Fusion Materials Sciences Proposed Budget

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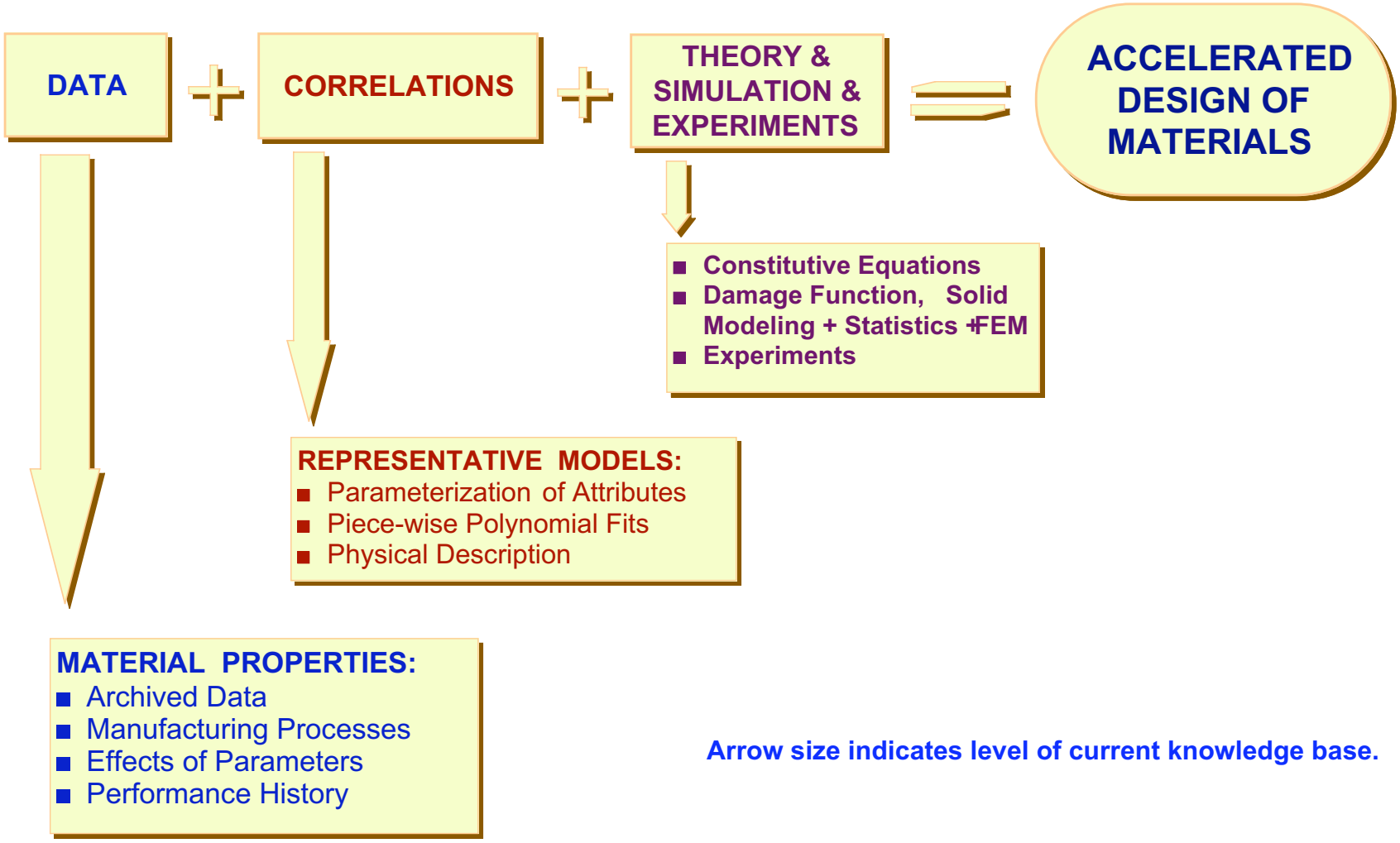
VLT Program Advisory Committee Meeting

