection of a container material, information gathering and key parameter identification is continued under activity E-20-21.

This activity will be conducted at QA Level III. The information that comes out of this activity will not be used directly in the license application, but it will identify those parameters that will be used in generating the QA Level I work in activities E-20-21.1, E-20-22, and E-20-23.

<u>Activity E-20-22 Development of plans for license application support tests</u>

After selection of an alloy(s) for advanced design work, a set of QA Level I tests must be planned in conjunction with the model integration work of Section 2.3 to allow eventual validation of the metal barrier performance model. Such tests cannot be conducted until a comprehensive set of test plans has been prepared, reviewed, and accepted. Preparation of these plans in activity E-20-22 'Development of plans for license application support tests' includes a review and comment process to ensure that the scope, accuracy and precision of the tests will be adequate for performance confirmation.

This planning activity will be developed at QA Level I. Documentation of how decisions were reached with regard to selection of test methods and selection of key parameters is needed to directly support the license application data (criterion for Level I). As indicated in the information flow diagram (Figure 1) and in discussions in the text on related activities, the plans will be periodically revised as important new information becomes available, for example from activity E-20-17 on technique development or from activities E-20-21 and E-20-21.1 on parametric investigations.

<u>Activity E-20-23 License application support tests</u>

The most intensive laboratory work in this task is in activity (E-20-23) 'License application support tests'. These tests, as planned in the activity described above, will be used to validate the metal barrier performance model, and will provide data to predict the expected long term metal barrier performance. The rationale behind these tests will be to test the alloy(s) chosen over a range of environment and time combinations to provide data for use in specially designed tests for validating the integrated performance model of the metal barrier, as described in activity E-20-25. Severe environments will produce measurable degradation in accessible times to validate models of the degradation process. Monitoring the decrease in the degradation kinetics as the environment tends toward that in the repository will provide validation of the time parameterization in the models. Long-time natural analogs, if available, will allow further validation in the time parameter. This activity will be conducted at QA Level I. The reason for this assignment is that this activity will generate license application design data.

In summary, the activities in the Metal Performance Testing area are:

Activity No.	Name	QA Level
E-20-17	Experimental technique development	III
E-20-18	Parametric degradation studies	III
E-20-22	Development of plans for license application support tests	I
E-20-23	License application support tests	I

It should be noted here that detailed plans for activities E-20-22 and E-20-23 cannot be developed until after the material selection process is completed.

2.5 Design Properties of Metal Barrier

This area comprises those properties of the metal barrier (as it is designed to be used in a waste package) that affect material selection and performance. These include the temperature and radiation field due to the radioactive decay, physical and mechanical properties of the metal, design details such as thickness of the container and the loads that it will experience, and microstructural characteristics such as grain size and internal precipitates both in the weld metal and the base metal. There are two activities in this area.

Activity E-20-14 Coordination with package design

The first activity in this area is 'Coordination with package design' (E-20-14). The rationale behind this activity is to ensure continued information exchange with the package design task. Examples of the kinds of information exchange are given in Section 3.5.1. This co-ordination is required to assure that the metal barrier selection and package design do not progress independently and end up with incompatible requirements.

This activity will be conducted at QA Level III as there is no license application design data being generated in the activity. This activity will continue throughout the active period of this SIP; the activity is not directly linked to any particular important scheduled milestone. However, this activity does serve to transmit information between the two tasks. Information from analyses being performed in other activities (e.g. E-20-18, E-20-21, and E-20-21.1) is used to determine 'key' parameters (especially metallurgical parameters). Information flows back from this activity to identify which of the mechanical and microstructural properties are central to making performance predictions (activity E-20-24).

Activity E-20-24 Determination of mechanical and microstructural properties of the selected metal barrier material

This activity is concerned with characterization and documentation of the important mechanical and microstructural properties of the selected container material in the as-fabricated and as-emplaced condition. Many of the activities concerned with survey of degradation modes, identification of key performance-related parameters, model development and integration, and testing to produce license application data and validation of the performance model depend on an accurate characterization of these key properties. This activity is closely linked with the Design, Fabrication, and Prototype Testing Task because the container fabrication process and the welding or other closure process have a significant influence on the mechanical and microstructural properties. Examples of mechanical and microstructural properties are given in Section 3.5.2. The particular properties that will be documented in this activity are those that are deemed important from the model development and integration activities (E-20-16 and E-20-20) and the parametric studies (E-20-18, E-20-21 and E-20-21.1). Additionally, from the point of view of fabricating, closing, and inspecting the container, there are certain desirable mechanical and microstructural properties, and these considerations must also weigh in the final material specifications.

Information from this activity will ultimately be used, in part, for establishing acceptance criteria for the waste package container. This information is provided to the Design Task and ultimately to those areas of the NNWSI Project responsible for the waste package manufacturing and handling facilities. Nearly all testing techniques for mechanical or microstructural properties are destructive. Therefore, a major contribution from this activity will be a technical basis for establishing a sampling program to assure that the finished container meets the specifications. Possible approaches to achieve this end are more fully explained in IN 1.4.1 of the SCP.

This activity will be conducted at QA Level I. The characterization and documentation of these properties serve as a basis for much of the modeling and testing work from which long-term performance behavior predictions are derived. Characterization of the starting conditions is a crucial point in establishing the validity of the predictions, and this meets the criterion for Level I (data for license application).

In summary, the activities under the grouping of Design Properties of the Metal Barrier are:

Activity No.	Name	QA Level
E-20-14	Coordination with package design	III
E-20-24	Determination of mechanical and microstructural properties of selected metal barrier material	I

3.0 Description of Tests, Models, and Analyses

3.1 Introduction

The thirteen activities defined in Sections 2.1 - 2.4 are described in the following sections. For those activities in which previous NNWSI work has been performed, that work is described. An outline of the work planned under this Investigations Plan is included. Detailed test, model, and analysis plans which will ultimately be required by this Investigation are listed in Section 5.0.

