Fusion materials science: overview of challenges and recent progress

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Abstract

A brief review is given of fundamental materials science concepts important for development of structural materials for fusion energy systems. Particular attention is placed on displacement damage effects associated with the unique deuterium-tritium (D-T) fusion environment. Recent examples of multiscale materials modeling results (closely coupled with experimental studies) are summarized. Fundamental differences in the behavior of body centered cubic versus face centered cubic crystal structures are highlighted. Finally, a brief overview is given of the high-performance reduced-activation materials being developed by fusion.

I. INTRODUCTION

Various energy analyses have concluded that the world energy needs will grow from current baseline power levels of ~14 TW to 25-60 TW by the year 2050.[1] Environmental concerns associated with fossil fuels are creating increased interest in alternative non-fossil energy sources. Potential environmentally sustainable large-scale energy options include solar, fission, and fusion energy. A common theme for all three of these options is the need for materials research to either improve capabilities (*e.g.*, Generation IV fission reactors) or to establish the technological feasibility for reliable baseline power. Other non-fossil alternatives have limited potential: hydroelectric power has already reached approximately full utilization in the U.S., and the estimated maximum power attainable from wind in the U.S. is less than 0.5 TW.[1] Although fusion energy certainly has the potential to fill anticipated worldwide energy needs in the second half of this century, it is often not included in energy assessments due to perceived technological immaturity. Along with the continuing sustained advances in plasma physics, materials research must become an increasingly important activity as part of the transition of fusion from being an important scientific venture to being a realistic candidate energy option for the 21st century.[2]

The challenging fusion reactor environment (radiation, heat flux, chemical compatibility, thermo-mechanical stresses) will require utilization of advanced structural materials in order to fulfill the promise of fusion energy to provide safe, economical, and environmentally acceptable energy. In the following section, a brief review is given of several key introductory materials science concepts. Some of the displacement damage physics principles are then summarized, followed by examples where multiscale materials modeling (closely coupled with focused experimental studies) is probing fundamental physical phenomena that control the stability of structural materials in a projected fusion reactor environment. Finally, a brief summary is given of the high-performance reduced-activation materials being developed by fusion (including materials that are being spun off for immediate commercial use in non-fusion applications). The focus in this paper is on mechanical behavior and microstructural stability of structural materials, including the dramatic changes that can be induced by fusion neutron irradiation. Ongoing work on chemical compatibility and joining is not reviewed. Important materials challenges also occur for numerous other materials systems in fusion machines, including plasma facing components, plasma heating systems, plasma diagnostics, and superconducting magnets.

The historical paradigm is that development of incrementally-improved materials for structural applications in non-irradiation environments typically requires a period of 10 to 20 years.[3,4] Considering the additional requirements for fusion structural materials to have good performance in the presence of high neutron irradiation and heat fluxes, the development of fusion structural materials may be the greatest challenge ever undertaken by materials scientists. This emphasizes the importance of utilizing a broad range of scientific tools to guide fusion materials development.

II. MATERIALS SCIENCE FUNDAMENTALS

Solids can be organized into two general categories, crystalline and noncrystalline. The latter category includes amorphous solids (*e.g.*, glass) and most polymers, which generally are not suitable for demanding structural applications and will not be discussed further. The atoms in crystalline materials are arranged in well-defined periodic configurations known as Bravais lattices. There are a total of 14 possible Bravais lattices.[5] Metals are approximately equally divided among three Bravais lattices: body centered cubic (BCC), face centered cubic (FCC), and hexagonal close packed (HCP).

Several types of crystalline defects can exert significant influence on the properties of materials, including vacancy and interstitial point defects and dislocation line defects.[6] A certain number of vacant lattice sites ("vacancies") are thermodynamically stable at nonzero temperatures due to statistical entropy considerations. Similarly, the concentration of atoms located in the interstices between lattice atoms ("interstitials") can be described by statistical mechanics. The thermal equilibrium vacancy concentration approaches 0.1% near the melting temperature of metals. The thermodynamic equilibrium concentration of interstitials is many orders of magnitude smaller than that of vacancies and generally can be neglected for nonirradiation conditions. For particle irradiation conditions, the concentrations of vacancies and interstitials are increased many fold over their thermal equilibrium values and their diffusion and agglomeration can introduce numerous profound changes to material properties.[7] A "dislocation" can be visualized as a line defect created when an incompletely formed plane of atoms is terminated in the interior of a crystalline solid.[6] Plastic deformation occurs in metals when they are subjected to loads that exceed the energy needed to induce motion of dislocations.

