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Multiscale Modeling of Radiation Damage in Oxide Dispersed Strengthened Steel Alloys: A Perspective

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***Abstract*—.** Currently, state-of-the-art reactors concept is based upon higher efficiency and better utilization of nuclear power. This energy is considered an alternate source replacing conventional methods. The materials used in nuclear power plants (NPP) suffer long term degradation due to radiation exposure and corrosive environments. This concerns the safety and reliability of NPP. The choice of material to sustain extreme conditions is crucial for developing safe and reliable systems. There are several candidate materials for advanced-generation reactors, out of which nano-dispersed oxides based have shown higher radiation stability at extreme irradiation conditions. This is due uniformly distributed nano oxides in the matrix having interfaces which make them a gutter for defects. The radiation damage is multiscale which requires integrated simulation and experimental techniques to understand and explain temporal/length scales for simulating the macroscopic nature of materials. For better visualization, it is necessary to have integrated multi-scale modeling and experimental approaches for explaining the associated mechanisms at atomic scales associated with dispersed oxides. This short review will summarize the current development state and modeling radiation damage studies to understand irradiation response of oxide-dispersed strengthened steels (ODS).

***Keywords*—**Molecular dynamics, oxide dispersed strengthened steels, atomic scale, nuclear power plant.

I. Introduction

Presently, the increasing energy crisis has led to a surge in alternate energy resources [1]. Nuclear energy can be considered an alternate source to meet the needs of the world. Nuclear fuels for current and advanced reactors are designed to have excellent structural properties which can withstand harsh environments including high temperatures and extreme exposure to irradiations [2]–[4]. Generation IV (GEN-IV) reactors are the advanced technology better than present reactors types which can have better energy utilization, reliability, lifetime, and excellent radiation resistance [5]. Due to the high safety standards required for NPP, it is preferable to use such material which has outstanding properties such as resistance to corrosion, mechanical properties, durability, and good radiation resistance and prevention against any accident scenario[6]–[8]. With the existing fission reactors, people are trying to develop materials for advanced reactors which will be able to produce more excessive, economical, and reliable sources of energy. To meet the requirement for harsh environments we need structural and fuel materials having excellent mechanical properties under high temperatures and dose per atom (dpa) [9]–[12]. The structural materials for fuel cladding material suffer very harsh environments due to extreme conditions which alter material properties. These changes are in the form of physical as well as chemical nature [13]. Stainless steel with chromium concentrations up to 10% has shown profound radiation stability observed for light water reactors. However, this scenario is a bit challenging for advanced-generation reactors (III, III+ IV). To overcome this requirement the mechanical properties of steel are enhanced by strengthening mechanisms that improve the suppression of voids during radiation. The high radiation resistance to sustain higher temperatures has been achieved by introducing nano dispersoids (Y_2O_3) ~20 nm in the iron matrix. This process is done by mechanical alloying followed by sintering and annealing processes [14]. Radiation damage is very crucial for developing radiation-tolerant fuel and structural materials for current and advanced reactors [11], [12], [15]–[20].

Most of the primary damage studies are reported by molecular dynamics simulations and experimental atomic probe tomography (APT). Atomic scale simulation methods have been considered a visible tool for understanding the nature of defects and their interactions at normal operating and elevated irradiation conditions [21]. Presently, researchers have proposed to improve the upper expected temperature limit of up to 1000K and 250dpa for advanced generation reactors.

The present review has summarized multiscale simulation and experimental studies on ODS, and problems associated with their behavior.