3.2 Metal Barrier Selection Process

3.2.1 Degradation mode surveys (E-20-13)

This activity is an analysis of all the degradation modes that are believed to pose a potential performance threat to one or more of the candidate metals for the container. These surveys will be a set of papers summarizing available information addressing whether any particular mode of degradation can be active under Yucca Mountain conditions, under what conditions it would be active, and what measures could be taken to avoid degradation. The surveys will become a baseline of information used to evaluate which degradation modes must be pursued in advanced tests and which can be eliminated from further consideration because they will not be active under postulated repository conditions. The surveys will also support the selection process, where they will provide input into a QA level I assessment of the degradation modes. That assessment will then be used to narrow the field of candidate metals to one or two. It is expected that some candidates will have more potential degradation threats than others. Selection criteria may favor those candidates that have few or no active degradation modes. A final application of the surveys will be as input to the Package Design Task to assist in evaluating design issues which could reduce or enhance the activity of degradation modes.

The candidate metals can be divided into two distinct alloy families, austenitic (iron-base and nickel-base) and copper-base. These families respond quite differently to the same environment. Because of this natural grouping, the assessments will be combinations of degradation mode and alloy family. While the fundamental mechanisms for corrosion resistance are similar within a family of alloys, individual members can exhibit substantial differences in behavior in certain environments. The common modes of environmental degradation can also be grouped into similar categories. Not all degradation categories apply to both alloy families, because some types of corrosion are not active with one of the families. Thirteen combinations of degradation mode and metal family have been identified that are at least conceivable under repository conditions. There is also a category of 'other' to allow continued survey of possible modes that appear remote now but that future investigations in this and other project tasks may reveal to be more important. Identified in this 'other' category are (1) additional mechanical degradation modes (e.g. low temperature creep) occurring at slow rates over long periods of time at the modestly elevated temperature in the repository and (2) the possibility of greatly enhanced corrosion degradation modes occurring because of substantial modification of the chemical environment by micro-organisms either native to the repository site or introduced during the construction and operational periods.

Survey papers to be prepared.

General Corrosion and Oxidation - Copper-base alloys.
Localized Corrosion - Copper-base alloys.
Stress Corrosion Cracking - Copper-base alloys.
Hydrogen Effects - Copper-base alloys.
Phase Stability and Ageing - Copper-base alloys.
Other Degradation (Creep) - Copper-base alloys.
- - - - -
General Corrosion and Oxidation - Austenitic alloys.
Localized Corrosion - Austenitic alloys.
Transgranular Stress Corrosion Cracking - Austenitic alloys.
Intergranular Stress Corrosion Cracking - Austenitic alloys.
Hydrogen Effects - Austenitic alloys.
Phase Transformation and Ageing - Austenitic alloys.
Other Degradation -Austenitic alloys.

3.2.2 Establishment of criteria for metal barrier selection (E-20-15)

The objective of this activity is the development of a methodology to select the container material from the list of candidate materials. A peer review group will be formed as provided for under the NWMP - QAPP (033-NWMP-P 2.2) to review this methodology and its use in arriving at the final material choice.

The following list is a preliminary list of the criteria for selecting a container material for the license application design and will serve as input to this activity:

1. Will the material meet the performance allocated to the container in achieving the containment objectives (substantially complete containment under anticipated processes and events occurring in the repository)?

    a. Resistance to oxidation.
    b. Resistance to general aqueous corrosion.
    c. Resistance to environmentally accelerated cracking (stress corrosion cracking and hydrogen embrittlement).
    d. Resistance to pitting, crevice, or other localized attack.
    e. Demonstration of adequate mechanical properties.
    f. Resistance to mechanical embrittlement.

2. Can the performance of the material under repository conditions be adequately predicted?

    a. Predictability of physical and chemical properties of as-emplaced container.
    b. Existence of models to explain and predict degradation phenomena, or ability to develop such models.
    c. Existence of models to extrapolate laboratory data relating to degradation phenomena to repository time scales and conditions, or ability to develop such models.

3. Will the container material interact favorably with other components?

   a. Interactions with waste form.
   b. Interactions with borehole liner.
   c. Interactions with the package environment.

4. Can a container be made of this material?

   a. Fabricability of container body.
   b. Weldability of container ("closeability" if a nonwelded closure).
   c. "Inspectability" of closure.

5. Are the container material and process for fabricating it practicable?

   a. Availability of container material.
   b. As-fabricated container costs.
   c. Quality control requirements (and costs).
   d. Repository handling costs.

6. How can confidence in the selection be gained?

   a. Previous engineering applications of the material.
   b. Available data base on the material.
   c. Favorable (or unfavorable) experiences with the material.

Weighting factors for each of the preceding criteria (and any others chosen) will need to be established. It is expected that the previously listed criteria in 1, 2 and 4 will have the heaviest weighting, but all of the criteria have some importance. One approach is to assign a maximum number of points to each item in the criteria list and a minimum number for each item that the material must pass. As a rather extreme example, it does no good to have a highly corrosion resistant material that cannot be fabricated and closed.

Where appropriate and available, examples of methods that have successfully been used to predict longer term behavior of materials from short-time laboratory or field tests will be used. Examples may derive from atmospheric corrosion testing, marine corrosion testing, underground testing, chemical process industry testing, or nuclear and fossil fuel power plant testing. These examples will provide information for some of the items listed in 1, 2 and 6.

Development of the selection criteria, weightings, and organization of the peer review group are the items to be completed in this activity. The Nevada Nuclear Waste Storage Investigations (NNWSI) Project will use its own staff and consultants to develop the selection criteria and weighting factors. The selection criteria and weightings will then be reviewed by the peer review panel as per the Quality Assurance Program Plan. Following revision, if necessary, the criteria will be used to assess the candidate materials and select a material or materials in activity E-20-19. The peer review panel will consist of approximately seven individuals with backgrounds in different areas of metallurgy and materials science and with different work experiences to achieve a balance of viewpoints and perceptions.