Dislocation motion involves localized lattice shear (bond breaking and reattachment) occurring over one atomic half-plane. The stress required to induce dislocation motion is more than one order of magnitude smaller than the stress needed to shear perfect dislocation-free crystals[6], thereby providing a low-stress deformation mechanism. However, the dislocation multiplication that normally occurs in metals during deformation typically leads to strengthening due to interlocking of dislocations and their stress fields in a process known as work hardening.

From lattice energy considerations, dislocation motion ("slip" or "glide") preferentially occurs along close-packed planes and in close-packed atom directions. A total of 12 primary slip systems exist for both BCC and FCC crystal structures.[8,9] In contrast, only three primary slip systems exist for HCP lattices. Since general plastic strain requires five independent slip systems,[8] HCP metals (*e.g.*, Be) generally have low ductility. Considering also the anisotropic properties associated with the HCP lattice, BCC and FCC metals are generally strongly preferred for structural applications.

Selection of a structural material involves compromise between strength and ductility. High strength materials generally have low ductility, and vice versa.[9] In general, FCC metals offer higher ductility whereas BCC metals offer higher strength (although wide variations in strength and ductility are achievable within any given metal by selective alloying additions or due to introduction of defects). For structural materials, a highly desirable feature is for the material to become stronger when plastically deformed up to elongations well above a few percent. This work hardening ability provides robustness in the event of unanticipated stresses (*e.g.*, high-current plasma disruptions). Very high strength materials generally provide little work hardening when plastically deformed, and begin to locally neck (leading to ductile fracture) after only a few percent deformation.[9] This low-ductility case requires application of more conservative engineering design rules[10] and hence the high strength cannot be fully utilized for safe engineering practice.

Of even greater concern is the tendency for high strength materials (particularly BCC metals) to exhibit prompt brittle fracture due to cleavage along atomic planes if the alloy strength exceeds a critical value.[11] Due to the rapid decrease in strength of unirradiated BCC metals with increasing temperature up to 300-400 K, a characteristic ductile to brittle transition temperature (DBTT) separates the low temperature brittle fracture regime from the high temperature ductile fracture regime. The DBTT is dependent on numerous factors, including strain rate, flaw size

and applied stress state.[12,13] For conservatism, most structural designs attempt to ensure that the exposure temperature is maintained above the DBTT whenever stress is applied. Internal flaws such as inclusions or microcracks from welding, etc. act as stress concentrators and often are the initiating points for fracture. The stress concentration factor $\sigma_{local}/\sigma_{applied}$ is equal to 3 for a spherical inclusion, and can become much greater for planar inclusions or cracks oriented with their plane perpendicular to the applied stress direction.[11] One of the most famous examples of brittle fracture involved catastrophic cracking in the Liberty ships constructed with welded hulls during World War II, which directly led to the advent of the field of fracture mechanics.[11]

III. OVERVIEW OF DISPLACEMENT DAMAGE PROCESSES

Energetic deuterium-tritium (D-T) fusion neutrons have a scattering cross-section with metals that results in a mean distance between collisions of a few centimeters. Each collision transfers substantial energy to the primary knock-on atom (PKA), which in turn causes additional displacements. Due to the high ion-ion scattering cross-section, the energy from the PKA is deposited within ~100 nm of the initial displacement event. The net result is a series of spatially separated "displacement cascade" regions.[14]

The international standard for quantifying displacement damage is displacements per atom (dpa).[14,15] The dpa calculation is based on straightforward binary hard sphere collision calculations with appropriate corrections for energy loss due to nondisplacive ionization events with lattice electrons. A dose of one dpa corresponds to stable displacement from their lattice site of all atoms in the material during irradiation near absolute zero, where no recovery due to thermally activated point defect diffusion can occur. The dose of 1 dpa corresponds to a 14 MeV neutron wall loading of ~0.1 MW-yr/m^2 in steels, *i.e.* less than one month of full power operation for currently envisioned fusion power plants. As reviewed elsewhere,[14] the initial number of atoms temporarily knocked off their lattice site during energetic neutron irradiation is ~100 or more times the dpa value. Most of these transient displaced atoms hop onto another lattice site during the few picosecond "thermal spike" phase as the kinetic energy transferred to the displacement cascade is dissipated and the atom energies become thermalized. This transient ballistic mixing is an important factor that must be considered in developing radiation-resistant materials containing nanometer-scale particles (i.e., the particles must be thermodynamically and

kinetically resistant to ballistic dissolution). At normal operating temperatures, many of the displacement defects diffuse and recombine so that the net surviving defect fraction is much less than the calculated dpa value.[14] As an aside, molecular dynamics simulations[14,16] and supporting experimental studies[14,17] have found that the binary collision approximation used in the dpa calculation overestimates the number of surviving defects remaining at the end of the "thermal spike" phase for fission and fusion neutron displacement cascade conditions by about a factor of four, due to many body effects and enhanced recombination within the displacement cascade. This reduction in primary defect production for displacement cascade conditions is routinely included in chemical rate theory models of radiation effects.[18]