II. DEVELOPMENT OF ODS ALLOYS

The material challenge for next-generation reactors is expected to handle the concerns relevant to core and cladding material at higher temperatures~1000K [4], [22]–[24]. Ferritic/ martensitic steels are proposed as a reference material for construction of the reactor's core and in and outlets of light water reactors (LWR) for the construction of reactor pressure vessel (RPV), ducts, and piping [25]. ODS alloys have a perspective for developing fuels and cladding materials for fast reactors and fusion reactors as reported by Ukai et al [26]. Future reactors requirement should have excellent structural and tensile properties, resistance to radiation, higher thermal conductivity, good creep strength, elevated temperature forbearance, low ductile to brittle transition temperature (DTBT), low residual activation, and cooling capability [27]–[29]. ODS steel, ferritic-martensitic steels, austenitic stainless-steel, and transition metallic alloys are potential candidates for next-generation reactors which have temperature and other conditions more severe than the current LWR [17], [18], [30], [31]. The presence of nano-size dispersoids in the matrix exists as secondary phases which act as a hindrance for defects and dislocations and entrap them due to the existence of coherent interfaces. These defect sink characteristics make them unique amongst other radiation-resistant materials [30-32]. Ferritic nano-oxides are considered as best dispersoids and act as sinks for dislocations because of their high temperature stability during irradiation [9], [11], [12], [15], [32]. The oxides of transition metals and semiconductors are better than metallic ones [32]. These oxides also provide hindrance and hence strengthening effects which in turn improve the mechanical properties. This occurs due to the interaction between dispersoid particles and dislocations in steels [10], [33]. This process can be described by the orowan unpinning and strengthening mechanism for crystal under plastic deformation to predict its strength [10][34]–[37]. Moreover, the grain boundaries (GBs) are reported to have defects/impurity trapping in steels with or without radiation [38].

Figure 1 displays the schematic layout of integrated multi-scale simulation and comparative experimental models over different time and length scales. Atomic scale simulations are the lowest time and length scale which involves electronic contribution (ab *intio* molecular dynamics (AIMD)/ density functional theory) while on the experimental counterpart atom probe tomography (APT). Each length scale provides relevant parameters for bridging length scales for a better understanding of the macroscopic properties of the material under neutron or ion irradiation observed in RPV.

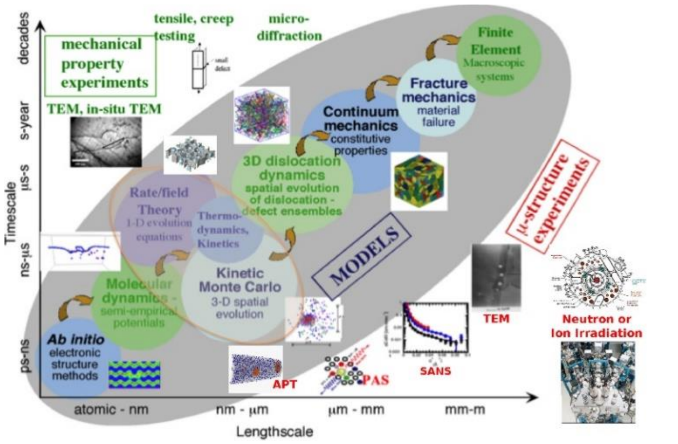

Figure 1. Multi-scale integrated computational-experimental hierarchical models over the different lengths and time scale observed for a material exposed to irradiation (adopted from Gilbert et al. [39]).

III. PRESENT STATUS OF DEVELOPMENT

ODS steels with a basic composition of Fe–Cr–W–Ti–Y_2O_3 are being reported for studying radiation effects under different conditions [9], [14], [40]–[50]. We have observed that most of the earlier studies reported so far have inconsistent findings since the conditions and routes for specific ODS are reported in different circumstances. Figure 2 displays a common route for the fabrication of ODS. This method used MA in the form of an inert atmosphere. The oxide in the ODS steel fine grains distributed in the form of dispersoids with an atomic radius of 50 nm [51]. The radiation stability of ODS is related to the size as well as interfacial orientation of the oxide during fabrication [10]. Furthermore, the size of yttria affects the different properties. The experimental studies have shown the addition of Y_2O_3 produces stable interfaces and better creep resistance while the presence of Ti improves the density and hence creep rupture strength [52], [53]. It was also reported that Zr-O improves the thermomechanical properties [54]. Additionally, Cr concentration (>12%) has a significant corrosion resistance [15], [16], [55]. There are some problems associated with the MA process such that it reduces the density of dispersoids with inhomogeneous structures. This can be handled through laser additive manufacturing [56].