3.2.3 Metal barrier selection (E-20-19)

This activity is the actual metal barrier selection step. The selection process will consist of applying the selection criteria to the list of candidate materials. As part of the process an assessment of degradation modes will be made for each material based on the survey papers from activity E-20-13. NNWSI Project personnel and consultants will perform the selection. Input will be the selection criteria and weighting factors from the previous activity, the degradation mode surveys from the first activity, consultant reports, NNWSI parameter studies, and existing literature information. There will be two components to the decision. First, each candidate will be examined to assure that its performance meets the minimum requirements, allowing a conservative margin for uncertainties. Second, it is proposed that a 'quantitative figure of merit' technique be used, in which each candidate alloy is judged on the established criteria. The quantitative scores, multiplied by the established weighting factors, are summed to provide the ranking total for the alloy. The selection process will be documented in a report on alloy selection. A peer review panel will be convened to review the report. It is expected that the same panel used for activity E-20-15 will be used for this review, but some additions might be made to address critical decision points. The selection, after review, revision if needed, and approval by the review group, shall be used to guide subsequent performance confirmation tests and degradation model development. The selected metal barrier material(s) and its physical, mechanical, and microstructural properties will also be used by the waste package design task as input into the advanced design work.

3.3 Metal Barrier Performance Modeling

3.3.1 Development of models for degradation modes, mechanical properties, and microstructure (E-20-16)

The analyses performed under this activity are directed toward producing a set of models for any degradation modes to which the container may be susceptible. The set of models will cover all degradation modes considered to be important for each candidate material in the repository environmental and thermal setting. The models will be preliminary in nature because of the large effort required to make them exhaustive, and because of the limited application required of these models before the selection step. Those models relevant to the selected alloy(s) will be further developed after selection, as described in activity E-20-20. This activity will also develop models to predict the mechanical properties and microstructure of the container material in the repository environment.

Prediction of the long-term performance of the metal barrier under repository conditions requires that all significant degradation mechanisms be identified and the probability of their occurrence be quantified. For all degradation modes that might be significant, a physical-chemical model must be developed that will allow extrapolation of data gathered in the laboratory to the times and conditions relevant to the repository. In many cases, the analysis to determine whether the degradation mode might occur requires the same model that will allow prediction of long-term behavior. Thus, in this activity analyses are included that both assess the relevance of particular degradation processes and develop models to describe their action under repository conditions. The tools that are developed under this activity will be used in the Performance Assessment Task to predict the condition of the containers as a function of time for both anticipated processes and events and for other, low probability cases for which source term data are requested by that Task.

The modeling activities discussed in this activity and the laboratory experiments discussed in E-20-18 are closely related. They are both described in fairly basic terms in Chapter 8 of the SCP (Information Need 1.4.3) with much greater detail to be provided in the laboratory test plan to be written for the activities. The results of this activity will be used in the selection of the alloy(s) for advanced work (activity E-20-19), and those portions of these models that apply to the alloy(s) selected will be used in activity E-20-20.

A fundamental element that transcends all the modeling of degradation modes that have some chemical features is a model for the corrosion potential. Various environmental parameters in the aqueous phase (e.g. pH, dissolved oxygen and other gasses, cation speciation, anion speciation, radiolytically produced species as well as temperature) influence the corrosion potential. Metallurgical parameters (e.g. alloy composition and phases -- including the effects of strain and prior fabrication history on these) also influence the corrosion potential. While more difficult to measure experimentally, the concept of corrosion potential also exists under "dry" oxidation conditions. The potential under dry conditions might be approximated by modeling the potential under conditions of a thin electrolyte layer as a function of thickness, and then letting the thickness approach zero. Initiation and propagation of non-uniform corrosion modes are governed by "critical potentials", so that models for these modes are based on the values of the critical potentials relative to the corrosion potentials. The values of the critical and corrosion potentials will change with time as environmental and metallurgical conditions in the repository and in the container material change. Many of the details depend on the material that is selected for the advanced designs.

Models for predicting critically susceptible microstructures for the onset of non-uniform corrosion modes (e.g. sensitization in stainless steels and nickel-base materials) are derived from considerations of the metallurgical reaction kinetics. These follow from nucleation-and-growth models based on diffusion of the critical component (diffusion of chromium to react with carbon). Particularly at the relatively low temperatures of interest in the repository, models must consider both high-diffusivity paths (grain boundaries, dislocations) and low-diffusivity paths (atom movements in the crystal matrix). Also, the reaction kinetics to form the carbide can become rate controlling at low temperatures. Models for sigma phase formation (a brittle phase) are based on nucleation and growth kinetics and will be developed by a similar approach. Some metallurgical reactions that are of interest (because the transformation products are brittle and are usually more prone to stress corrosion and/or hydrogen embrittlement) are diffusionless (e.g., martensitic reactions in stainless steels and possibly in aluminum bronze), and the modeling approach is therefore different. Martensitic reactions are usually considered in the context of critical temperatures to begin the transformation and to complete the transformation. High strains greatly increase the critical temperatures, so that they can coincide with the repository temperatures for the more susceptible materials (304L). Models for these are built upon the effect of temperature, strain, and alloy composition with evidence for the formation being resolution by optical microscopy.

The extent to which the modeling activities will be carried out depends on the material selected for advanced designs and the results of degradation mode assessments for the materials and different degradation modes being considered.

3.3.2 <u>Integration of models for selected material (E-20-20 and E-20-20.1)</u>

The analyses of this activity follow those of the preceding one (E-20-16) and the metal barrier selection step (E-20-19). This activity involves taking those degradation mode models that are relevant to the selected alloy, completing them, and integrating them with required input from activity E-20-21 and E-20-21.1 concerning the material and repository conditions to provide performance predictions for the metal barrier. This activity will interface with the Performance Assessment Task to produce container performance models consistent with the needs of that Task.

The work of this activity is closely related to the information gathering and laboratory testing activities of E-20-21, E-20-21.1 and E-20-23. They are described in general terms in Chapter 8 of the SCP (Information Need 1.4.2) and will be detailed in the individual test and analysis plans to be written for the material(s) selected for the advanced designs. Particularly in the case of localized corrosion and stress corrosion cracking, there is a considerable need to select detailed test methods as well as materials, and this selection is best left until after the final material is selected.