The magnitude of the challenge for developing radiation-resistant fusion materials capable of withstanding exposure doses of ~100 dpa (~10 MW-yr/m^2) is clear: approximately 99.9% of the "stable" displacements as calculated by the dpa value must recombine in order for the material to maintain dimensional stability (*e.g.*, <10% volumetric swelling). Conventional off-the-shelf materials typically exhibit 90-99% recombination of the displacements as calculated by dpa. The proposed operating conditions for a demonstration fusion reactor are significantly more challenging than first generation fission reactors. The structural materials in the first commercial fission reactors were exposed to maximum doses of ~1 dpa and maximum temperatures of ~300˚C. Existing (2nd generation) fission power light water reactors have core internal structure maximum doses of ~30 dpa and temperatures of <350˚C, and fast breeder reactor internal structures have displacement damage levels up to ~100 dpa with maximum temperatures of ~600˚C. The common theme for proposed fusion, Gen IV fission, and space fission reactors is the need to develop higher temperature materials with adequate radiation resistance. The first demonstration fusion reactor is expected to have a maximum structural dose of ~50 to 150 dpa at maximum temperatures of 550 to 1000˚C, depending on the design. A further challenge for fusion reactor structures is the high amount of H and He produced by transmutation reactions between the energetic D-T fusion neutrons and the structure (up to ~1500 appm He for metals in a fusion demo reactor compared to <10 appm He for most fission structures). Helium and hydrogen tend to impede the recombination of point defects, and can promote embrittlement over a broad temperature range. The proposed maximum temperature and doses for structures in future Gen IV fission reactors is comparable to that contemplated for fusion, but the transmutant He generation is approximately two orders of magnitude smaller than the fusion case.

There are five major radiation damage phenomena that can degrade structural materials.[19] Low temperature radiation hardening and embrittlement is of primary concern for doses above 0.1 dpa and temperatures up to ~0.35 T_M, where T_M is the melting temperature. Phase instabilities from radiation induced segregation and radiation induced precipitation are of particular concern for damage levels above 10 dpa at temperatures between 0.3 and 0.6 T_M. Irradiation creep (permanent deformation that is proportional to dose and applied stress) is of major concern for doses >10 dpa and temperatures up to ~0.45 T_M. Volumetric swelling from void formation (three dimensional aggregates of vacancies) can introduce unacceptable dimensional instability for doses >10 dpa at temperatures from 0.3 to 0.6 T_M. Finally, high temperature He embrittlement of grain boundaries can cause intergranular fracture at low stresses, particularly for doses >10 dpa (He concentrations >100 appm) and temperatures above 0.5 T_M. The relatively high transmutant He generation rates for fusion reactors promote low temperature embrittlement (via additional matrix hardening), void swelling, and high temperature He embrittlement. The higher He generation rates can also alter radiation-induced precipitation processes over a wide temperature range[20] and may cause a reduction in the fast fracture resistance of metals at temperatures well below 0.5 T_M due to enhanced grain boundary decohesion effects.[13]

IV. MULTISCALE MATERIALS MODELING AND EXPERIMENTS

Radiation damage is inherently a multiscale phenomenon, with interactions encompassing timescales from femtoseconds to years and length scales from sub-nanometer to meters. The current science-based approach for investigating radiation effects phenomena is based on utilization of a series of specialized models (each tailored for examining a discrete range of length and time scales) that are closely linked to a complementary set of multiscale experimental approaches.