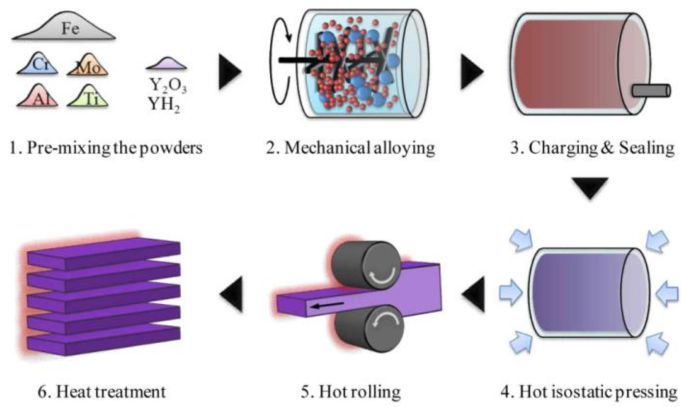

Figure 2. Route for fabrication of ODS steel (adopted from Noh et al. [43]).

The International Thermonuclear Experimental Reactor (ITER) Program for building advanced engineering thermonuclear tokomak fusion and EURO fusion-based materials have proposed ODS steel for plasma-facing wall and diverter [57]–[59]. The distribution of temperature variation as a function of radiation doses for GEN-IV reactors is displayed in Figure 3. There are six prototype GEN-IV fast reactors. They are more advanced, reliable, and economical reactors than LWR. The expected materials type for these reactors must have excellent mechanical properties and higher tensile strength against neutron irradiation [60].

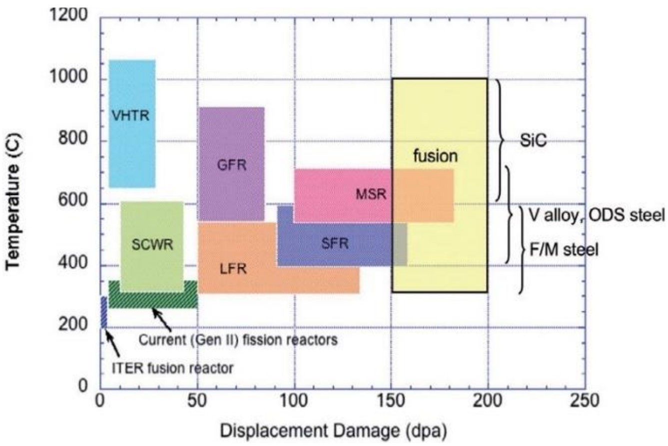

Figure 3. Relation of temperature and displacement per atoms (dpa) for GEN-IV reactors (adopted from Zinkle et al. [61]).

Table 1. Summary of GEN-IV reactor's coolant and neutron spectrum [62]–[64].

Reactor	Coolant	Neutrons	System pressure (MPa)	Core outlet Temp. (^{O}C)
GFR (Gas-cooled fast reactor)	Gas -Helium	Fast	7	~850
LFR (Lead-cooled fast reactor)	Liquid metal- Lead, lead/Bismuth	Fast	0.3	480–800
MSR (Molten salt reactor)	Molten Salt-Fluoride	Epithermal	0.6	700–800
SFR (Sodium-cooled fast reactor)	Liquid metal -Sodium	Fast	0.3	~550
VHTR (Very high temperature reactor)	Gas -Helium	Thermal	8	>900
SCWR (Super-critical water-cooled reactor)	Water	Thermal/Fast	25	510–626
LWR (Light water reactor)	Water	Thermal	8-16	325

Table 1 displays a summary of GEN-IV coolant and neutron spectrum and outlet temperatures and its comparison to LWR. It can be seen that the conditions expected for GEN-IV reactors are quite challenging and different materials are required for each component as per circumstances. The desired material for these reactors must have high strength, radiation stability to void and creep resistance, and many more characteristics mentioned elsewhere [58][62].