3.3.3 Performance parameter studies (E-20-21 and E-20-21.1)

The QA Level III portion of this activity (E-20-21) consists of information collection and tests to support the development of degradation models but which do not support the validation and license application. This activity serves a role after the selection step similar in nature to the role of activity E-20-18 before selection. This activity continues those experiments from E-20-18 which apply to the selected alloy to assist model development. The experiments can be divided into eight categories of degradation, and can be further divided naturally into the two families of candidate alloys (austenitic and copper-base). The eight categories are:

1. Metallurgical aging and phase transformations.
2. Low temperature oxidation
3. General aqueous corrosion.
4. Intergranular attack and intergranular stress corrosion cracking.
5. Hydrogen entry and embrittlement.
6. Pitting, crevice, and other localized attack.
7. Transgranular stress corrosion cracking.
8. Other potential degradation modes

The QA Level I portion of this activity (E-20-21.1) consists of information collection and tests to support the completion and integration of degradation models including any data which supports the validation (E-20-25) or the license application design. Details of this activity will not be available until the preliminary models are complete (E-20-16), the alloy(s) for advanced design work is chosen (E-20-19), and model integration (E-20-20) is ready to commence. Until that time, the parametric information needs for this task will not be known. When appropriate, analysis and or test plans will be prepared and reviewed to assure that the parametric input into the metal barrier performance model is adequate and accurate. This activity is a QA Level I analog of activity E-20-18 and will gather or generate data on critical issues such as chromium diffusion, phase stability, and chloride ion effects (austenitic materials) and such as rates and concentrations of nitric acid or ammonia formation (copper-base materials). The data will be used in the development and integration of the performance model (E-20-20.1) but are not distinct validation tests (E-20-25).

3.3.4 Validation of model (E-20-25)

This activity will conduct QA Level I metal barrier material tests and compare the results with the predictions of the degradation model. The purpose is validation of the model for long term waste package performance predictions. Substantial variance of the model from the test results must be investigated and explained. A peer review process will monitor the results and review the validation. Input into this activity will be the long term material performance model from E-20-20.1 and the test results from E-20-23.

3.4 Metal Barrier Performance Testing

3.4.1 Experimental technique development (E-20-17)

This activity involves the development of custom laboratory techniques for degradation testing and examination of metal barrier candidates. It involves both analyses of requirements and existing techniques and laboratory testing to develop techniques. One portion of this activity will be an ongoing review of the experimental requirements for metal barrier testing. As the investigation progresses, there may be an evolution of test requirements, since they are dependent upon the results of activities E-20-13, E-20-19, and E-20-16. As these experimental requirements are identified, an assessment of existing techniques will be made to determine whether the need is already filled. Established techniques that are required but not already available to the NNWSI program will be obtained, either by installing and developing expertise at LLNL or by contract to other laboratories with established capabilities. It is possible that needs will be identified that are not met by established techniques. In this case, an effort will be made to develop the required capability either at LLNL or at a contractor facility. The work under this activity will be done at QA level III. However, any techniques developed here that will be used for activities E-20-21.1 or E-20-23 will have QA Level I procedures written for them.

Examples of experimental requirements that may lead to developmental work include:

1) use of microelectrodes to measure and monitor electrochemical potentials in small areas. A great deal of technical literature is concerned with measurement of electrode kinetics as a function of statically or dynamically applied electrochemical potentials. On this basis, potential regions are established. These regions are bounded by so-called 'critical potentials' that govern where particular kinds of corrosion can occur. In conventional electrochemical techniques, potentials are measured on areas with a linear dimension of approximately 1 mm, while advanced techniques allow potential measurements on area with linear dimensions of 10 micrometers, and considerably less in the most advanced techniques (about 30 nanometers). This advancement permits an experimenter to monitor the potential distribution that would occur around a freshly initiated crack, crevice, pit, or other surface feature on a corroding metal surface. Conventional electochemical techniques will complement the microelectrode work.

2) use of advanced microanalytical techniques to measure and monitor the concomitant environmental chemical concentration gradients along with the electrochemical potential gradients existing in a crack, crevice, pit or other surface feature on a corroding metal surface. Such techniques involve selective ion probes or intense light sources.

3) use of advanced microscopic techniques to investigate changes occurring in the metal or alloy. These techniques include advancements in scanning and transmission electron microscopy to examine and analyze very small precipitates, transformation products, or other microstructural features of interest. With the latest "state of the art" microscopes, resolution to 10 Angstroms (and lower) is possible. Resolution of these small particles is important in establishing credibility of metallurgical models (e.g. sensitization in stainless steels; martensitic transformations in stainless steel and possibly aluminum bronze) proposed for predicting changes in the container material with time.

4) use of advanced surface and analytical techniques to investigate the chemical and structural composition of protective films and layers on corroding metal surfaces. From this information, the kinetics of film formation and re-formation when broken can be determined. Of possible interest are advancements in scanning tunneling electron microscopy to examine in situ surfaces exposed to aqueous environments, and spectroscopic ellipsometric techniques to investigate in situ the structure and growth kinetics of passive films. More conventional in vacuo techniques, e.g. Auger electron spectroscopy and ESCA techniques, will be used to supplement the in situ techniques, as needed.

The intent in developing the above techniques is to allow examination of grain boundaries, arrays of dislocations, sub-critical size precipitates, local anodes and cathodes, and other fundamental factors in elucidating the mechanisms for corrosion and other degradation modes. These advanced techniques are to be used in conjunction with more established and conventional corrosion test methods (as discussed in the next section)

3.4.2 Parametric studies of metal degradation and microstructure (E-20-18)

The work in this activity will be QA level III experiments to provide specific corrosion data needed throughout the model development phase, and to act as input to the selection process. Those studies to be used in the selection process are needed in the near term. Some of these are currently planned and should begin soon. Examples of these near term studies include:

Identification of the sensitization rate-determining step in austenitic stainless steel at low temperatures (Cr diffusion within grains, Cr diffusion along dislocations, rate of carbide formation, etc.) and develop a means to show this microscopically.

Determine the lowest critical chloride ion concentration (lowest critical potential) that will cause 1) pitting, 2) crevice, 3) transgranular SCC in the three austenitic alloys and develop means to demonstrate this.

Verification that a high radiation field will not cause a high oxidation or general corrosion rate, or onset of SCC by ammonia formation in copper-base materials.

A substantial amount of previous work has been done by the NNWSI Project on experiments to examine these issues in relevant environments. A variety of experiments were conducted at Lawrence Livermore National Laboratory from 1982 to 1986. Additional experimental work was conducted at several contractor sites (Pacific Northwest Laboratory, Westinghouse Hanford Co., Ohio State University, San Diego State University, University of Minnesota, and the University of Florida). These are described in a general way in the Site Characterization Plan (Section 7.4.2) and some of the reports from these experimental activities are cited in Section 7.0 of this SIP. Several additional reports are in preparation. These reports will serve as input to the 'Degradation mode surveys' of activity E-20-13.