At this juncture, it is appropriate to briefly review the current state of the art of computational materials science in order to investigate the feasibility of utilizing powerful supercomputers and massively parallel codes to unilaterally address the key radiation damage physics issues via first principles models. The goal of *ab initio* models is conceptually simple: solve the Schrödinger equation (or the Dirac equation, if relativistic effects are important). This

is trivial for the case of hydrogen (where an analytical solution exists), but is exceeding difficult for higher atomic number elements due to many-body effects in the Hamiltonian.[21] Although electrons can be decoupled from ions using the adiabatic Born-Oppenheimer approximation with high accuracy, reducing the many-electron problem to an effective one-electron system requires approximations that can introduce significant errors.[21,22] Quantum chemistry atomistic models provide the best accuracy, but are computationally very expensive with ~$O(N^6)$ scaling where N is the number of electrons in the system. This limits the simulation to ~100 atoms on currently available computers. The current "standard model" for condensed matter physics is density functional theory (DFT) using the local density approximation (LDA), which exhibits $O(N^3)$ computational scaling. It is generally successful in predicting structures and macroscopic properties, but it tends to underpredict band gap energies, overpredict lattice parameters, and predicts the wrong ground state for some magnetic materials (*e.g.*, Fe).[21] The computationally more expensive generalized gradient approximation (GGA) in DFT fixes some of these errors but in some cases underestimates the magnitude of binding forces. The DFT-LDA and DFT-GGA models are currently limited to ~1000 atoms due to their $O(N^3)$ scaling. The largest known DFT molecular dynamics simulation to date involved 1080 boron atoms (N=3480 electrons) and required two weeks run time on a 2000 cpu Linux cluster.[22] Accurate modeling of the behavior occurring within one individual grain of a fusion material requires simulation of ~10^{12} to 10^{15} atoms, which would require >10^{27} improvement in computational performance using $O(N^3)$ scaling. Similarly, molecular dynamics modeling is currently limited to time scales <1 μs. This highlights the motivation within the condensed matter physics computational sciences community to find approximate methods exhibiting linear O(N) scaling that introduce acceptably small errors,[21,22] and to utilize innovative time step acceleration techniques[23] that may enable near-first-principles examination of processes occurring on time scales beyond nanoseconds.

Due to the absence of first principles methods that can be applied to large time and length scales, a suite of discrete computational codes have been developed to investigate radiation effects phenomena at different time and length scales. Each transition to a larger-scale model involves introduction of simplifying assumptions for some of the physical processes. It is therefore essential to utilize complementary experiments to validate the model predictions at the different scales. For example, Mössbauer spectroscopy or electron paramagnetic spectroscopy experiments performed at low temperature can be used in some cases to confirm atomistic

predictions of the most stable point defect configurations. At larger scales, positron annihilation spectroscopy, small angle neutron scattering, atom probe tomography, and high-resolution transmission electron microscopy (TEM) can be used to validate molecular dynamics predictions regarding nascent defect cluster and precipitate geometries. Similar experimental tools can also be used to validate predictions obtained from higher-scale kinetic Monte Carlo and dislocation dynamics codes.

Recent atomistic modeling work has determined the <111> dumbbell interstitial is the most stable configuration for vanadium, in contrast to earlier lower-precision predictions that the <110> or <100> configuration was most stable.[24] Similar atomistic modeling of Fe-He has found that the tetrahedral site is preferred for He when magnetic interactions are considered, as opposed to earlier simulations that predicted the octahedral site was most stable.[25]

Molecular dynamics (MD) calculations (in concert with experimental studies) have been instrumental in determining that the primary damage state created by fission (~0.1 MeV neutron energy) and fusion (up to 14 MeV neutron energy) neutrons are quantitatively similar.[26] Figure 1 compares the displacement cascade structures in Fe near the peak of the displacement event (~0.5 ps) for PKA energies of 10, 50 and 200 keV, which correspond to displacement events for typical fission reactors, the average displacement event in a D-T fusion blanket structure, and near-peak-energy D-T fusion (12 MeV neutron) conditions.[27] At PKA energies above 10 keV, the displacement cascade forms localized lobes of displacement damage each of which is spatially similar to the average fission neutron case. The formation process of "fission-like" subcascades at high PKA energies signifies that correlation of fission and fusion neutron results using the international dpa parameter is justified. Experimental tensile and TEM results obtained on fission, 14 MeV fusion neutron, and high energy spallation proton irradiated specimens have been shown to agree well when compared on a dpa basis, providing experimental support that there are no large differences in the primary damage state for fission vs. D-T fusion neutrons.[26,28] This conclusion is significant because it validates the use of existing fission reactors for exploratory studies on new fusion materials regarding fundamental stability of fine scale structure to ballistic dissolution, *etc*. However, a critical unresolved issue is the effect of the higher transmutant solute (in particular, H and He) on the microstructural evolution of materials at moderate to high doses in a fusion reactor spectrum. The resolution of this question will require significant advances in computational modeling along with experimental validation in an

intense fusion-relevant neutron facility. Several focused fission reactor experiments currently in progress are utilizing He injection and isotopic tailoring[29] to provide some experimental information on helium effects on microstructural evolution in ferritic/martensitic steels. In addition, further work is needed to determine if there may be moderate self-interactions between subcascades for energetic D-T neutrons that could modify the production efficiency of radiation damage.