IV. MICROSTRUCTURE AND MECHANICAL PROPERTIES

The improved mechanical properties in ODS are due to the presence of nano oxides which are stable at elevated temperatures. The ability of a material to resist its microstructures depends on the evolution of defects [48]. The tensile strength of ODS as a fuel cladding material has displayed high radiation resistance at elevated temperatures [65]. The improved high temperature limit in ODS compromises the ductility and hence it is very important to identify the contribution affecting it. Figure 4 displays a graphical representation of the microstructural evolution of the strengthening mechanism in ODS (Fe-9%Cr) through experimental characterization through SANS (Small-angle neutron scattering), EBSD (Electron backscatter diffraction), TEM, and APT. The number density as a function of oxide radii is represented by SANS (top right). The APT display a heterogenous structure of Y and TiO (top left). EBSD shows average grain size distribution (right lower bottom). The TEM representation displays homogenous particle distribution (left lower bottom).

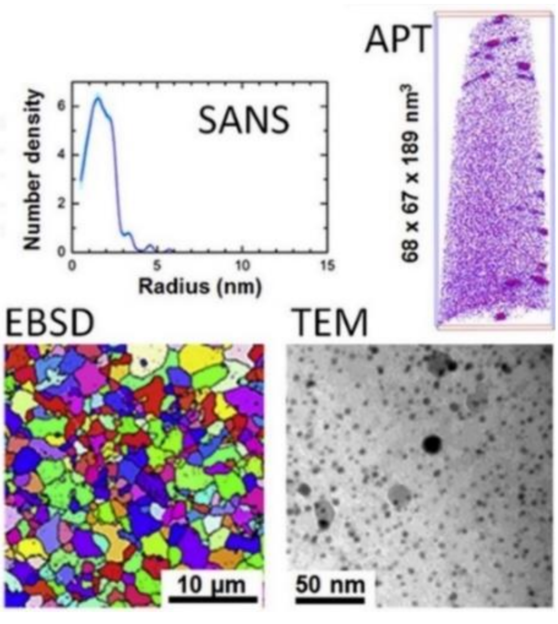

Figure 4. Microstructural characterization of strengthening in ODS (adopted from Chauhan et al. [66]).

The microstructural characterization was observed to determine the strengthening effect of ODS and was investigated and compared. The mechanical response of ODS in a radiation environment is shown in Figure 5. The tensile strength of 18%Cr-ODS was reported by Nagini et al found that samples with dispersoids were more stable and had higher strength than non-ODS, where ODS $_{(F, C, M)}$ display fine, coarse, and medium microstructures [67].

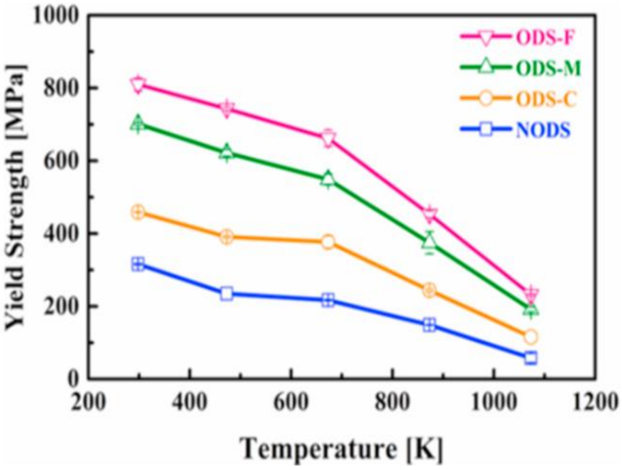

Figure 5. Relation between yield strength (YS) as a function of temperature (adopted from Nagini et al. [67]).

The concentration of alloying content also affects the properties of ODS under various compositions have been reported in earlier experimental and simulation studies [52]–[54], [56]. Chromium concentrations up to 16% improve the tensile strength and corrosion resistance with embrittlement. Another study reported that the supplement of aluminum content improves strength and decreases embrittlement [68]. Figure 6 represents the effect of Cr concentration in the presence of nitric acid solution [55].

