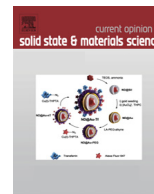




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Atomic-level heterogeneity and defect dynamics in concentrated solid-solution alloys

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ABSTRACT

Performance enhancement of structural materials in extreme radiation environments has been actively investigated for many decades. Traditional alloys, such as steel, brass and aluminum alloys, normally contain one or two principal element(s) with a low concentration of other elements. While these exist in either a mixture of metallic phases (multiple phases) or in a solid solution (single phase), limited or localized chemical disorder is a common characteristic of the main matrix. Fundamentally different from traditional alloys, recently developed single-phase concentrated solid-solution alloys (CSAs) contain multiple elemental species in equiatomic or high concentrations with different elements randomly arranged on a crystalline lattice. Due to the lack of ordered elemental arrangement in these CSAs, they exhibit significant chemical disorder and unique site-to-site lattice distortion. While it is well recognized in traditional alloys that minor additions lead to enhanced radiation resistance, it remains unclear in CSAs how atomic-level heterogeneity affects defect formation, damage accumulation, and microstructural evolution. These knowledge gaps have acted as roadblocks to the development of future-generation energy technology. CSAs with a simple crystal structure, but complex chemical disorder, are unique systems that allow us, through replacing principal alloying elements and modifying concentrations, to study how compositional complexity influences defect dynamics, and to bridge the knowledge gaps through understanding intricate electronic- and atomic-level interactions, mass and energy transfer processes, and radiation resistance performance. Recent advances in defect dynamics and irradiation performance of CSAs are reviewed, intrinsic chemical effects on radiation performance are discussed, and direction for future studies is suggested.

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1. Introduction

Since civilization began, development of metallic alloys with better structural strength or improved functionality have repeatedly changed human culture and capacity. Scientific breakthroughs are increasingly required to meet the population's ever-growing industrial and technological demands. Many useful alloys are comprised of single or multiple phases with one principal element

modified by small additions of other elements or with two dominant elements, such as Fe–Cr and Ni–Cr based alloys with precipitates. Conventional approaches have historically taken a material with empirically good properties, and made small changes in composition and microstructure to achieve a more desired performance, such as improved radiation tolerance. For discussion purposes in this work, most of these alloys with the major element acting as a solvent and alloying elements as solutes are termed **traditional alloys**, or dilute alloys.

In sharp contrast to traditional alloys, concentrated solid-solution alloys (CSAs) consist of two to five (or more) elemental species all at high concentrations or near equiatomic composition. CSAs have recently attracted increasing attention and intensive research efforts [1–3]. Some of the newly developed multi-component systems are commonly termed high entropy alloys (HEAs), wherein the configurational entropy is higher than the

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entropy of melting in most common metals [4–6]. Contrary to ordered intermetallics from classical physical metallurgy, a direct consequence of thermodynamic stabilization of some high-entropy phases is a reduction of the thermodynamic driving force toward oxidation and phase transformation. Both face-centered cubic (fcc) and body-centered cubic (bcc) CSAs, including HEAs, with a strong tendency toward solid solution strengthening, have been produced. These **non-traditional alloys** exhibit strong resistance to softening (high strength and low plasticity) at high temperatures, and excellent tensile strength at low temperatures, which make them candidate materials for many potential applications, including those requiring thermal stability and hardness at elevated temperatures [7–9], enhanced fatigue, strength, ductility, and fracture resistance [3,10,11], improved irradiation resistance [2,12–14] and excellent corrosion and wear resistance [5].

Intense radiation in nuclear fission and fusion power systems transfers energy to electrons and atoms in the material, and produces defects. Structural materials, such as iron-based alloys (currently the primary basis for structural materials in advanced nuclear reactors), must demonstrate long-term stability and tolerance to radiation damage at elevated temperatures over long lifetimes. It is known that the accumulation of defects may ultimately compromise the material's strength and performance lifetime. Historically, the development of traditional alloys with improved radiation performance has been focused on the addition of alloying elements or nano-scale features with complex microstructures to mitigate damage. In order to move beyond the limitations afforded by current knowledge and incremental radiation resistant property improvements in traditional alloys, we must better understand how the constituents interact in alloys and how their atomic-level heterogeneity affects defect evolution in a radiation environment.

