OVERVIEW OF THE US FUSION MATERIALS SCIENCES PROGRAM

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Highlights of recent U.S. fusion materials research activities are summarized, including multiscale materials modeling and experimental results. Recent first principles atomistic calculations on vanadium and iron-helium have found that previous interatomic potentials incorrectly predict several important point defect properties. Molecular dynamics simulations of displacement cascades are now approaching energies equivalent to 14 MeV fusion neutrons. Considerable effort is being devoted to understanding the fundamental mechanisms of low temperature radiation hardening and embrittlement. Work is also in progress to determine the allowable temperature and dose operating regimes for candidate reduced activation structural materials (including transmutant helium effects). New compositions of reduced activation steels and vanadium alloys with potential for significantly improved properties are being investigated. Due to recent improvements in SiC/SiC ceramic composites, engineering-relevant mechanical property tests are being introduced to replace historical qualitative screening tests. Materials research in support of the ITER burning plasma physics machine is briefly described.

I. INTRODUCTION

The primary mission of the U.S. fusion materials sciences program is to 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. Some effort is also directed toward assessment of facilities needed for this development, which recently involved work on the conceptual design of the international fusion materials irradiation facility (IFMIF) **[1]**. A third activity involves support of materials research needs for existing and near-term devices, ranging from small-scale plasma physics machines to ITER. Institutions involved in U.S. fusion materials research in 2004 included three national laboratories and 7 universities. To a large extent, the performance limits of the structural material in the fusion blanket region controls the response of the overall reactor power generation system. Therefore, research on structural materials is the main focus of the fusion materials program. Research on important nonstructural fusion technologies (including materials), such as plasma facing components, tritium breeders, plasma heating systems, and plasma diagnostics, is primarily carried out in other fusion technology programs.

About 25% of current research is directed toward cross-cutting multiscale materials theory and modeling. The remainder of the research activity is split among experimental studies on advanced reduced activation structural materials (ferritic/martensitic or oxide dispersion strengthened ferritic steels, vanadium alloys, and SiC/SiC ceramic composites), functional materials (insulator coatings to mitigate magnetohydrodynamic effects between channel walls and conductive coolants flowing across magnetic field lines, improved ductility Mo alloys for high heat flux applications, copper for various high conductivity applications), ITER machine-specific R&D, and support of the IFMIF activities. The research in the fusion materials program is highly leveraged with two Japanese collaborations (DOE/JAERI and JUPITER-II), along with a wide range of non-fusion U.S. programs including DOE (Basic Energy Sciences, Nuclear Energy, Science and Technology, Naval Reactors), Nuclear Regulatory Commission, National Science Foundation, and NASA programs.

The following provides a brief overview of recent experimental and modeling research highlights on advanced structural materials for fusion energy systems.

II. MULTISCALE MODELING ACTIVITIES

Multiscale modeling activities are investigating defect production and migration mechanisms, plastic deformation mechanisms, and fracture mechanics behavior. Recent atomistic first-principles calculations have been performed on vanadium [2] and Fe-He [3] in order to investigate fundamental point defect behavior in these important reduced activation materials (e.g., formation and migration energies of vacancies and self-interstitial atoms), and to provide fitted interatomic potentials suitable for molecular dynamics simulations. The <111> dumbbell was found to be the most stable interstitial configuration in vanadium, whereas previous potentials predicted <110> or <100> configurations to be most stable [2]. The predicted vacancy and interstitial

migration energies with the new vanadium potential were found to be in good agreement with experimental estimates [2]. In the Fe-He calculations, the energetically stable location for He atoms was found to be the tetrahedral site instead of the octahedral site predicted by previous interatomic potentials [3]. Similar results have recently been reported using a different atomistic code [4]. Magnetism was found to play a crucial role in determining He interaction properties in iron [3]. Helium located in the tetrahedral interstice produced the least perturbation on the magnetic moment of Fe. Figure 1 shows the large change in calculated electron density associated with the octahedral site [3]. A fitted Fe-He interatomic potential incorporating three-body interactions was derived.