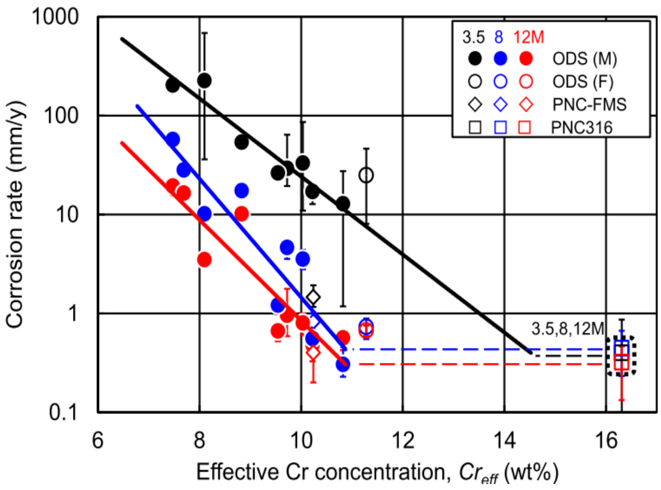

Figure 6. Relationship between cession rate with Cr concentration in acidic solution (adopted from Takashi et al. [55]).

The microstructural change in Fe-12Cr-2W-0.3Ti-0.25Y_2O_3 observed through the tensile test at room temperature (RT) at a strain rate of 10^{-4}/s is expressed in the form of the stress-strain curve displayed in Figure 7. The values of YS are approximately 1100MPa, which is 5 times higher than Fe [69], [70]. Thus, higher unpinning stress is required for defects in ODS steel.

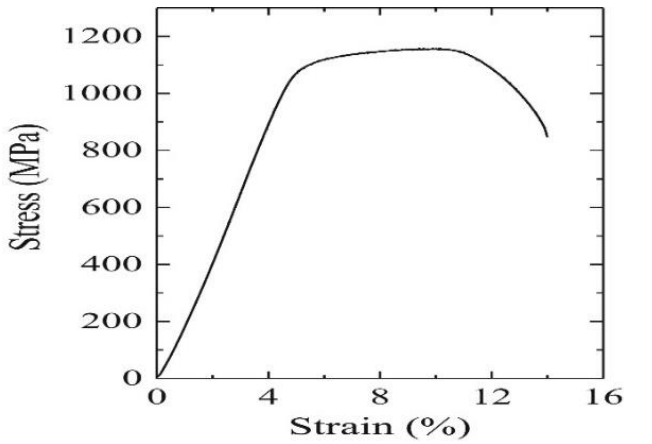

Figure 7. Stress-strain curve for 12% Cr ODS at RT (adopted from Shen et al. [69]).

It was reported that the presence of oxides in the matrix results in strengthening and grain stability at higher temperatures[71]. This effect is more prominent at high temperatures where oxide hinders the movement of dislocations. This phenomenon is called precipitate strengthening. The orowan is the minimum value of stress required for dislocations to bypass in the presence of oxides (also known as precipitates) [10][72]. The concentration of other alloying elements affects the stress response. The stress-strain behavior for 16Cr-ODS is plotted in Figure 8. It can be seen in Figure 8 that more strengthening was observed for higher Zr concentration. There is an increase in yield stress, and it is reported that this is related to grain boundary strengthening following the Hall-Petch relation [54].

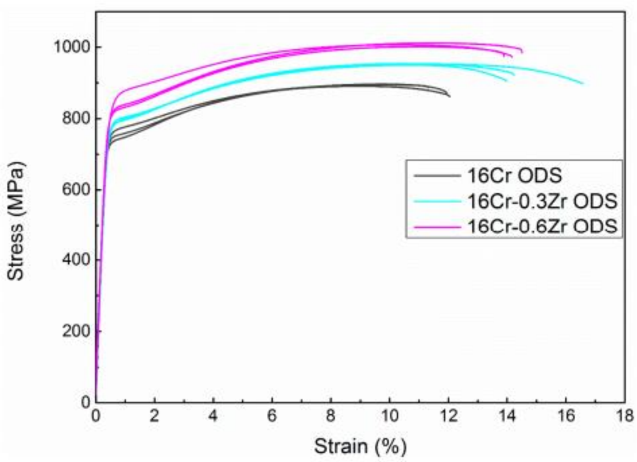

Figure 8. Stress-strain curve for 16% Cr-Zr ODS at RT (adopted from Ren et al. [54]).

The microstructural evolution observed for Fe–14Cr–(0.3-0.06)Ti–0.3Y_2O_3-ODS displayed dislocation density and crystallite size is temperature dependent.