March 2-3, 2004

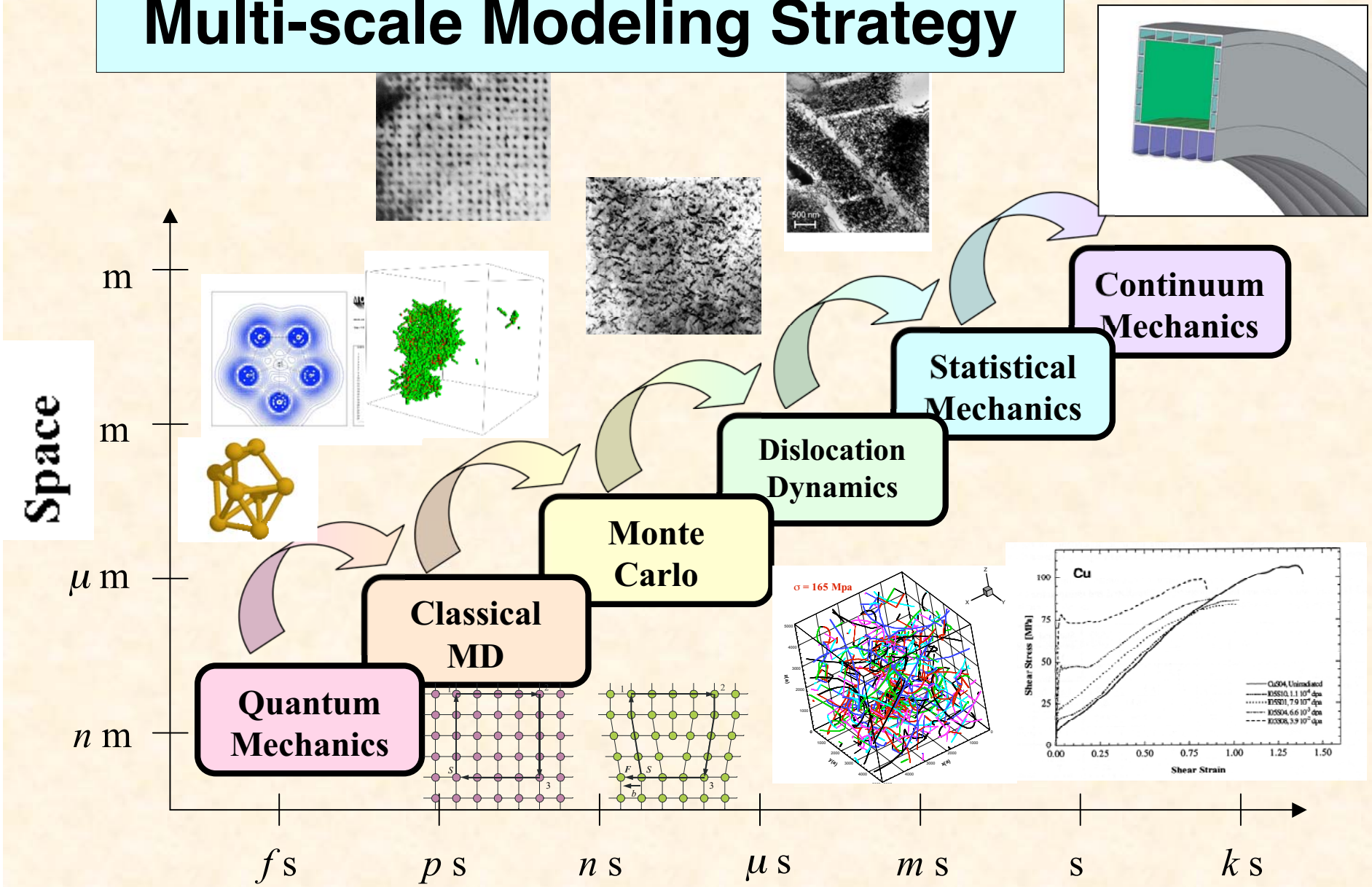
Fusion Materials Science Mission Statement

- **Advance the materials science base for the development of innovative materials and fabrication methods that will establish the technological viability of fusion energy and enable improved performance, enhanced safety, and reduced overall fusion system costs so as to permit fusion to reach its full potential**
- **Assess facility needs for this development, including opportunities for international collaboration**
- **Support materials research needs for existing and near-term devices**
- **Performance measures:**
  - **must provide timely information on operational limits for a wide variety of materials in prototypic fusion environments**
  - **Develop improved-performance materials to enable mission-critical components to satisfactorily function**

Accelerated Design Of Materials with Physical and Statistical Confidence



Multi-scale Modeling Strategy



Principal FY03/04 Achievements

- State-of-the-art computational research and experimental studies have uncovered the physical mechanisms responsible for flow localization in metals irradiated at low temperatures (e.g. dislocation channeling). This can lead to the design of materials that are resistant to these radiation-induced flow localization processes.