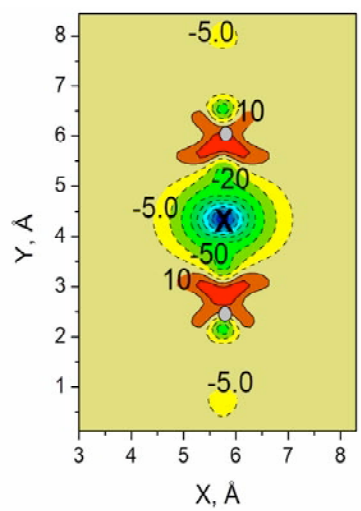

Fig. 1. Spatial distribution of charge density (electrons/Å^3) for He in octahedral site of BCC Fe lattice.

Molecular Dynamics (MD) simulations up to neutron displacement damage energies of 12 MeV, much higher than the average primary knock-on atom (PKA) energy in a fusion blanket and approaching the maximum PKA energy associated with a 14 MeV neutron collision, have recently been performed for iron [5]. These new results provide further support for the conclusion drawn from earlier experimental and MD simulation studies [6,7] that the primary damage state created by fusion neutrons is similar to that produced by fission neutrons. For PKA energies in iron above ~10 keV (corresponding to the average PKA energy from fission neutron irradiation), localized lobes of displacements known as subcascades are generated. Each of these subcascade lobes is spatially and temporally similar to the cascades produced by fission neutrons. This causes the fraction of defects surviving in-cascade recombination events (time scale > ~5 ns) to become constant relative to the international standard Norgett-Robinson-Torrens displacement damage per atom (dpa) value, and therefore validates the use of dpa as a means to compare displacement damage obtained in widely varying types of irradiation sources (fission, fusion, and spallation neutron). Figure 2 compares the displacement cascade structure for the average fission and fusion blanket conditions [7]. A critical unanswered question for fusion irradiation conditions [6] is the effect of the higher transmutant solute production (in particular H and He) on the microstructural evolution at moderate doses (above 1 to 10 dpa). Fundamental modeling and experimental studies are in progress to determine the migration and trapping behavior of helium in metals, in order to design materials with improved resistance to void swelling and high temperature helium embrittlement in fusion reactor irradiation environments [8].

At higher length and time scales, kinetic Monte Carlo [9-12] and three-dimensional dislocation dynamics [13-16] models are being used to investigate the microstructural evolution during neutron irradiation and interactions between dislocations and defect clusters. Chemical rate theory models are being used to investigate long-term defect accumulation and helium transmutation effects [17,18].

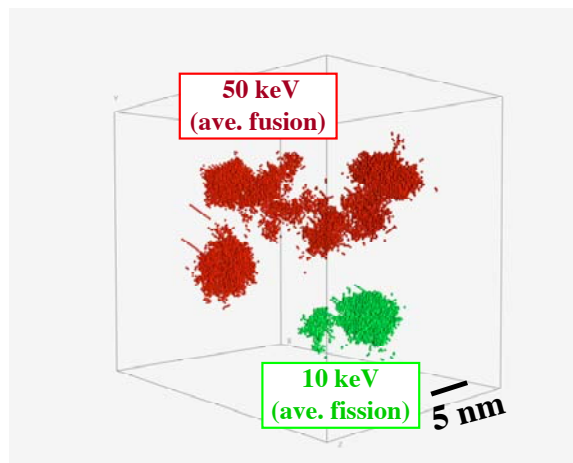

Fig. 2. MD simulation of displacement cascades in Fe at peak damage condition (~0.5 ps) for two PKA energies.

III. DEFORMATION AND FRACTURE BEHAVIOR OF IRRADIATED METALS

Due in part to the near-term needs for ITER, deformation and fracture issues for materials irradiated at low to intermediate temperatures have been the focus of several recent experimental and modeling investigations. In-situ straining experiments performed in electron microscopes [19-22] have directly observed annihilation of defect clusters by gliding dislocations, which is a key step in the formation of cleared dislocation channels in metals irradiated and deformed at temperatures below ~0.3 T_M where T_M is the melting temperature. These cleared dislocation channels are thought to be a key factor

in the low ductility of metals irradiated below 0.3 T_M. Supporting MD simulations are investigating the effects of experimental parameters such as dislocation type (screw vs. edge), deformation temperature, and strain rate (dislocation velocity) [19,20,23]. Fig. 3 shows the double superjog and debris created after a single interaction by a gliding dislocation that reduced a 4.2 nm (136 vacancy) stacking fault tetrahedron to 2.75 nm (55 vacancies) [24], demonstrating the efficiency of the cleared channel formation process. Fig. 4 shows the tensile stress-strain curves for F82H ferritic/martensitic steel after neutron irradiation to 5 dpa [25]. Very low uniform elongation occurs after irradiation at 573 K for doses above 0.1 dpa. Cleared dislocation channels were observed in the deformed gage regions of the irradiated specimens [25].