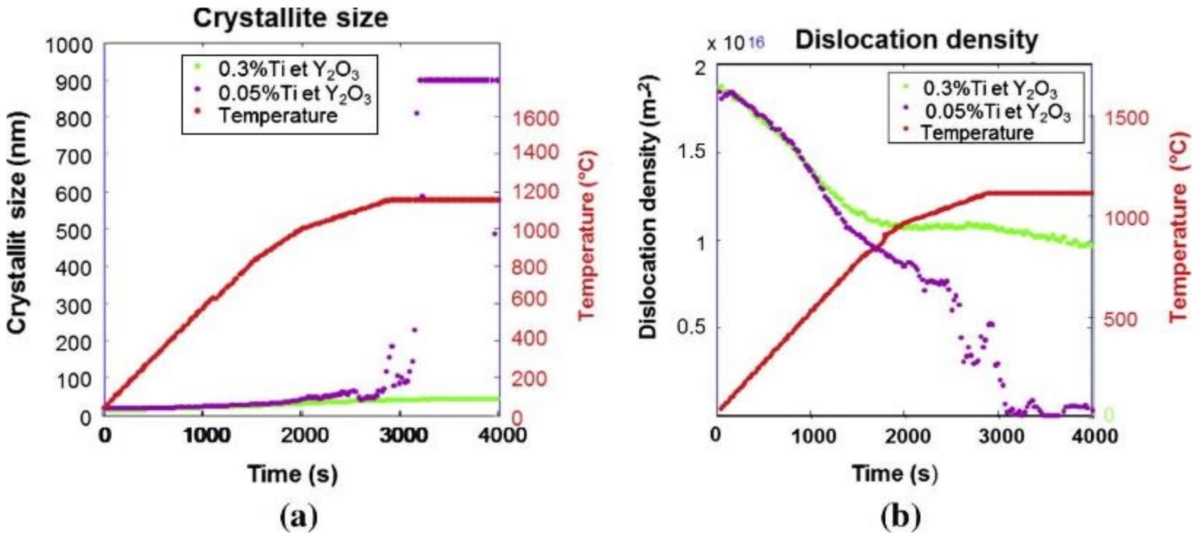

Figure 9. Variation in crystallite size and dislocation density as a function of time (adopted from Boutard et al. [73]).

The mechanical properties of ODS-Tungsten were reported at different temperatures (RT & 500ºC) and found that tensile stress is proportional to the sintering temperature. This establishes that tensile strength at high sintering temperatures is higher at RT. We conclude that ODS has higher temperature strength. The relation between stress-strain at RT and 500ºC is plotted in Figure 10.

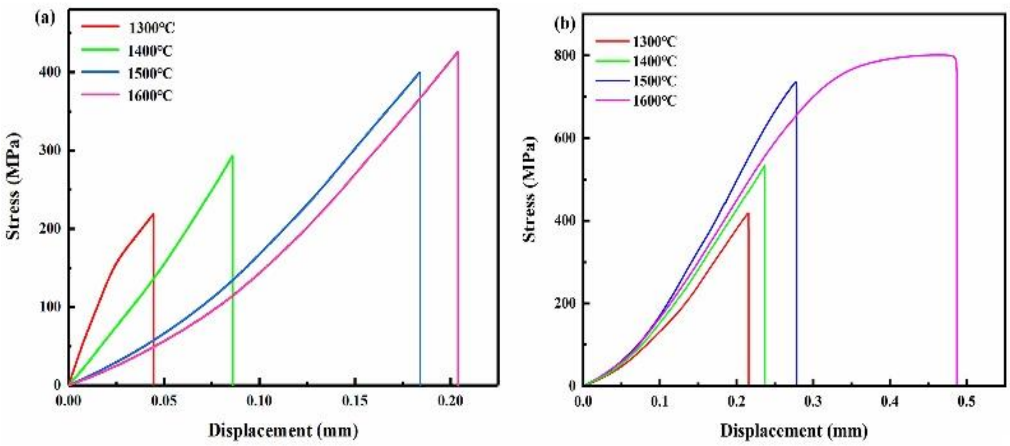

Figure 10. Stress-strain relation of ODS-tungsten at different temperatures (adopted from Liu et al. [74]).