MD simulations have also clearly revealed a significant difference in the defect configurations created in BCC vs. FCC metals. The FCC lattice is close-packed and contains the maximum possible atom packing density (74%), whereas the BCC lattice has less compact stacking that results in an atom packing density of 68%. In addition, BCC metals exhibit higher stacking fault energies than FCC metals which leads to different preferred defect cluster morphologies. As shown in Fig. 2 for a PKA energy of 25 keV, the displacement event in the close-packed FCC metal (Cu) is relatively compact and consists of one or more large planar vacancy clusters near the center and several well-formed interstitial clusters near the periphery of the cascade.[30] In contrast, the defects produced in the non-close-packed BCC metal (Fe) are more diffuse and consist of much smaller cluster sizes.[16,31] In particular, large (>10 defect) vacancy clusters are not observed to directly form in MD simulations of Fe, although nanoscale 3-dimensional vacancy cavities can form during subsequent aging. Defect yield experiments based on TEM observations of irradiated Cu and Fe specimens have similarly concluded the efficiency of producing visible clusters directly in displacement cascades is greater in FCC Cu than in BCC Fe.[14,32]

These observations have wide-reaching ramifications regarding design of radiation-resistant materials. The predominant formation of point defects and small mobile defect clusters in the case of BCC Fe significantly enhances the probability of vacancy-interstitial recombination compared to the largely clustered (segregated) defect configuration in FCC Cu. This immediately implies that BCC metals such as Fe and V should have inherently better radiation damage resistance than FCC metals such as Cu and austenitic stainless steel. It is difficult to modify the microstructure with moderate alloying additions to prevent significant defect cluster formation if in-cascade cluster formation occurs in the base alloying material (as in the case for most FCC metals). Conversely, introduction of a high number density of nanoscale precipitates that serve as point defect recombination sites would be a very effective way to minimize the amount of

surviving defects at intermediate and high temperatures in materials such as BCC Fe that exhibit initially dispersed vacancy and interstitial populations. Numerous experimental studies performed at intermediate temperatures have found that BCC metals generally have significantly higher resistance to radiation damage compared to FCC metals, based on tests such as void swelling and irradiation creep.[33] Alloying additions can have a strong effect on modifying the intrinsic radiation resistance of a material (*e.g.*, swelling resistant FCC austenitic steels have been successfully developed for fission reactor applications). However, it is prudent to focus on materials such as medium atomic weight BCC alloys (V, Fe) as the major alloying constituent for challenging fusion reactor structures since they have superior propensity for radiation damage resistance compared to pure FCC metals.

At low irradiation temperatures (<0.3 T_M), high concentrations of sessile defect clusters are formed in irradiated metals (due to in-cascade formation or from diffusion and coalescence of point defects or glissile clusters). These sessile defect clusters act as obstacles to dislocation motion and therefore produce significant hardening. Unfortunately, the large radiation hardening is typically accompanied by dramatic reductions in ductility, with the uniform elongation (amount of plastic extension when the peak engineering stress is achieved in a tensile test, corresponding to the onset of localized necking) decreasing to <1% in many cases.[34-37] Furthermore, the radiation hardening can induce dramatic increases in the DBTT for BCC metals and decreases in the toughness in the "ductile" regime for both FCC and BCC metals.[13,36,38] Pronounced hardening and embrittlement effects can occur for doses as low as 0.01 dpa in non-optimized materials.

A number of experimental studies have linked the loss of uniform elongation in irradiated metals with the formation of cleared "dislocation channels".[34,39] The experimental studies suggest that a gliding dislocation emitted from a source can somehow annihilate the radiation –produced defect clusters. Although a high stress is required to propagate a dislocation through the defect clusters, once the initial dislocation has passed and annihilated the defects subsequent dislocations emitted from the same source will experience a relatively soft defect-free channel. This would lead to pronounced flow localization and would suppress normal interactions between dislocations emitted from different sources that are the basis for usual work-hardening behavior in deformed metals. Interest in low-temperature hardening phenomena was rekindled by materials research in support of the international thermonuclear experimental reactor (ITER)

engineering design. Numerous MD simulations and supporting in-situ deformation studies in transmission electron microscopes have recently been performed in order to investigate possible physical mechanisms responsible for defect annihilation by gliding dislocations.[40]