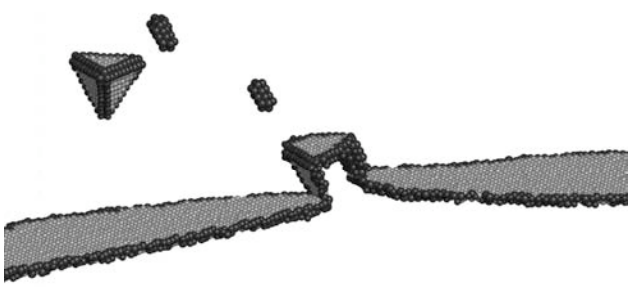

Fig. 3. MD simulation of partial destruction of a 4.2 nm SFT due to gliding edge dislocation at 450 K.

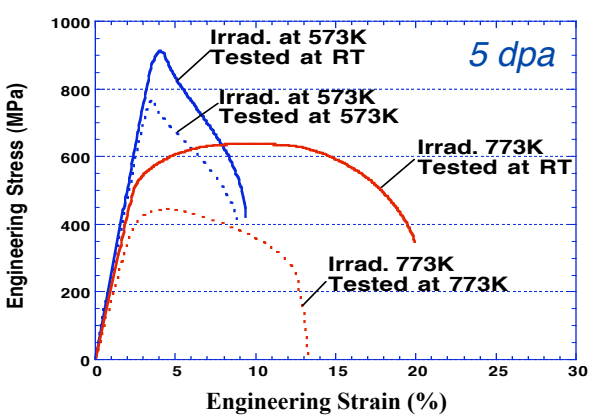

Fig. 4. Engineering stress-strain curve for F82H ferritic martensitic steel after neutron irradiation.

The effect of irradiation dose, temperature and deformation level on the predominant deformation mode has been investigated for a wide range of metals [25-31]. The general effect of neutron irradiation at temperatures below ~0.3 T_M is to inhibit dislocation glide and multiplication processes. This can cause alternative deformation processes such as twinning to appear in irradiated metals. Despite the pronounced hardening and change in the shape of the engineering stress-strain tensile curve that occurs in metals following neutron irradiation at low temperatures, it was found that the stress to induce localized necking (plastic instability stress) was similar for annealed, cold-worked, and irradiated materials [27,28]. The shapes of the true stress-strain plastic deformation curves were also found to be comparable for unirradiated and irradiated metals when shifted to account for initial radiation strain hardening, which suggests that radiation-induced defects and deformation-produced network dislocations produce similar post-yield strain hardening effects.

Recent fracture mechanics investigations have focused on determination of the applicability to vanadium alloys [32-35] and reduced-activation ferritic/martensitic steels [36-39] of the "master curve" methodology that was developed for fission reactor pressure vessel steels. These studies have demonstrated that the master curve method is applicable to 9Cr ferritic/martensitic steels. Adoption of the master curve method greatly reduces the required number and physical size of specimens that must be tested [39]. Fig. 5 shows the temperature-dependent fracture toughness of different sized F82H steel specimens after correction for constraint and small scale yielding effects [39]. A multiscale model was developed to link macroscopic fracture behavior with atomic-scale initiating mechanisms [38]. The key physical parameters controlling the fracture mechanics behavior of structural metals are the true stress-strain constitutive equation (including temperature and strain rate effects), coarse-scale inclusions that act as stress-concentrating initiation sites for fracture, and geometric size effects. Physical size effects arise from weakest-link statistics (the probability of encountering a critical-sized inclusion is proportional to the tested volume) as well as constraint loss. One important outcome of geometric size effects for thin-walled fusion structures is that the benefits of radiation hardening may offset the reduction in elongation [38].