The candidate materials in the NNWSI Project are regarded as corrosion resistant materials, as opposed to corrosion allowance materials. This means that the oxidation and general corrosion rates for the candidate materials in all the anticipated environments (and in many of the credible, although unanticipated, environments) during the containment and isolation periods are sufficiently low that perforation of the container wall in the time periods of concern by these mechanisms is very improbable. However, these modes will occur continuously from the time of emplacement, and they are of interest in establishing the background conditions (including the characterization of protective films and their change with time) for the metal surface.

The more serious concerns for container failure during the time periods of interest are the other corrosion modes listed above as well as metallurgical aging and transformation reactions leading to structures that are brittle or more subject to localized corrosion and stress corrosion modes. Many of the advanced techniques listed in the previous section are planned to be used for the purpose of investigating under what conditions these corrosion modes are initiated and propagated. The bulk of this activity is analysis of the rates of initiation and propagation, as they apply to the environmental conditions (including temperature and radiation fields) and the population of containers (including their fabrication history and mechanical stress distribution). These conditions will not be uniformly distributed on the surface of a given container and will vary among the population of emplaced containers in the repository. Localized corrosion, stress corrosion, and hydrogen embrittlement have important statistical components, related to the distribution of environmental, metallurgical, and strain conditions from point to point, and the manifestation of these is a distribution in the rate of attack by these modes.

As discussed under activity E-20-16 'Development of models for degradation modes, mechanical properties, and microstructure', the fundamental "tie line" between the different degradation modes is the relationship between critical potentials for the initiation and propagation steps of the different modes of localized and stress corrosion and the electrochemical corrosion potential. Measurement of the corrosion potential and the various critical potentials is the key link between the modeling and performance activities. This means that, for example, a series of pre-cracked stress corrosion cracking tests will be conducted on a suitable fracture mechanics-type of specimen at different applied potentials in a given set of otherwise constant environment conditions. The crack propagation rate will then be measured as a function of time and applied potential. The critical potential for initiation of measurable crack growth is then determined. Other pieces of information, such as the crack propagation rate, the crystallographic path, continuity or discontinuity of the propagation, and tendency toward crack branching, will be used eventually to estimate the time-to-failure of a container. Several metallurgical parameters can be introduced into the test series to indicate the effects of key microstructural parameters such as degree of sensitization (stainless steels) or aluminum segregation (aluminum bronze) on the crack propagation rate and critical potential. The effect of mechanical factors such as stress intensity and size of the plastic zone on crack propagation and critical potential can also be obtained from the same series of experiments. Thus, a single set of experiments (with parameters well chosen and with a high degree of sensitivity to crack growth measurements) can yield an impressive amount of information that can be used to predict failure rates. Also, all three of the basic factors (susceptible microstructure, aggressive environment, critical stress) needed in determining stress corrosion susceptibility will be present in the test series.

3.4.3 Development of plans for license application support tests (E-20-22)

The purpose of this activity is to produce the test plans for the long term tests of metal barrier performance. After the selection process has chosen one (or two) metal alloys for advanced work, tests will be required to determine the behavior of that metal in a variety of environments. The plans for those tests must be sufficient to provide the data needed to model the performance of the metal barrier. These plans will be developed by NNWSI personnel and contractors as a QA level I task.

Detailed preparation of these plans will not be possible until activities E-20-13 and E-20-19, that serve as input to the plans, are complete, and results are available from the early portions of E-20-17 and E-20-18. Some examples of tests that might follow are sensitive weight loss coupon tests, crevice tests (with controlled crevice gap sizes), and constant load stress corrosion tests (on both smooth and pre-cracked specimens). In several cases, these will be designed as "null tests", where the prediction is that no measurable effect should occur. The credibility of the null tests is established on the sensitivity of the measurement and the time over which the tests are conducted. It is impossible to demonstrate long-term predictions on null tests alone, but null tests conducted in accordance with a credible model that predicts no effect should add substance to the demonstration.

3.4.4 License application support tests (E-20-23)

This activity is the QA level I performance testing of the selected metal barrier. After the candidate alloys have been found to meet minimum performance requirements and have been ranked against one another, one (or two) alloy(s) will become the selected metal barrier material(s) for advanced design work (see activity E-20-19). The job of this investigation beyond that point is to concentrate on this selected alloy to produce a validated model for its long term performance in the Yucca Mountain environment and to produce the data required by the model to predict that performance. Data required for the model to support the license application is the product of this activity. The previous activity (E-20-22) describes the preparation of the plans for these tests. Details of the tests will not be available until completion of the plans. Note that data used specifically for the model validation (activity E-20-25) will be produced in activity E-20-25.

Until completion of the metal barrier selection process, the description and goals of these tests cannot be finalized. It is expected that the tests will include both anticipated repository service environment and material conditions which should yield null results for material degradation, and more aggressive conditions which should yield a result predictable by the performance model. Material conditions include simulated or actual weld microstructures, as well as representative base metal conditions.

Examples of types of tests which might be selected are:

> weight loss coupon tests (general aqueous corrosion and oxidation, also indicates pitting and other localized attack), crevice cell corrosion tests, slow strain rate tests (stress corrosion cracking), constant load stress corrosion tests, constant deformation stress corrosion tests (C-rings, U-bends, bent beam), fracture mechanics tests (stress corrosion and hydrogen embrittlement), electrochemical polarization tests (general and localized corrosion), various stress corrosion tests at constant applied potentials, localized and stress corrosion tests in irradiated environments, "scratch" potential or other tests to indicate the mechanical and electrochemical breakdown of passive films, straining electrode tests (film rupture and repassivation kinetics in analysis of localized and stress corrosion analyses), hydrogen permeation tests, double cantilever beam tests (hydrogen embrittlement and stress corrosion cracking susceptibility), corrosion tests using AC impedance techniques (general corrosion for determining passive film characteristics), multiple sample techniques using stochastic analysis (probability for localized corrosion), scanning electrode imaging (localized pH and other chemical changes in sequestered regions), analysis of electrochemical noise (pitting frequency), in situ Raman spectroscopy (speciation in passive films particularly on copper-base alloys to show selective leaching), low-angle X-ray (oxidation films), stress wave emission (discontinuity of stress corrosion crack propagation), ion chromatography (determination of anions and cations in solution), and band gap measurements (identify film species).