Initial MD simulations did not observe defect cluster annihilation by dislocations except for unusual truncated defect cluster geometries.[41] However, in-situ TEM studies during deformation conclusively showed that defect cluster annihilation could occur even for a single dislocation interaction. Conversely, defect cluster annihilation was sometimes not observed in these experimental studies even for multiple dislocation interactions. Understanding the physical mechanism(s) controlling whether or not annihilation occurs may be key for developing materials with improved resistance to low temperature irradiation embrittlement. These experimental observations stimulated follow-on MD studies with lower dislocation velocities (more computation-intensive) and a variety of simulation conditions (edge vs. screw dislocations, with and without adjacent free surfaces) that successfully observed defect cluster annihilation.[42] The detailed mechanisms responsible for cluster annihilation are currently under investigation.

At higher scales, kinetic Monte Carlo (KMC) methods have been used to follow the microstructural evolution of irradiated materials up to moderate doses (~0.1 dpa).[43,44] The advantage of KMC methods compared to mean-field chemical rate theory approaches is that the spatial location of lattice structure can be included in the simulation. However, both of these higher-scale models require specification of all potential mechanisms and their activation energies (typically obtained from MD simulations or experiments). Three-dimensional dislocation dynamics simulations[44,45] can provide insight on defect cluster interactions with dislocations and plastic deformation mechanisms. Finally, finite element modeling is being used to investigate material behavior including work hardening and flow localization effects[46] as well as fracture mechanics studies of localized stresses near crack tips in a variety of different specimen geometries.[13,47] These modeling efforts are linked to experiments investigating the mechanisms responsible for flow localization and necking in irradiated metals.[37,48] The experimental studies suggest plastic instability (prompt necking) occurs when the yield stress exceeds a critical value. The critical value frequently appears to be similar for a given metal independent of initial thermomechanical state (annealed, cold-worked, or neutron irradiated).

V. REDUCED ACTIVATION MATERIALS FOR FUSION

Substantial work was performed in the 1980s on Type 316 austenitic stainless steel, including effects of fusion-relevant helium production and displacement damage on the properties and microstructural stability.[49] Many of these studies utilized a thermal neutron induced two-step transmutant helium production reaction that occurs in nickel-containing alloys as a means to investigate helium effects in fission reactors.[29] These studies formed the basis for selection of austenitic stainless steel for the first wall structures in ITER. However, austenitic stainless steel exhibits relatively high levels of long-lived radioactivity due to the presence of Ni and other elements, and has poorer thermomechanical properties compared to ferritic/martensitic steels. Therefore, austenitic stainless steel is not a candidate for fusion energy demonstration power reactors.

Based on considerations of long-term radioactivity burden and short-term radionuclide safety as well as practical considerations regarding which elements can form the basis of a structural material,[50] three classes of high-performance reduced activation structural materials have emerged for fusion energy:[4,26,51] ferritic/martensitic steels (containing 8-9%Cr and 1-2% W,V, and Ta), vanadium alloys (containing 4-10% Cr and Ti), and SiC/SiC ceramic composites. It is worth noting that none of these materials existed in their current formulation 15 years ago. As reviewed elsewhere,[3,4,26,52] these reduced-activation materials have properties comparable or superior to commercial materials that exhibit high induced radioactivity following neutron exposure, and therefore these materials are also attracting attention for a variety of non-fusion structural applications. The steels are suitable for a variety of coolant and tritium breeding options and have good mechanical strength up to 500-550˚C. Oxide dispersion strengthened steels may enable even higher temperatures up to 650-800˚C to be considered if fabrication and joining issues can be satisfactorily resolved. Vanadium alloys are best suited for use in self-cooled lithium breeding systems and may operate at temperatures up to 700-750˚C, which provides improved thermodynamic efficiency compared to conventional steel systems. Silicon carbide composites offer potential for operating temperatures greater than 1000˚C. The fusion-formulated steels share many fabrication and mechanical design characteristics found in commercial steels, and therefore are technologically mature relative to the other reduced activation material options (the main unknown issues being effect of ferromagnetism on plasma

performance and stability under intense fusion neutron irradiation). The vanadium alloys, as with all refractory alloys, have limited industrial infrastructure but have demonstrated attractive properties and fabricability. Silicon carbide composites have the most feasibility issues of the three material systems due to their technological immaturity, but offer the greatest potential for high thermodynamic efficiency systems. Recent assessments of the current status and critical issues for development of ferritic/martensitic steels,[53] vanadium alloys,[54] and SiC/SiC composites[55] are given elsewhere.