- A Master Curve methodology was developed to treat constraint loss effects in fracture toughness specimens, and a critical stressed-volume model was established that successfully described the behavior in V alloys and ferritic-martensitic steels.

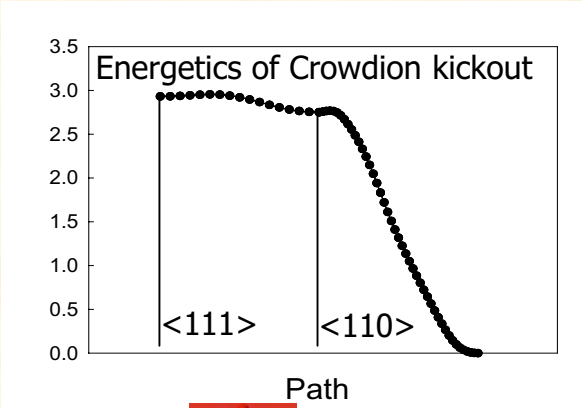
- Evidence for new thermodynamic processes at the nanoscale (e.g., dissolution of Y_2O_3 particles during processing) have been obtained in nanocomposited ferritic steel. The new alloys may increase the upper operating temperature limit of steels by ~200˚C.

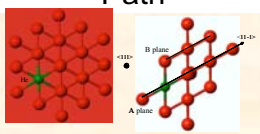
- A science-based program has led to the development of radiation-resistant SiC/SiC composites (for doses up to 10 dpa). These improved composites utilize 3rd-generation SiC-based fibers and tailored fiber/matrix interphase regions (e.g., SiC multilayer interphases). Work with Japanese colleagues (Jupiter-II program) has resulted in the first SiC/SiC composites that have sufficiently low bulk permeation constants for He gas.

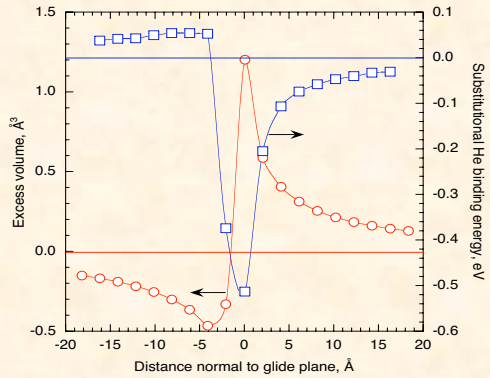
- Scoping compatibility experiments for candidate V/Li MHD insulators have identified several candidates which may perform satisfactorily for temperatures up to 800˚C, including AlN, Y_2O_3 and Er_2O_3. Work is underway to expand their upper use temperatures by doping the Li with suitable concentrations of Ca, O, Al or N solutes.

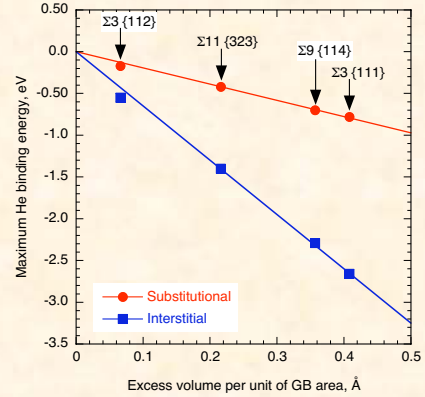
- New atomistic computational methods are revealing the mechanisms of transport and retention of helium in irradiated ferritics.