Other possible techniques of an advanced nature are discussed under activity E-20-17.

3.5 Design Properties of Metal Barrier

3.5.1 Coordination with package design (E-20-14)

This activity is the interaction and information interface between the metal barrier task and the package design task. The purpose of this activity is to provide an ongoing analysis of the interaction between the decisions and information gained by the Metal Barrier Selection and Testing task and the Waste Package Design task. There are many potential impacts, both beneficial and adverse, that these two tasks could have on each other. The Metal Barrier Selection and Testing Task interfaces with several other tasks (as indicated in Figure 1); these interfaces are handled by communication between the affected Task Leaders. However, the interface with the Design, Fabrication, and Prototype Testing Task is regarded as the most important one, and therefore warrants a special activity.

Some examples of these Metal Barrier - Design interactions include the criteria of "fabricability" and "weldability" for the container material selection. In many cases, small changes in the alloy composition (particularly in micro-constituents) play an important role in determining the weldability of different candidate materials and may influence (and improve) the corrosion performance of the material. The metallurgical and microstructural features of the weld are important parameters in selecting a technique for non-destructive evaluation of the weld. The choice of the methods used for fabricating and for welding the metal container (or other closure method) are important considerations in evaluating the performance of the container material, because of the close relationship between composition (and its variations in the welded region and heat affected zone), microstructure, residual stress, and the susceptibility to the forms of corrosion (localized corrosion, stress corrosion cracking) that are important in limiting the container integrity. Furthermore, the processes for fabricating and closing the container are viewed as having an important influence on metallurgical reactions (such as phase transformations and precipitation of carbides and other phases) in the metallurgically metastable candidate materials. Non-welded closure methods also have important implications in the corrosion performance of the closure region.

Handling and emplacement operations in the repository also need to be considered in establishing the long-term container performance, since these operations may impart some degree of surface defects and contamination on the container. Some aspects of the repository design work (not a responsibility of LLNL, but closely monitored by the Waste Package Design Task) also influence the performance of the container. These include the emplacement geometry, areal power loading of containers, and the borehole liner configuration. Also, the choice of cements, grouts, or other materials to support the borehole liner need to be reviewed as to their effect (favorable or unfavorable) on the container material performance.

It is, therefore, the function of this activity to review all of the issues and activities of the two tasks, document their interaction, and insure communication of that interaction. Information will be gathered from the design task under this activity, sorted by QA Level and application, and passed on to other activities of this plan. No specific tests or analyses are planned for this activity.

3.5.2 Determination of mechanical and microstructural properties of metal (E-20-24)

This activity provides information about the mechanical and microstructural condition of the container material at the time of emplacement. After the container material and the fabrication and closure processes have been selected this activity will determine those material properties that affect the performance of the container, and in many cases set limitations on the acceptable range of those properties. This information will be used as input to the performance model and will also be used by the Package Design Task. The results of this activity may also form a set of specifications and tolerances for material production, fabrication, and closure.

The principal mechanical properties of interest are the following:

1. Yield strength.
2. Ultimate tensile strength.
3. Elongation (or other measure of ductility, such as reduction in area).
4. Modulus of elasticity.
5. Impact strength (or other measure of fracture toughness).

Knowledge of the effect of metal fabrication processing and inter-relationships between mechanical properties and microstructural properties is also required. This includes the effect of such factors as phase distribution, grain size, inclusion content, and previous plastic deformation. The effect of the strain rate on the mechanical properties is also needed. While individual mechanical properties are listed above, the entire stress-strain relationship merits attention in order to enable one to evaluate the toughness of the material when subjected either to low strain rate or to high strain rate processes during handling or that can later develop in the containment period.

Because the microstructure is intimately related to fabrication process variables and, in some cases, to relatively small compositional variations, this dependence will be documented. The microstructures of the fusion zone and heat-affected zones around the weld must also be characterized; characterization of these depends strongly on the welding process variables, and in some welding processes, on the composition of the filler materials. The microstructural features of importance include the following:

1. Primary phases present and their distribution.
2. Secondary phases and evidence of precipitation reactions.
3. Segregation effects.
4. Grain size and distribution of grain size.
5. Evidence of preferred orientation.
6. Identification and distribution of nonmetallic inclusions.

The time at elevated temperature (during the container fabrication and closure process) is influential in determining the above features.

4.0 Application of Results

The activities of this investigation directly address Issue 1.4 of the Site Characterization Plan. The primary applications of the results will be: 1) to select a material(s) for advanced design work for use by the Waste Package Design Task, and 2) to provide a validated model (and data for use by the model) of that material's long-term behavior in the repository environment to the Performance Assessment Task. The secondary application of the results is to indicate what changes (if any) the presence of the metallic container produces on the package and repository environment. These changes would be incorporated into the EQ3/6 geochemical code and its subsequent use in establishing performance of other waste package components. The information, test results, and models obtained in this investigation will also be applied in several other ways:

1. To provide, along with a considerable amount of information supplied by the Design, Fabrication, and Prototype Testing Task, a description of the "as-emplaced" container for use in predicting repository performance.

2. To establish meaningful laboratory test conditions for activities discussed under the grouping 'Metal Barrier Performance Testing'. Results from these tests input into the models for the different degradation modes. These test conditions specify the environmental, metallurgical and strain conditions that govern the susceptibility to certain forms of localized corrosion, stress corrosion cracking, and hydrogen embrittlement (those forms of corrosion are expected to be most important in limiting the container lifetime in the time periods of concern in demonstrating containment and controlled release). For some of the candidate alloys, projections of microstructures that may develop over the long-term containment period are important because of either potential embrittlement problems or greater susceptibility to different corrosion modes. Analysis of the expected as-fabricated, as-welded (or otherwise assembled), as-emplaced structure serves as the basis for beginning these projections.