V. MODELING AND SIMULATION OF ODS ALLOYS

Computational modeling of the material is the predictive capability when exposed to extreme radiation environment and estimate time of the component being used. The atomic scale modeling provides an in-depth understanding of the mechanism associated with radiation build-up at extreme conditions. It can assist in understanding the response of material at different conditions. Moreover, we can pre model the material as required assumptions and handle the risk associated with experiment. So, atomic scale methods take advantage of high-power computing to perform virtual experiments at a microscopic level for problems in a few hours which take days/months in experimental reactors. Atomistic level simulations have been able to investigate mechanism associate with formation of nanoclusters in ODS. Different thermodynamics models for ODS have been used to predict the phases using CALPHAD. It was found that the concentration of transition metal-oxide control thermodynamic equilibrium properties [75]. The generic compositional of Fe-Y-Ti-O nanoclusters having a high density at the interface is reported as a sink. The process defect recombination occurs in nanocrystalline alloys [76]. Atomic scale simulations were performed to observe the structural evolution of defects near the interfaces and creep behavior under applied stress and temperatures. It was found that interfaces play very important role [77]. The size distribution of oxides at different temperatures in ion radiation were observed through TEM and it was found that stable structure were found at RT [78].

Defect creation is the process where the displacement cascade starts. The displacement cascade studies observed in ODS with sizes >2 nm with recoil energy (5keV) generate shock waves. It was seen that cascade propagation area is proportional to the displacement cascade energy. Figure 11 (a-d) shows defect evolution for Fe-Y-Ti-O nano ferritic alloy (NFA) with incident PKA of energy 20keV. It was seen that all Fe atoms remain at their position near the interface [79]. DFT results display interfaces act as defect trapping region known as 'catalyst' as reported by Brodrick et al., as adjoining Klimiankou interfaces $[110]_{Y2O3} \parallel [111]_{Fe}$ [80].

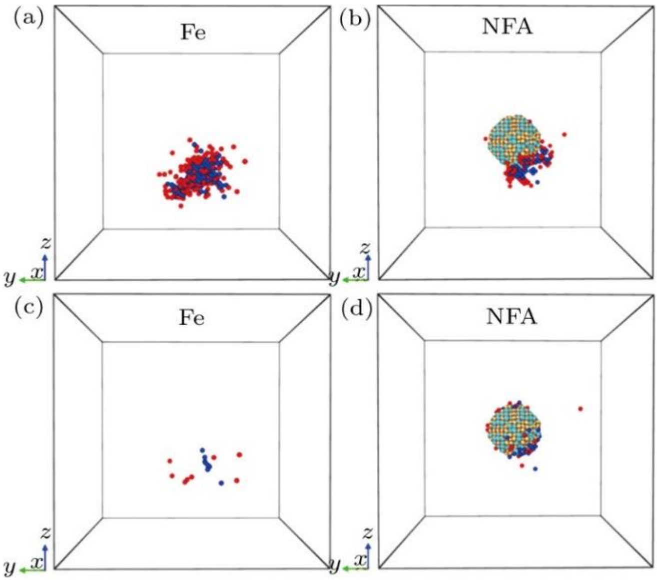

Figure 11. MD snapshot of displacement cascades observed for pure Fe and ODS at 20ps (adopted from Sun et al. [79]).

The number of defect evolution for case of Fe-Y-O-Ti model under displacement cascades of E_{pka} of composition constituents with hot energy (> 0.2432eV). After attaining the maximum number of displaced atoms ,defect annihilation leads to fewer surviving defects after cascade cools down. The number of surviving defects for O atoms are higher whereas Ti atoms are smaller than all as displayed in Figure 12. The studies have reported that region near the interfaces is more amorphous due to lattice mismatch. This defective part of the model which have overlapping atoms. In most cases, such region has been counted while performing Weigner Seitz's analysis [79].