The Fate of Helium in Ferritic Steels

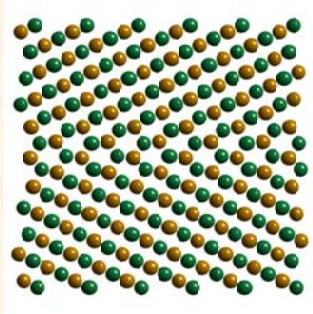








Helium's interaction with dislocations and grain boundaries correlates with the "excess volume" in these defects



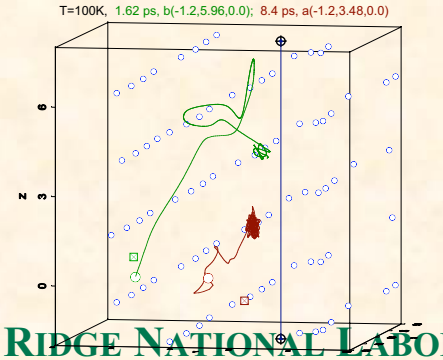
Fe crowdion interstitials "kick" He out of the lattice to interstitial sites where it is highly mobile

Molecular Statics

Potential Energy Surface Mapping

Molecular Dynamics

Helium is attracted to stable positions along dislocations

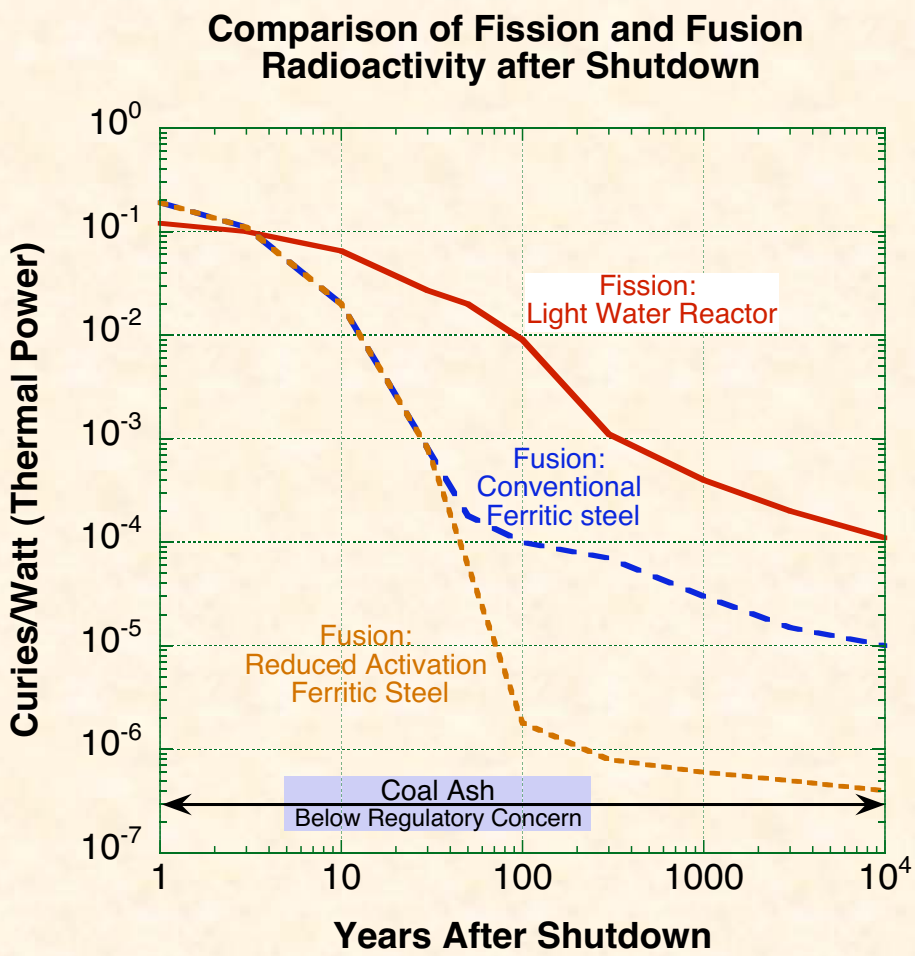


These atomic-scale models of He transport and He interactions with grain boundaries, precipitates, dislocations and defect clusters provide quantitative information on:

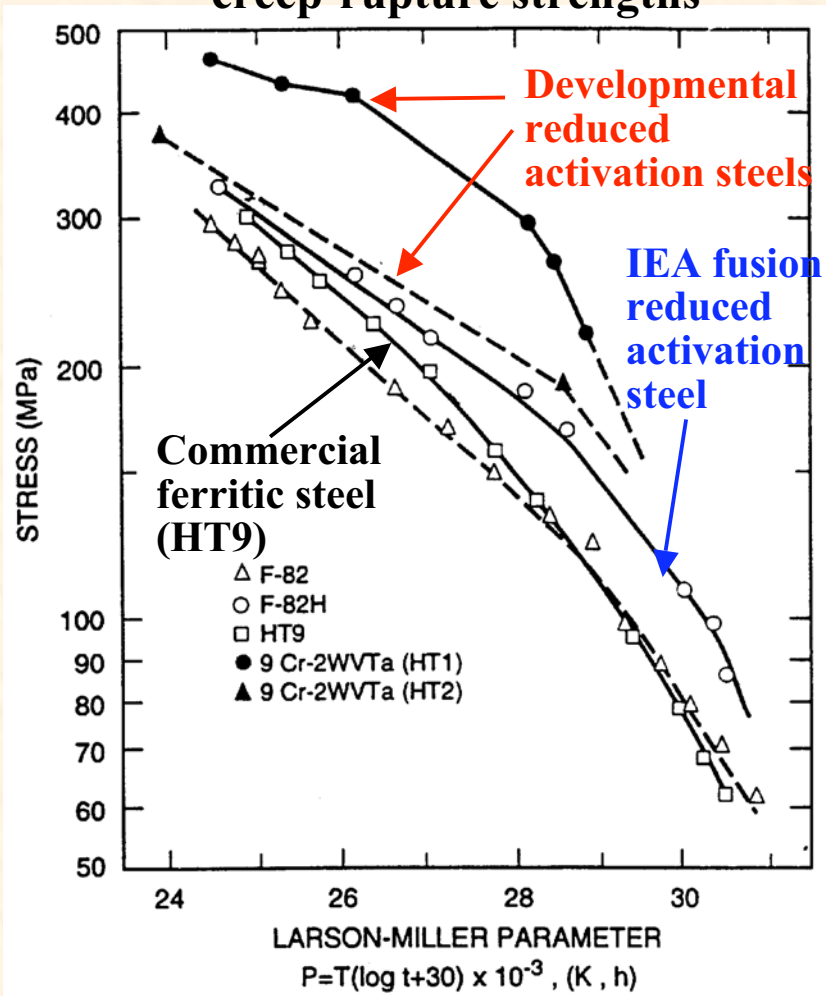
- Mechanisms of the interactions
- Energetics
- Kinetics

This is the basic input required for higher-scale predictive models of microstructure evolution and mechanical property changes.

Ferritic/martensitic Steels with Reduced Radioactivity and Superior Properties Compared to Commercial Steels have been Developed by Fusion