3. To form part of the basis for materials selection for final waste package designs, and to complete that selection. The selection process is discussed in activities E-20-15 and E-20-19. As discussed in section 3.2.2, it is anticipated that the performance under expected repository conditions, the predictability of the performance, and the fabricability of the material will be the paramount criteria, but considerations of mechanical and physical properties plus other practical considerations may be expected to play an important role in the selection process. An important part of the fabricability and weldability issues relates to whether or not unfavorable mechanical-microstructural features are produced in an otherwise resistant material.

4. To form a basis for establishing any additional specifications on the composition and mechanical properties of the candidate materials beyond the normal industry specifications.

5. To provide guidance in selecting the industrial processes for forming, joining, and handling the container. These results will further serve as input to information needs under Issues 2.1 (Options for retrievability), 2.6 (Preclosure design criteria), 4.3 (Waste package production technology), and 4.5 (Waste package costs).

6. To complete certain elements of the waste package design which are materials-dependent. Most waste package design features, at the conceptual level, are not sensitive to which material is eventually selected. At the advanced design stage, detail on the selected material and processes for producing and handling the container is needed. These results are input into Information Need 1.10.2.

7. To complete considerations in several repository design-related options. These include a decision on whether the containers are emplaced horizontally or vertically in the boreholes, and the use and configuration of borehole liner materials (currently it is suggested to use comparable materials for the container and borehole liner to eliminate any galvanic corrosion effects). Also, the emplacement and operational activities in the repository may be partly influenced by the container material selected, to insure that projections on its performance are not compromised.

8. To provide to the Waste Package Environment Task a description of the corrosion products that are expected to form in the near-package environment. These species may influence the performance of other waste package components and are of interest in assessing the modification to the natural environment caused by degradation of the waste package container.

5.0 *List of Test Plans to Support this Scientific Investigation Plan*

The following test and analysis plans will describe in detail the activities forming this investigation:

Metal barrier selection review plan

Metal barrier test plan (for selected material)

Metal barrier degradation model development and integration plan (for selected material)

Metal barrier performance model validation plan

The test plan and plan for model development and integration depend very much on which material is selected for advanced design work. Plans for testing and modeling are centered around the appropriate and applicable degradation modes for the different candidates, so that it is not possible to give many details until the material selection is completed. However, it is envisioned that each of the plans listed above will be completed in stages, the initial stage being an umbrella plan that covers the broad aspects of the planned activities. This will be followed by more detailed plans for testing and modeling that will cover particular aspects, such as pitting corrosion, crevice corrosion, or stress corrosion.

6.0 History of Metal Barrier Candidate List

The set of materials selected as candidates for waste package containers in the tuff repository has undergone some evolution over the course of the NNWSI project, and it is helpful to briefly review the history of candidate selection.

In late 1982 the NNWSI Project selected a repository horizon in the Topopah Spring member of the Paintbrush Tuff. This horizon lies in the unsaturated zone, well above the permanent water table. Initially, the NNWSI project selected AISI 304L stainless steel as its reference material and a relatively thin-walled design for its containers. A number of factors contributed to these choices. First of all, it was known that there would be no significant lithostatic or hydrostatic pressure on the containers if emplaced in tuff above the water table. Therefore, thick walls would not be necessary for the prevention of buckling, as is the case for most other proposed deep geologic sites. This situation seemed to lend itself to use of a thin, corrosion resistant material rather than a thicker, corrosion allowance material. Secondly, the Defense Waste Processing Facility at Savannah River had already selected AISI 304L stainless steel as the reference material for borosilicate glass pour canisters for its defense waste. It appeared likely at that time (and has since been established as policy by the federal government) that defense waste and commercial waste would be emplaced in the same repository. NNWSI's initial proposal was thus to use the pour canisters as the metal barriers for defense waste, and to fabricate containers of the same material (AISI 304L stainless steel) for the spent fuel. Past experience with austenitic stainless steels in hot air and dry steam environments had been very satisfactory, and it appeared that this material would serve well in the unsaturated tuff environment at temperatures above the boiling point.

The process by which AISI 304L stainless steel was selected as the reference material also resulted in the selection of three other alternatives: AISI 321, AISI 316L, and Alloy 825. These were chosen for their increased resistance to particular types of corrosion, should this be found necessary after more detailed testing, particularly if extensive contact with an aqueous phase was found to be likely, or if the environment turned out to be more severe than anticipated.

This candidate selection process involved the comparison of 17 commercial alloys according to the criteria of mechanical properties, weldability, corrosion resistance, and cost. In the absence of enough detailed information to establish relative weights for these four criteria, all four were considered to be equally important. Using available corrosion data, which in some cases was rather sparse, the 17 candidates were ranked and resulted in the selection of the four austenitic alloys AISI 304L, 321, 316L, and alloy 825 for further consideration.

As the project proceeded it became clear that the AISI 304L stainless steel of the borosilicate glass pour canisters would have been subjected to a thermal history that might lead to sensitization of the material to intergranular stress corrosion cracking and that differential thermal expansion during cooling of the poured glass and the canister would put the canister walls into hoop tension, aggravating this situation. It was therefore decided to modify the waste package design for the glass waste forms to include an outer container surrounding the pour canister. The thermal history and the stress state in this container could be better controlled, so as to reduce the threat of intergranular stress corrosion cracking.

In 1984 at the request of OCRWM, NNWSI began to investigate the feasibility of using copper-base materials for waste package containers. After consultation with the Copper Development Association, Inc. and the International Copper Research Association, Inc., three copper-base materials were selected for further consideration: CDA 102 (oxygen-free copper), CDA 613 (aluminum bronze), and CDA 715 (70-30 copper-nickel). Copper-base materials appeared to offer several potential advantages. First of all, among the available engineering metals, copper alone is able to co-exist thermodynamically with water (under some conditions). The driving force for corrosion and oxidation is thus smaller for copper than for materials such as Fe-Cr-Ni alloys that depend on passive film formation for their corrosion resistance. Localized and stress-assisted forms of corrosion are thus generally less severe for copper-base materials. Evidence for survivability of copper materials can be seen in the existence of native copper deposits and in copper and bronze artifacts recovered from the ruins of earlier civilizations.

Another potential advantage of the copper-base candidates is the simpler microstructures compared to the austenitic materials. Unlike iron, copper has no phase transformations. Thus the phase stability of copper-base materials appears to be of a lesser concern than it is with the iron-base austenitic materials.