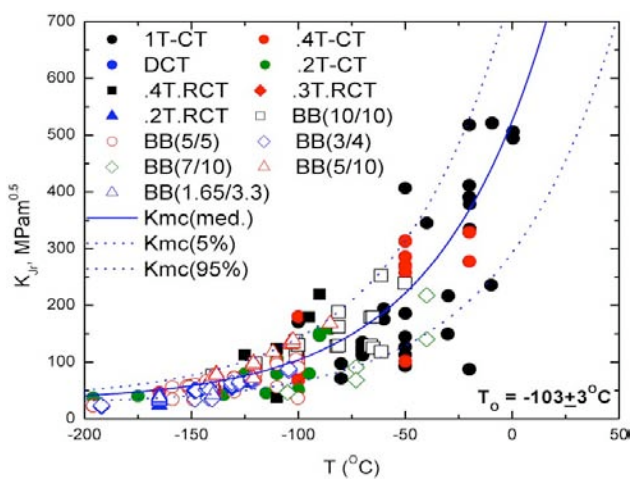

Fig. 5. Fracture toughness of F82H ferritic martensitic steel corrected for size effects.

IV. REDUCED ACTIVATION STRUCTURAL MATERIALS AND COMMERCIAL SPINOFFS

As reviewed elsewhere [40-42], consideration of the limited number of elements that have acceptable radiological safety performance and low long-term radiation levels following exposure to intense fluxes of fusion neutrons, along with the demanding structural requirements, leads to three classes of candidate structural materials: reduced activation steels, vanadium alloys, and SiC/SiC ceramic composites. Within the reduced activation steel class, ferritic/martensitic and bainitic steels and nanocomposited oxide-dispersion-strengthened (ODS) ferritic or martensitic steels have been developed with favorable radioactivation characteristics, improved radiation resistance, and comparable or superior unirradiated properties than existing commercial steels [42-44]. The DOE/JAERI US-Japan collaboration is investigating effects of fusion-relevant helium generation rates on the mechanical properties and microstructures of neutron irradiated advanced ferritic/martensitic steels [45]. A V-4Cr-4Ti alloy with good radiation resistance, good low-temperature fabricability and toughness, and adequate high-temperature strength has been developed [6,46-48]. The potential for further improvements in V alloy radiation resistance via nanoscale precipitates is currently being investigated [49]. A sustained program on the fundamental behavior and radiation damage mechanisms in SiC/SiC composites has recently led to improved mechanical behavior by utilizing advanced fibers and fiber-matrix interfaces [50-53]. Recently developed experimental tests have focused on measurement of specific properties that control the composite constitutive behavior, including interlaminar shear, in-plane shear, and various miniaturized tensile and compressive tests [54]. This also enables acquisition of engineering-relevant data (uniaxial tensile, etc.) instead of qualitative screening tests (e.g. bend flexural strength) that have historically been used for SiC/SiC [54].

Recent chemical compatibility tests have identified several promising new candidates for magnetohydrodynamic (MHD) insulators in lithium-cooled systems [55,56], and have determined that SiC has good chemical compatibility with Pb-Li up to very high temperatures [56].

Although fusion materials R&D is focused on long-term fundamental and applied research, several high-performance materials directly enabled by fusion are being introduced into near-term commercial applications. For example, the phase evolution knowledge obtained on stainless steels during elevated temperature irradiation provided the foundation for development of several new austenitic stainless steels (wrought and cast) with dramatically improved high temperature strength. The new cast steel has very high thermal creep resistance (e.g., 23000 h creep rupture time at 850˚C for an applied stress of 35 MPa, versus 500 h for standard material) [57]. The improved creep resistance is due to the formation of a fine dispersion of stable nanoscale MC precipitates. This improved steel uses reactive Ti, V and Nb solute that enhance MC precipitate formation, and also utilizes catalytic effects (i.e., Si enhances Fe_2Mo or M_6C formation during irradiation). Selective additions of Nb in place of Ti promote formation of fine-scale NbC instead of globular TiN. Modified wrought austenitic steels have been developed for microturbine recuperators and other high temperature applications [58]. Figure 6 shows the nanoscale precipitate structure of wrought Type 347 stainless steel foil after a modified process treatment that reduced thermal creep at 732˚C by over one order of magnitude. A 3Cr bainitic steel developed by fusion is being commercialized due to its superior tensile and thermal creep strength compared to existing 2 1/4Cr steels [59,60]. This steel is also attractive because joining of large sections may not require a post weld heat treatment.