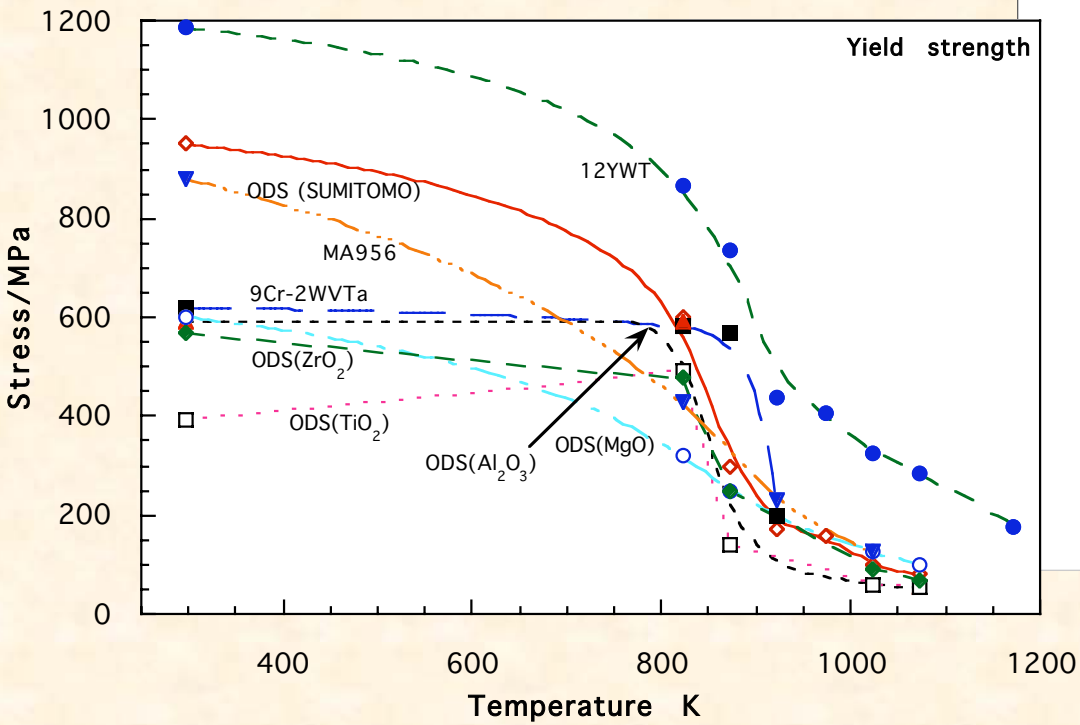


Comparison of thermal creep-rupture strengths

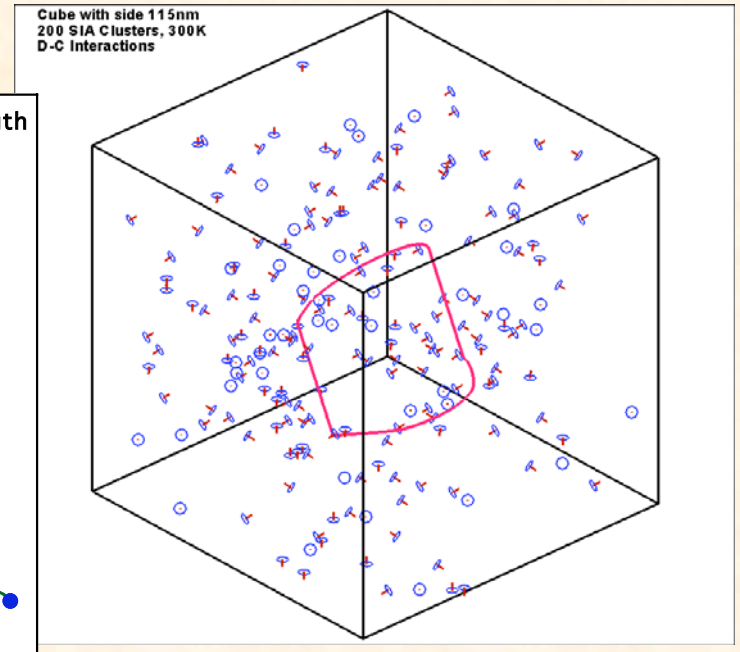


Fusion-developed steels also have superior tensile strength, irradiated fracture toughness, and thermal conductivity

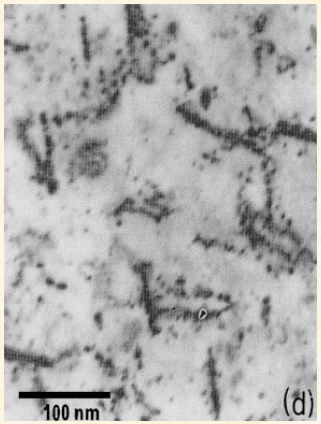
Design of Radiation-Resistant Materials: A Combined Computational & Experimental Approach



Comparison of Tensile strength of New 12YWT Nanocomposited Ferritic Steel vs. other ODS steels



Computer simulation of defect evolution



FY03 Funding Profile

FY2003 Funding by Institution ($000)

	Structural Materials R&D	Neutron Source R&D	Crosscut Theory & Modeling	Functional Materials (MHD ins.)	DOE/JAERI & Jupiter-II tech. support
ORNL	2120	180[a]	450	150	1200
ANL	105(CO)	–	–	300	–
PNNL	990	–	300	–	90
LLNL	–	–	290	–	–
UCSB:	205	–	225	–	50
UCLA:	–	–	270	–	
Princeton:	–	–	141	–	
Wash. State	–	–	40	–	
Merrimack U.	–	–	24	–	
RPI	50	–	–	–	
Mat.Sci.Init.	258**	–	200**		
Totals	**3728**	**180**	**1940**	**450**	**1340**