The underlying fusion materials development philosophy is based on formation of a high density of uniformly distributed nanoscale particles that are highly stable to long-term thermal and neutron exposures. Certain categories of solutes and precipitate phases are known to be susceptible to radiation-induced dissolution or coarsening effects due to their solubility and diffusion behavior. Precipitate phases that can cause embrittlement (*e.g.*, delta-ferrite, chi and $M_{23}C_6$ phases in ferritic/martensitic steels)[56] should be avoided. Commercial thermodynamic modeling codes are typically used to identify intrinsic equilibrium structures in the absence of irradiation and to determine promising compositions for further study. The multiscale materials modeling codes summarized in Sec. V are then used to probe radiation effects behavior. Targeted neutron and ion irradiation experiments on simple model alloys and complex engineering alloys are used to validate computational predictions and to probe conditions unsuitable for quantitative computational analysis. Since the nanoscale precipitate structures necessary for radiation damage resistance generally also improves the unirradiated mechanical properties, several high-performance commercial alloys have recently been spun off from the fusion materials research.[3]

The knowledge base on materials exposed to fusion-relevant operating conditions is very limited (mainly austenitic stainless steels, as summarized above). Therefore, although a closely integrated theory and modeling program combined with targeted experiments in existing ion accelerator, fission, and spallation neutron facilities would certainly accelerate the development of fusion materials needed for a demonstration fusion reactor, a recent international workshop concluded that it would not replace the need for a dedicated fusion neutron facility such as the proposed accelerator-based (D-Li) international fusion materials irradiation facility.[22]

VI. SUMMARY AND CONCLUSIONS

The key issues for structural materials in future fusion energy machines are largely centered on structural stability and property changes associated with intense thermal and energetic neutron exposures. Coordinated experiments and multiscale modeling activities are being utilized to investigate defect production and migration mechanisms, plastic deformation mechanisms, and fracture mechanics behavior. Based on this understanding of performance-limiting degradation phenomena, a series of high-performance structural materials have been developed by fusion scientists over the past ten years with significantly improved properties compared to earlier materials. Similar to the portfolio approach used for examining various attractive plasma physics configuration options, three different categories of fusion structural materials are being investigated: steels, refractory alloys, and ceramic composites.

Molecular dynamics simulations and experimental studies have shown the body centered cubic lattice generally conveys improved radiation resistance compared to the close-packed face centered cubic lattice, due to a reduction in the amount of vacancy and interstitial defect clustering that occurs directly within displacement cascades as well as higher stacking fault energy. This supports continued development of ferritic/martensitic steels and vanadium alloys as promising BCC candidates for fusion reactor structures. First principles atomistic computational materials science simulations are currently limited to less than 1000 atoms and timescales less than 1 microsecond. Although work is continuing to derive accurate methods to eliminate the $O(N^3)$ scaling for these atomistic simulations, this requires extensive use of a suite of multiscale materials models to investigate larger length and time scales. Since these larger scale models utilize numerous approximations to minimize computational expense, experimental validation is critical to test the multiscale model predictions.

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Figure captions

FIG. 1. Comparison of MD simulations of displacement cascades in Fe for different PKA energies.[27]

FIG. 2. Comparison of surviving (>2 ps) defect configurations in FCC (Cu) and BCC (Fe) medium-weight metals for a 25 keV displacement cascade.

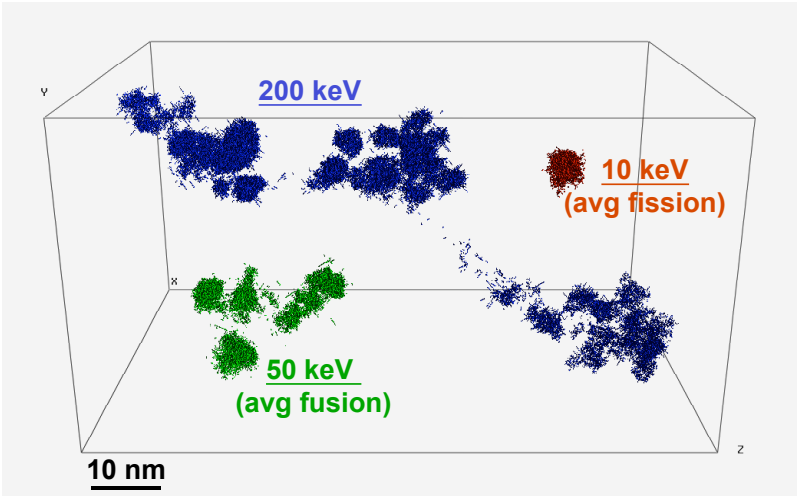

FIG. 1. Comparison of MD simulations of displacement cascades in Fe for different PKA energies.[27]