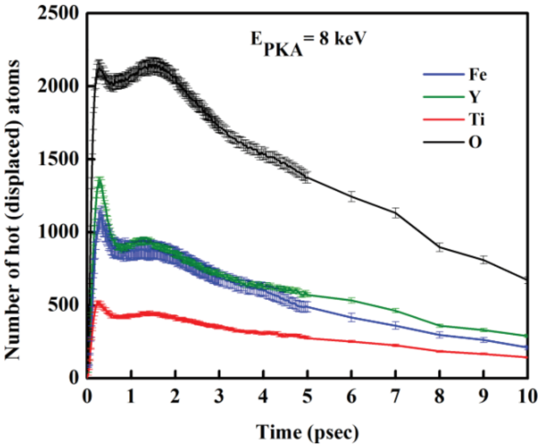

Figure 12. Evolution of defects as function of time for each bombarded species (adopted from Manan et al. [83]).

During the initial phase a lot of defects are created and then defects start subsiding as soon as cascade cools down. There are a greater number of vacancies than interstitial. Most of the defects recombine within a few picoseconds. After the surviving defects recombine they are trapped at the interface which is the reason for grain boundaries act as defect sink [81], [82].

The study on the dislocation interaction reported in earlier studies display that stability of the structure is obtained through atomic scale simulation require charge distribution instead of neutral models. Moreover, the interaction in the presence of oxide follows orowan unpinning mechanism for dislocation to bypass followed by a loop which increase the dislocation density at the interface and, hence strengthening is observed. Additionally, radiation stability is proportional to the size of the oxide. The critical unpinning stress is higher for oxides than any other obstacle (void) [9], [10], [19], [84]. Figure 13 (a-d) represents the interaction mechanism for oxide of different sizes, where r>2nm orowan mechanism during dislocation interaction was observed. The area around the oxide is proportional to the size.

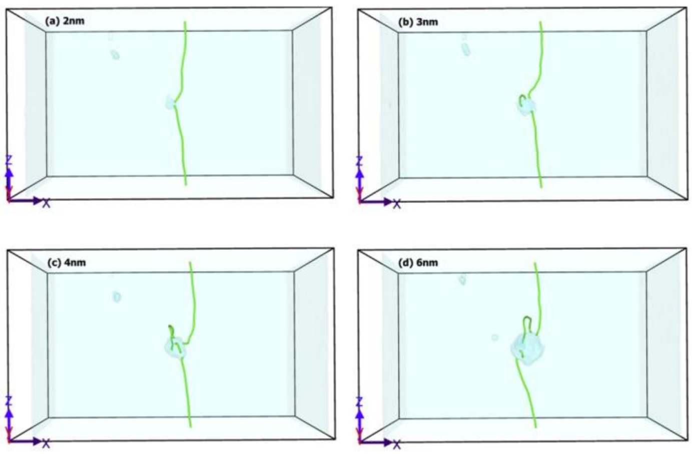

Figure 13. Evolution of defects as function of time for each bombarded species (adopted from Azeem et al. [10]).

There are numerous studies on the radiation effects in ODS steels with inconsistent finding due to conditions and circumstances. The studies based on the ODS steels are inconsistent in atomic scale as well as on experimental studies[85]. The atomic simulations are dependent on the realistic potentials. Recently machine learning based interatomic have been considered more accurate than empirical. More research is required to explore the resistive nature of ODS by considering the methods in experimental as well as through atomic scale methods. Off course the electronic contribution always plays important role and it's beyond empirical molecular dynamics potentials. Therefore , multiscale simulation methods are required to bridge scales and reveal the macroscopic nature of the material.

CONCLUSION

We have summarized current state of ODS steels which are nanostructure alloys having resistive nature at higher temperature and radiation conditions .Advanced ODS F/M alloys strengthened by dispersoids have displayed radiation stability, improved microstructure, and creep strength at elevated temperature. These nano-dispersoids have shown outstanding stability, creep resistance after long-term exposure to radiation for high energy neutrons and ions. Nanoclusters (dispersoids) trap He ions and help in the recombination of defects induced due to radiation. Due to certain limitations determining the phenomenon related to nanoclusters' behavior is still unknown and under research. The innovative design and construction of GEN-IV reactors are based on the vision of a longer lifetime, safety, economical, carbon-free environment-friendly systems. Our study has summarized and serve as predictive atomic model for developing better radiation-resistant materials.

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