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Status of materials handbooks for particle accelerator and nuclear reactor applications

Stuart Maloy [a,*], Berylene Rogers [b], Weiju Ren [c], Philip Rittenhouse [d]

[a] Los Alamos National Laboratory, MS H816, Los Alamos, NM 87545, United States
[b] Los Alamos National Laboratory, MS E578, Los Alamos, NM 87545, United States
[c] Oak Ridge National Laboratory, MS-6155, Oak Ridge, TN 37831, United States
[d] 346 Myers Road, Kingston, TN 37763, United States

A B S T R A C T

In support of research and development for accelerator applications, a materials handbook was developed in August of 1998 funded by the Accelerator Production of Tritium Project. This handbook, presently called Advanced Fuel Cycle Initiative (*AFCI) Materials Handbook, Materials Data for Particle Accelerator Applications*, has just issued Revision 5 and contains detailed information showing the effects of irradiation on many properties for a wide variety of materials. Development of a web-accessible materials database for Generation IV Reactor Programs has been ongoing for about three years. This handbook provides a single authoritative source for qualified materials data applicable to all Generation IV reactor concepts. A beta version of this *Gen IV Materials Handbook* has been completed and is presently under evaluation.

1. Introduction

The purpose of this paper is to briefly describe two energy-related materials handbooks being supported by the US Department of Energy (DOE). These are: (1) the *AFCI Materials Handbook, Materials Data for Particle Accelerator Applications* and (2) the *Gen IV Materials Handbook*. The complexities and scope of these handbooks are of such magnitude that it will be impossible to discuss them here fully, but the intent is to provide sufficient detail to give the flavor of the content and use of these databases. The *AFCI Materials Handbook* will be treated in Part 1 and the *Gen IV Materials Handbook* in Part 2.

2. Part 1: AFCI Materials Handbook

2.1. History of the AFCI Handbook

The purpose of the *AFCI* (*Advanced Fuel Cycle Initiative*) *Handbook* is to provide a controlled quality source of materials data and information for use in all phases of the AFCI project. A materials handbook is the most logical and efficient method of ensuring that data and information used in connection with target and structural materials are both highly qualified and consistent. This handbook was first issued as the *APT* (*Accelerator Production of Tritium*) *Materials Handbook, Materials Data for Particle Accelerator Applications, Revision 0* in August 1998. Its preparation and publication was a cooperative effort among materials experts at a large number of DOE National Laboratories; later revisions also involved cooperating government laboratories in Germany and Switzerland. The physical form of the *AFCI Materials Handbook* is a CD with separate chapters as PDF files. Revision 5 of the *Handbook* was issued in June of 2006 and is available with demonstrated need through Stuart Maloy at LANL – maloy@lanl.gov.

2.2. Content of the AFCI Handbook

The materials and properties included in the *AFCI Materials Handbook* were selected on the basis of guidance and requirements provided by the designers of accelerator components and systems. Data for incorporation into the *AFCI Materials Handbook* came from a broad range of carefully considered sources including existing handbooks. Data from industry-accepted standards such as the *ASME Boiler and Pressure Vessel Code* were adopted wherever possible.

The *Handbook* currently consists of 22 chapters as shown in Table 1. The chapters on Alloy 718, 304L and 316L stainless steels, 6061 aluminum, and HT9 ferritic/martensitic steel were developed based upon their application as structural and cladding materials in accelerator systems. Tantalum, tungsten, and lead–bismuth eutectic were included as leading candidates for target materials of spallation neutron sources. Other material chapters address a wide variety of needs and applications (e.g., titanium for cryogenics and graphite for beamstops and for producing pions and muons at the Paul Scherrer Institut (PSI)).

For each of the materials covered in the *Materials Handbook* there are sections addressing the following:

* Corresponding author.
E-mail address: maloy@lanl.gov (S. Maloy).

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Table 1
Materials Handbook Chapter listing

Chapter	Material/subject	Comments/applications
1	General information and handbook guide	Purpose, scope, etc.
2	Alloy 718	Beam window/clad
3	316L stainless steel (SS)	Structural/clad
4	6061 aluminum	Structural/clad
5	316L SS to 6061-T6 aluminum weldment	Structural/clad
6	Lead	Blanket
7	Tungsten	Neutron source
8	Niobium	RF cavity
9	Titanium and titanium alloys	Cryogenics
10	Graphite	Beamstop
11	RF window alumina	RF window
12	Fiber optic materials	No data provided
13	Accelerator component materials	No data provided
14	Tritium system materials	Hydrogen isotopes
15	Coolants and fluids	General
16	304L SS	Structural/clad
17	AISI 1040 carbon steel	No data provided
18	HT9 and Russian ferritic/martensitic steels	Structural/clad
19	Modified 9Cr–1Mo Ferritic/martensitic steel	Liquid target vessel
20	Untitled	Placeholder only
21	Tantalum	Neutron source
22	Lead–bismuth eutectic	Neutron source