The current opinions and developments outlined in this article focus on single-phase CSAs, with HEAs containing five or more elemental species as part of the CSA family. The constituent elements in these CSAs are distributed randomly on a crystal lattice, such as fcc, bcc, or hexagonal close-packed (hcp). While retaining a simple macroscopically crystalline structure, such random occupancy of different elemental species (**chemical complexity**) creates unique site-to-site lattice distortion (atomic displacements and heterogeneous stresses) and locally disordered chemical environments (lack of translational periodicity), leading to intrinsic complexity at the electronic and atomic levels [2,12,15,16]. In extreme cases such as found in HEAs, no element will have the same nearest and second nearest neighbors [2,15]. Such unusual lattice distortion has demonstrated significantly improved radiation resistance attributed to the high atomic-level stresses facilitating rapid recrystallization and preventing extended dislocation formations.

Recent research has focused on how alloy complexity (the number of major alloying elements, the actual alloying species and concentrations) in single-phase CSAs affects defect dynamics and microstructure evolution by varying the number, type and concentration of alloying elements [2,12–14,17]. This article reviews compositional effects on radiation performance in traditional alloys and reports on current progress of radiation effects in CSAs, including the unique energy landscape of CSAs and atomic-level understanding of defect dynamics at both short- and long-time scales. Challenges and future directions are also discussed.

2. Radiation effects in traditional alloys

2.1. Radiation effects in metals and metallic alloys

When materials are bombarded with energetic particles, the materials are normally damaged and their properties degrade

[18]. Radiation damage in materials has been studied intensively for over 70 years, yet there are still important issues to be addressed both in terms of practical issues and in the fundamental science of radiation effects, including segregation, precipitation, void swelling and embrittlement, etc. [18–28].

The interaction of energetic electrons, ions and neutrons with solids initiates energy transfer processes in both the electronic and atomic subsystems. For the energy transfer to the target atoms, the evolution of radiation-induced defect concentration in metals and metallic alloys can be described by three simplified stages in competing processes: defect production from the collision cascades; subsequent vacancy and interstitial recombination within the diffusion volume; and point defect absorption after diffusing to extended defects (sinks) such as dislocations, additional phases, interfaces, grain boundaries, and precipitates [18]. In the defect production process (the 1st stage), the energy transfer from an incident particle can displace one or more lattice atoms, called primary knock-on atoms (PKA) or recoils, from their original lattice location. These energetic recoils can further collide with other lattice atoms, creating additional displaced atoms in a displacement cascade. In this process, a large amount of interstitials, vacancies and small defect clusters are produced. In the diffusion process (the 2nd stage), interstitials recombine with vacancies, leading to significant annihilation of point defects [18,19]. In addition, defects can also react with defect sinks (the 3rd stage) that leads to annihilation or accumulation of defects along with residual damage build-up. In recent years, intensive studies have concentrated on this 3rd stage to increase the density and strength of defect sinks by introducing nanostructures with a large number of additional precipitates or grain boundaries [28–31]. In other words, the interaction of energetic particles with materials leads to the production of defects, atomic mixing, disordering and possible amorphization that can cause material failure. Radiation effects have been investigated at the atomic level, and, to a large extent, microstructure evolution of irradiated materials are attributed to defect production, diffusion and interaction [19,23–31].

Research on ion-induced irradiation damage has largely focused either on nuclear energy deposition at keV energies (displacement cascade events), or on electronic energy deposition at much higher energies (0.1 to several GeV). In both of these regimes it is generally assumed that nuclear and electronic damage processes are fully separable. In the intermediate energy regime where energetic particles deposit simultaneously a significant amount energy to both electronic and atomic subsystems, the conventional understanding is that the large amount of energy deposited will ultimately be dissipated by a non-damaging mechanism (electron excitation and heat dissipation without causing lattice defects) and by a damaging mechanism (direct atomic displacements); but the two mechanisms have long been assumed independent and non-correlated. The significant amount of energy deposited into the electronic subsystem (dominant fraction for ions with collision energies above a few tens keV) is often poorly approximated or even ignored in conventional atomic-scale models of radiation damage. For metallic targets, although electronic effects have been neglected for a long time, it is well demonstrated that high electronic excitations can play a dominant role in the damaging processes of some metal targets [32–35]. Even for low-energy (~10 keV) radiation damage events, the effects of electronic energy deposition are not negligible and the slower cooling results in enhanced defect recombination [35]. In many radiation events, although non-monotonic effects of the electron-phonon coupling strength or non-adiabatic processes on the residual damage are predicted, there is no understanding on if such electronic effects can be ignored or safely taken out as heat from molecular dynamics simulations. Such a lack of knowledge originates from the complex nature of ion irradiation, where electronic energy transfer

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