[a]subcontracted to Univ. Tennessee ($40 K), Advanced Energy Systems ($90 K) and private consultant ($50 K)

**performing institutions to be determined by competitive review process

FY05 Tasks

Reference Budget:	7400 k$
Principal Milestones	**Crosscutting Theory & Modeling** • Complete first round of detailed comparison of computational and experimental studies on the interaction between moving dislocations and dislocation loops, bubbles, voids, defect clusters and precipitates responsible for hardening, embrittlement and plastic flow localization in alloys (April 2004) • Complete model-based analysis of sink strength effects on high temperature He embrittlement and creep behavior and report recommendations of optimum microstructures (June 2004) **Structural Materials** • Complete SANS, TEM and 3D atom probe analysis of the physical origins of the superior mechanical properties of nanocomposited ferritic steels, and make a preliminary assessment of the influence of nanoscale features on thermodynamics (December, 2004) • Complete evaluation of thermal conductivity data and develop experimentally-validated models for prediction of thermal conductivity of ceramic composites (October 2004) • As part of the Jupiter-II program, investigate the irradiation behavior of new SiC/SiC composites possessing low gas permeability, high strength, high toughness, and high thermal conductivity (Aug. 2004) • Determine the elevated-temperature (900-1300?C) swelling behavior of irradiated SiC (Sept. 2004) • Complete irradiation of the Jupiter-II Li-bonded capsule (primary emphasis: deformation and fracture mechanisms, including irradiation creep and radiation effects on V alloy weldments) and two DOE/JAERI irradiation capsules (primary emphasis: effect of He generation of deformation and fracture behavior of ferritic/martensitic steels)--(Aug. 2004) **Neutron Source** • Provide engineering validation data on the performance of the accelerator system for IFMIF (Aug. 2004) **Functional Materials (MHD insulators)** • In conjunction with the DOE/MEXT Jupiter-II program, utilize modeling and experimental studies to determine the maximum allowable flaw concentration in MHD insulator coatings, and establish the viability (chemical compatibility, integrity, electrical resistivity, and self-healing capability) of candidate MHD insulators (AlN, Y_2O_3, Er_2O_3) for Li-cooled V alloy blanket systems (April, 2004) **ITER** • Complete principal milestones in support of ITER materials agreement G 74 TD 07 FU ❋ Participate in anticipated future requested ITER materials tasks. ❋ Continue development of Materials Database and VISTA.

Fusion Materials Sciences
-Enhanced (>10%) FY05 budget scenario

- Establish a fusion materials science center, modeled after the NSF materials science centers (500 k$)
  - research priorities may include nanoscale and other innovative materials research, fundamental experiments/modeling on deformation and fracture
  - This center would involve multi-institutional participation, and would provide critical leveraging of the concepts proposed in items 2 and 3 in the 10% increase budget scenario
  - Tangible focal point for Virtual Laboratory for Materials

FY06 Milestones

• **Reference Budget:**	7400 k$ - 10%
• **Principal Milestones**	**Crosscutting Theory & Modeling** • Complete initial multiscale modeling of He transport and fate in advanced BCC metals (Dec. 2005) • Complete investigation of possible microstructural changes to minimize the effect of low temperature radiation embrittlement in metals (Nov. 2006) **Structural Materials** • Investigate the effects of trace element composition variables on the DBTT behavior and the mechanical properties of V alloys from 450 to 700?C (November 2005) • Gain a preliminary understanding of the efficacy of joining processes for SiC composites, including the effect of irradiation on first-generation joints (Feb. 2006) • Begin exploration of hermetic coating techniques for SiC composites and joints (Nov. 2005) • Complete investigation of alternative (less costly) processing routes for synthesis of nanocomposited (oxide dispersion strengthened) ferritic steels (Jan. 2006) • Determine the effect of helium additions on the low temperature radiation embrittlement of ferritic-martensitic steels, as part of the DOE/JAERI program and modeling initiative (July 2006) **Neutron Source** • Provide critical engineering validation data and engineering design support for the IFMIF ion source, accelerator, target system, and test cell (Apr. 2006) **Functional Materials (MHD insulators)** • Complete examination of the integrity and electrical resistivity (including self-healing capability) of leading candidate MHD coatings in flowing loop facility (September 2006). **ITER-Related Materials Engineering**: Continue development of the Digital Materials Database and implementation of the VISTA Structural Evaluation Process.