- Application – typical uses of the material in accelerator systems.
- Materials biography – description of the characteristics of the material, common applications, etc.
- Composition, product forms, and specifications.
- Physical properties as appropriate (e.g., density, thermal conductivity and thermal expansion, specific heat, and electrical resistivity).
- Mechanical properties as appropriate (e.g., elastic, tensile, fatigue, creep, and fracture toughness.)

For most of the materials in the *AFCI Handbook,* the effects of temperature, thermal exposure, exposure environment, and irradiation (including neutron, proton and mixed neutron–proton irradiations) are presented for each property. References are provided to each of the data categories. Perhaps most importantly, the effects of irradiation on properties are treated in great detail. In many instances (e.g., Alloy 718, 316L SS, and tungsten) this involved the generation and analysis of new radiation effects data in the Los Alamos Neutron Science Center (LANSCE). Most recently (Revision 5) radiation effects data were added for high-purity (99.95%) tungsten (irradiated in LANSCE at doses to 23 dpa), for HT9 and similar Russian ferritic/martensitic steels (EP 823) irradiated in both the Fast Flux Test Facility (FFTF) (67.5 dpa maximum dose) and the SINQ Target Irradiation Program (STIP)-II in Switzerland (19.5 dpa max), and reduced activation ferritic/martensitic steels irradiated in the FFTF to 67. 3 dpa (Chapter 9).

The AFCI handbook has served as an important materials resource for many US programs including the Accelerator Production of Tritium, the Spallation Neutron Source and the Advanced Fuel Cycle Initiative and international projects like MEGAPIE (MEGAwatt Pilot Experiment). It will also be an important resource in the new Global Nuclear Energy Partnership for the development of a new handbook for the Advanced Burner Reactor, which is a sodium-cooled reactor designed to burn minor actinides in nuclear waste.

3. Part 2: Gen IV Materials Handbook

3.1. Development of the Gen IV Materials Handbook

The development of Gen IV Nuclear Reactor Systems for the DOE will require and benefit significantly from modern materials data management techniques. Many material types (metals, ceramics, graphites and composites) are involved in Gen IV reactor development and activities such as material selection, component design, and stress analysis will be conducted. It was recognized at an early stage of the Gen IV Program that a material property database that provides an authoritative single source that is internally consistent, validated, and highly qualified is necessary to efficiently manage all the materials data and to facilitate the coordination of materials-related design activities. A task supported by the DOE was therefore established to develop a database named *Gen IV Materials Handbook*. Because constant updates are expected in the *Handbook* as the Gen IV Program develops, and, further, because *Handbook* users may be scattered across the US and around the world in Gen IV International Forum (GIF) countries, it was decided that the database would be constructed electronically using specialized computer software and that it would be remotely accessible through the Internet. Most recently, all GIF member countries agreed to support the use of the *Gen IV Materials Handbook* as the GIF data depository.

The early activities in establishing the *Handbook* database framework included efforts on two fronts: developing software functionality specifications and investigating the marketplace for customizable software products. As a result of these efforts, it was concluded midway through 2005 that the Granta Materials Intelligence (MI) System software developed under the guidance of the Material Data Management Consortium (MDMC) could provide the basic functionalities required for the *Handbook* with desired flexibility for customization and future enhancement. It was further concluded that adopting the MI System as the base software for the *Handbook* and obtaining MDMC membership would reduce overall cost and expedite the development of the Gen IV materials database. The MI hardware and software were acquired and assembled at ORNL and the *Handbook* task officially joined the MDMC.

3.2. Handbook content and plans

The "*Gen IV Materials Handbook* Implementation Plan" [1] defines information that should be contained in the *Gen IV Materials Handbook*. This includes the following:

- Description of the characteristics of the material (e.g., usual applications, crystal structure and phases present, and response to heat treatment).
- Chemical composition.
- Relationship of processing and structure (e.g., effect of architecture in composite materials) on properties.
- Product forms and sizes available.
- Applicable ASTM, ASME, and other technical specifications and code cases.
- Physical and thermal properties (e.g., melting point/range, density, thermal conductivity, electrical resistivity, thermal expansion, specific heat, and emissivity).
- Elastic properties including Young's Modulus, Poisson's Ratio, and shear modulus.
- Mechanical properties (tensile and compression properties, high- and low-cycle fatigue and creep-fatigue behavior, fracture toughness, creep and cyclic crack growth rates, and creep properties).