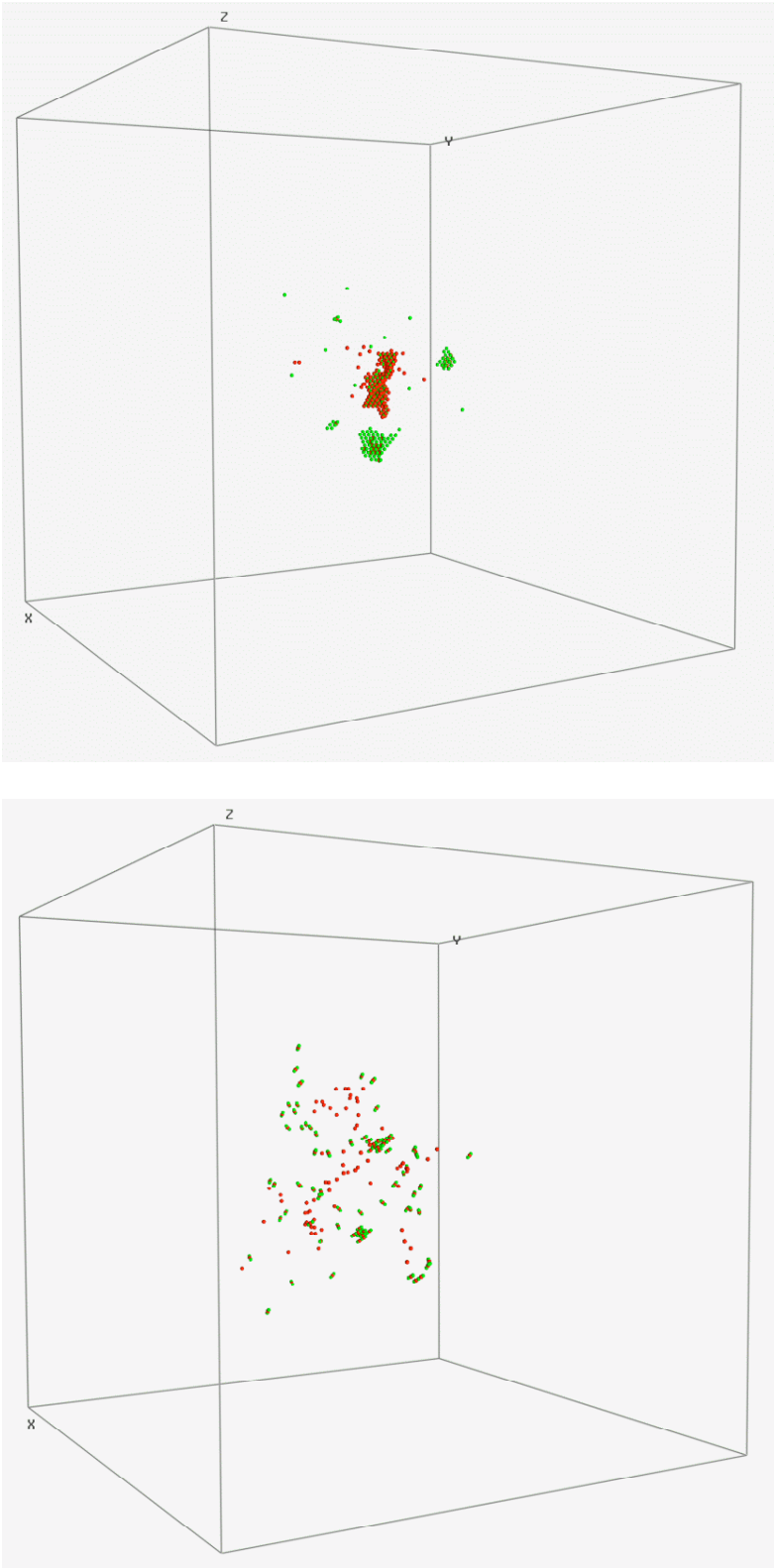

FIG. 2. Comparison of surviving (>2 ps) defect configurations in FCC (Cu, top) and BCC (Fe, bottom) medium-weight metals for a 25 keV displacement cascade.