FY06

-Enhanced budget scenario (at FY05 Level)

1. Establish a significant US participation level in the engineering validation / engineering design activity for the IFMIF neutron source project. The required FY05 resources for a "full-partner" participation with EU, Japan and Russia is ~3.2 M$ (see major initiatives section below).

2. Expand functional responsibilities for materials engineer task group, currently funded at 150 k$/year (interface between materials community and enabling technology/near term plasma experiments). The increased budget would enable materials science experts not currently funded by fusion to apply their expertise to key near-term issues, such as the ITER blanket module design. – additional funding of $200 K

3. Provide support for maintenance and upgrading of key experimental facilities, with preference for facilities used in international collaborations (hot cell equipment, etc.). One of the key outcomes of this initiative would be to enable a Virtual Laboratory for Materials to become functional for the US research team and international collaborators ("lab without walls initiative"). A milestone would be to establish full remote (internet-accessible) control and operation of a mechanical property test machine located in a hot cell by August, 2006 --$300 K

FY06

-Enhanced budget scenario (cont)

4. Continue to build upon the successful theory and modeling initiative launched three years ago, which is already generating numerous significant results. The new initiative (based on peer-reviewed proposals) should preferentially increase support for universities, postdocs & younger staff (knowledge transfer for the future). Areas of emphasis could include modeling of deformation and fracture of irradiated materials (including effects of helium), and modeling of radiation damage, swelling and thermal conductivity degradation of SiC.—$200 K

5. Determine underlying mechanisms responsible for the Radiation-Induced Electromotive Force (RIEMF) in irradiated plasma diagnostic components (gamma ray and thermal annealing tests), which is a critical R&D issue for ITER. Effective methods to minimize the current drift associated with RIEMF are needed for long-pulse burning plasma experiments. Research results obtained on in-core fission flux monitors can be utilized to minimize the drift that occurs in insulated cables. An FY05 milestone would be to 1) complete a critical analysis of the in-core fission detector data and results obtained by fusion researchers on RIEMF (Feb., 2003), and 2) recommend alternative cable geometries and/or materials that would minimize the RIEMF effect (Aug. 2006)--$100 K

Reduced FY06 budget scenario

- Significant negative impact on the ability of the Materials Science program to meet its international commitments (DOE-JAERI and DOE-MEXT Jupiter-II programs). These collaborations (which bring over 2 M$/year into the US) require a mixture of personnel with different technical areas of expertise. Since the average research staff member on the Materials Science program is currently only funded at a level of ~0.4 FTE/yr, further cuts would cause irreparable harm.
- US support for the IFMIF neutron source project would be cut (it should be noted that the EU, Japanese, and Russian budgets for IFMIF have increased in the past year, due to the impending engineering validation / engineering design activity that is scheduled to begin in late 2004.

FY06

-Enhanced budget scenario (above FY05 Level)

- The engineering validation / engineering design activity (EVEDA) of the international fusion materials irradiation facility is scheduled to begin in the fall of 2004. In order for the US to participate as a full partner with the EU, Japanese and Russian parties, an estimated FY06 US budgeted effort of ~3.2 M$ would be required. Active participation in the IFMIF EVEDA phase is essential in order for the US to commence on an R&D program that would produce electrical power from fusion within ~35 years.

- Establish a fusion materials science center, modeled after the NSF materials science centers (research priorities may include nanoscale and other innovative materials research, fundamental experiments/modeling on deformation and fracture). This center would involve multi-institutional participation, and would provide critical leveraging of the concepts proposed in items 2 and 3 in the 10% increase budget scenario--$500 K

Interface Issues and Miscellaneous

- Materials engineer initiative (viewed as positive step; initially funded by Materials program and MFE Chamber technology)
- The activity can play a positive role in the interface with ITER-related tasks.