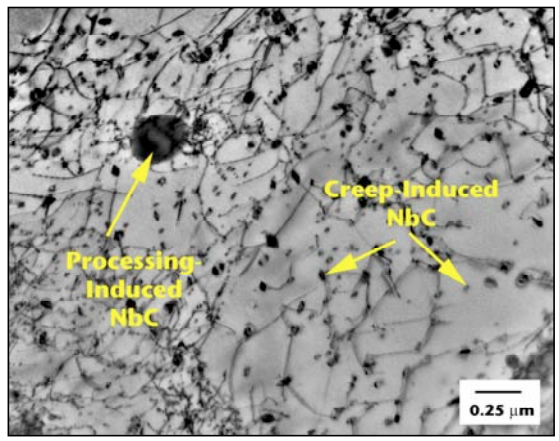

Fig. 6. Microstructure of wrought Type 347 austenitic stainless steel after creep testing at 732˚C for 10,000 h.

V. ITER-RELATED R&D

The fusion materials program generated data for the engineering design of ITER, and is continuing to provide key data and supporting analyses on the structural materials (Cu alloys, stainless steel) and functional materials (plasma diagnostics, plasma heating) for ITER. The DOE/JAERI program provided much of the radiation effects data on austenitic stainless steel base metal and weldments at ITER-relevant conditions that served as the foundation for the ITER engineering design [31,61-70]. Additional ITER R&D is summarized below:

- Cu alloy R&D (CuCrZr, GlidCop) [71-80]: Research was performed to determine the most appropriate heat treatment conditions for CuCrZr that retained acceptable strengths. Substantial mechanical properties data was obtained on unirradiated and irradiated ITER-grade GlidCop oxide dispersion

strengthened copper (US/Russia and US/EU collaborations). Mechanical fatigue studies on Cu/stainless steel layered structures and monolithic Cu alloys were also performed.

- Ceramic insulator radiation-induced electrical degradation (RIED) studies and other plasma diagnostics radiation effects R&D (including US/Japan JUPITER and DOE/JAERI collaborations) demonstrated that RIED was not an issue for ITER conditions [81-83]. If the RIED effect had proven to exist for ITER conditions, ITER operation would have been restricted to a few full power days of full power DT operation.
- Irradiated Be mechanical properties studies (at ITER-relevant low temperatures) demonstrated that no catastrophic embrittlement or thermal conductivity degradation occurred [84].
- Research on the effect of irradiation temperature on graphite thermal conductivity degradation (modeling and experimental data) substantially improved the understanding of the potential operating temperature regimes for graphite tiles in ITER [85-87].

Current ITER-relevant aspects of the US fusion materials program include both ITER machine-related tasks and test blanket module (TBM) R&D activities. The ITER machine tasks include a critical assessment of data for the ITER materials properties handbook, establishment of design methodologies for joints of irradiated and dissimilar materials, targeted R&D on specific metallic systems, and research on ceramic insulators for plasma heating and diagnostics.

One of the main ITER TBM tasks is examining effects of neutron irradiation on the deformation and fracture behavior of ferritic/martensitic steels. The results from this research program are applicable for both near term (e.g., ITER) and long-term (e.g., Demo) machines. Additional ITER TBM tasks include exploration of the high temperature chemical compatibility of SiC with Pb-Li, measurement and modeling of the thermal and electrical conductivity degradation in neutron irradiated SiC composites (pertinent to flow channel inserts for the dual coolant TBM), and initiation of 3-dimensional finite element simulations of stress conditions and deformations in provisional ITER TBM designs.

VI. CONCLUSIONS

The U.S. fusion materials program is increasing activities related to ITER (machine and test blanket modules). Underlying deformation and fracture mechanisms at low temperatures are a major research emphasis. High temperature deformation and fracture (He embrittlement) is also of concern, but is not a current major activity due to funding limitations. SiC/SiC ceramic composite R&D has progressed from initial qualitative screening studies to measurement of engineering-relevant mechanical properties (unirradiated and irradiated). On-going U.S.-Japan collaborations (DOE-JAERI and JUPITER-II programs) are important and mutually beneficial for advancing fusion materials progress for ITER and follow-on machines.

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