After it was decided to include copper-base materials as candidates for further consideration, it became necessary to reduce the number of the other candidates in order to bring the scope of the testing program within the range of available resources. It was decided to eliminate AISI 321 from further consideration because AISI 316L offers the same benefits as AISI 321, as well as additional ones, so that the range of qualities has been preserved within the austenitic family. This decision leads us to the present six candidates for the metal barrier: AISI 304L and 316L stainless steels, high-nickel austenitic alloy 825, oxygen-free copper CDA 102, 7% aluminum bronze CDA 613, and 70-30 copper-nickel CDA 715. Within this field of candidates we thus have materials based upon three different metals: iron, nickel (essentially), and copper. We have corrosion-resistant materials, and we also have one (CDA 102) that can be viewed in some respects as a corrosion allowance material (CDA 102 would likely be used with a greater wall thickness than the others, anyway, because of its lower strength).

7.0 Annotated Reference List

The content of this SIP complements material prepared for Chapter 7 (Section 7.4.2) and Chapter 8 (Issue 1.4 and Information Needs 1.4.1-1.4.5) of the SCP that are currently undergoing final review by the NNWSI Project Office and the DOE Office of Geological Repositories. The material in Chapter 7 reviewed the choice of candidate materials, preliminary analyses of degradation modes for the materials in the context of the Yucca Mountain repository environment, and the results of experimental activities (mostly corrosion testing activities). The Chapter 8 material covered the information flow to and from other waste package and repository task elements and outlined the work to be done in the next several years. The material in this SIP breaks down this work into discrete activities.

A reference list for some related publications by selected subject areas is given below. This is by no means an exhaustive source on the subject, but is given as a guide for further reading.

1. Materials Selection

The first paper gives the rationale used to select the first candidate materials (austenitic materials) for the NNWSI Project.

E. W. Russell, R. D. McCright and W. C. O'Neal, "Containment Barrier Metals for High-Level Waste Packages in a Tuff Repository", Lawrence Livermore National Laboratory Report UCRL 53449, (October, 1983).

This work was followed up with additional explanation on corrosion considerations by:

R. D. McCright, H. Weiss, M. C. Juhas, and R. W. Logan, "Selection of Candidate Canister Materials for High-Level Nuclear Waste Containment in a Tuff Repository", Lawrence Livermore National Laboratory Report UCRL 89988, (November, 1983)

Further reading on principles in selecting stainless steels and nickel-base alloys is found in:

A. J. Sedriks, Corrosion of Stainless Steels, Chapter 2, John Wiley and Sons, New York (1979)

Copper-base materials were added as candidate materials to the NNWSI Project, and the rationale for their addition was discussed in:

R. D. McCright, "FY-85 Status Report on Feasibility Assessment of Copper-Base Waste Package Container Materials in a Tuff Repository", Lawrence Livermore National Laboratory Report UCID 20509, (September, 1985)

A very informative discussion of many engineering materials and their potential application as nuclear waste containers is found in:

K. Nuttall and V. F. Urbanic, "An Assessment of Materials for Nuclear Fuel Immobilization Containers", Atomic Energy of Canada, Ltd., report AECL-6440, (September, 1981).

2. Degradation Modes

Several good texts exist that discuss corrosion modes and causative factors. The ones that we most frequently refer to are:

M. G. Fontana and N. D. Greene, Corrosion Engineering, 2nd edition, McGraw-Hill, New York (1977). A new edition of this is due to be published this year.

L. L. Shreir (editor), Corrosion, Newnes-Buttersworth, London and Boston (1976). This is in many ways, the text on the subject and is very complete in its treatment of the phenomenology and preventive measures. It is a thick two-volume set; volume 1 is on metal/environment reactions and is the one most applicable to the present work.

An older text, but one which is chock full of information and contains lots of engineering data (most newer texts concentrate more on explaining mechanisms), is:

F. L. LaQue and H. R. Copson, Corrosion Resistance of Metals and Alloys, 2nd edition, Reinhold Publishing Co., New York, (1963).

3. Corrosion Test Results

Some reports from NNWSI-sponsored work that have been used in establishing preliminary analyses on important degradation modes are:

M. C. Juhas, R. D. McCright, and R. E. Garrison, "Corrosion Behavior of Stressed and Unstressed 304L Specimens in Tuff Repository Environmental Conditions", Lawrence Livermore National Laboratory Report UCRL 91804, (November, 1984).

R. S. Glass, G. E. Overturf, R. A. Van Konynenburg, and R. D. McCright, "Gamma Radiation Effects on Corrosion: Electrochemical Mechanisms for the Aqueous Corrosion Processes of Austenitic Stainless Steels", Corrosion Science, vol. 26, p. 577 (August, 1986).

C. F. Acton and R. D. McCright, "Feasibility Assessment of Copper-Base Waste Package Container Materials in a Tuff Repository", Lawrence Livermore National Laboratory Report UCID 20847 (September, 1986).

R. E. Westerman, S. G. Pitman, and J. H. Haberman, "Corrosion Testing of Type 304L Stainless Steel in Tuff Groundwater Environments", Pacific Northwest Laboratory Report PNL-5829, LLNL Report UCRL-21005 (November, 1987).

R. D. McCright, W. G. Halsey, and R. A. Van Konynenburg, "Progress Report on the Results of Testing Advanced Conceptual Design Metal Barrier Materials Under Relevant Environmental Conditions for a Tuff Repository", LLNL Report UCID-21044 (December, 1987).

The authoritative source on corrosion test methods is:

W.H. Ailor, Handbook on Corrosion Testing and Evaluation, John Wiley and Sons, New York, (1971).

4. Modeling Activities

The model of sensitization of stainless steel is discussed in:

T. A. Mozhi, W. A. T. Clark, K. Nishimoto, W. B. Johnson, and D. D. Macdonald, "The Effect of Nitrogen on the Sensitization of AISI 304 Stainless Steel", Corrosion, vol. 41, p.555 (October, 1985).

T. A. Mozhi, H. S. Betrabet, V. Jagannathan, B. E. Wilde, and W. A. T. Clark, "Thermodynamic Modeling of Sensitization of AISI 304 Stainless Steel Containing Nitrogen", Scripta Metallurgical, vol. 20, p. 723, (May 1986).

The model of corrosion potentials is discussed in:

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