To manage all of the information noted above and the data requirements that may emerge in the course of Gen IV Materials Program development, the *Handbook* data management overview schema is structured as shown in Fig. 1. It should be pointed out that the boxes in the figure are only conceptual entities used to represent grouping of certain types of data in the *Handbook*. They

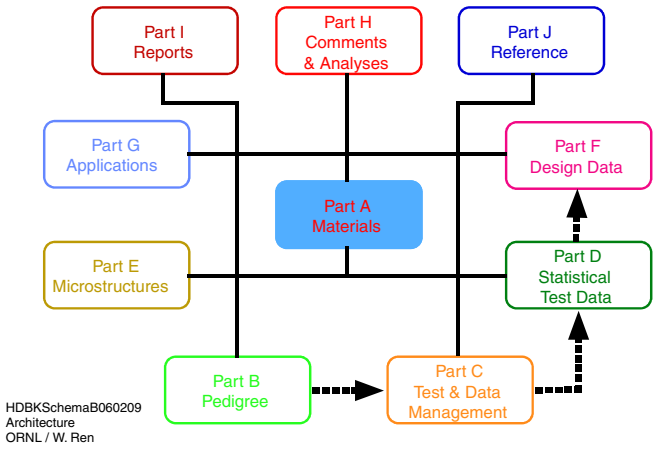

Fig. 1. Overview of *Gen IV Materials Handbook* database schema.

are not real electronic boxes and can be considered as chapters or parts in a book.

The Materials box (Part A) contains general materials information and acts as a conventional main point of entry to the *Handbook* database. The Pedigree box (Part B) contains detailed information on the materials including specification, supplier, processing, joining process and product form; it is heat, product, or batch specific. The Microstructures box (Part E) contains detailed heat, product or batch, and process specific microstructure information. The Test and Data Management box (Part C) contains all relevant information on testing and test data. The Statistical Test Data boxes (Part D) differ from their Test Data box counterparts in that the former stores statistical summaries of the raw test data of the latter. The Design Data box (Part F) contains information generated from the statistical test data for design and analysis. Information on the Gen IV Nuclear Reactor applications of a candidate material is stored in the Applications box (Part G). The Reference data box (Part J) provides the sources for the data while the reports box (Part I) contains a list of relevant reports generated in the Gen IV Nuclear Reactor Program. A separate designated area (Part H) is provided for users to communicate and to leave their comments, analyze results, and discuss data stored in the *Handbook*.

The database schema above is presented in great detail in a report "*Gen IV Materials Handbook* Architecture and System Design" [2] along with discussion of the *Handbook* Home Page and Materials Tree, structure of the three-tier base software architecture, data container hierarchy, data processing functionalities, and access control. Another important report is "*Gen IV Materials Handbook* Beta Release for Structural and Functional Evaluation" [3]. It describes the current status of *Gen IV Handbook* website construction and discusses *Handbook* components and access control of the beta version. Detailed instructions and examples are given to provide guidance for evaluators to browse the constructed parts and use all the currently developed functionalities of the *Handbook* in their evaluation.

This beta version release is focused on demonstration of the base software functionalities, the basic *Gen IV Handbook* structure, and the completed components using primarily Alloy 617 data. The components loaded include the following with reference to the database schema discussed above:

(Part A) Materials – several metallic materials loaded with their data.
(Part B) Pedigree – several metallic materials but only Alloy 617 loaded with pedigree data for several heats.
(Part C1) Test data/creep – Alloy 617 loaded with creep test data at various temperatures and test loads in both air and helium environments.
(Part C3) Test information – specimen information for creep test data of Alloy 617 contained in Part C1-test data/creep.
(Part E) Microstructure – optical and scanning electronic micrographs of Alloy 617 from the heats contained in Part B.

The beta version of the *Gen IV Materials Handbook* was released to selected Gen IV Program stakeholders for evaluation late in 2006. Requests for access to the beta version may be made to Weiju Ren at ORNL – renw@ornl,gov.

4. Summary

Revision 5 of the *AFCI Materials Handbook, Materials Data for Particle Accelerator Applications*, contains relevant data on materials properties for a wide variety of materials. It has served as an important materials database for many US programs and some international projects. It exists in CD form and is available by request through Stuart Maloy at LANL.

Development of a web-accessible materials database for Gen IV Reactor Programs has been ongoing for about three years. A beta version of this *Gen IV Materials Handbook* has been completed and was released to selected stakeholders for evaluation late in 2006.

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