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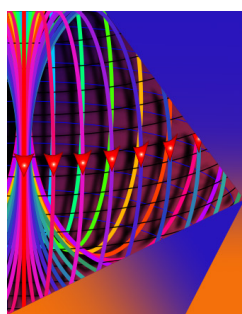


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ABSTRACT

Extensive experimental and computational studies have demonstrated outstanding physical and chemical properties of the novel materials of compositionally complex carbides (CCCs), enabling their promising applications in advanced fission and fusion energy systems. This perspective provides a comprehensive overview of radiation damage behavior reported in the literature to understand the fundamental mechanisms related to the impact of multi-principal metal components on phase stability, irradiation-induced defect clusters, irradiation hardening, and thermal conductivity of compositionally complex carbides. Several future research directions are recommended to critically evaluate the feasibility of designing and developing new ceramic materials for extreme environments using the transformative “multi-principal component” concept. Compared to the existing materials for nuclear applications including stainless steels, nickel alloys, ZrC, SiC, and potentially high-entropy alloys, as well as certain other compositionally complex ceramic families. CCCs appear to be more resistant to amorphization, growth of irradiation defect clusters, and void swelling.

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I. INTRODUCTION OF COMPOSITIONALLY COMPLEX CARBIDES

Since the discovery of “high-entropy” ceramics in 2016, these ceramic materials with multi-principal metal elements have sparked international, extensive research activities, as they introduce promising opportunities for designing and developing novel ceramic materials for structural, electric, and energy storage applications. It has also become a widely debated topic whether the newly observed physical properties originate from the thermodynamic effect such as “high configurational entropy” or “entropy stabilization.” According to the perspective of Schneider,¹ the term “high-entropy ceramics” is not consistent with the classical definition² of “high-entropy alloy” as the molar configurational entropy is only a fraction of 1.61 R, where R is the gas constant ($8.3145 \text{ J mol}^{-1} \text{ K}^{-1}$), for ceramic compounds with one type of

non-metal element. The computation studies by Tang *et al.*³ suggested that the formation of these carbides is controlled by the competition between entropy and enthalpy of mixing. Therefore, the terminology of “compositionally complex ceramics” or “multi-principal component ceramics” may be better used to describe the unique characteristics of these ceramic materials, which can also include non-equimolar compositions.⁴

The compositionally complex carbides (CCCs), including (HfZrTaNbTi)C⁵ and (HfTaZrTi)C,⁶ were first synthesized using spark plasma sintering (SPS) from monocarbide powders in equimolar concentrations in 2018. As an example, (HfZrTaNbTi)C was synthesized using the following route: HfC, ZrC, TaC, NbC, and TiC powders were mixed with an equimolar composition (HfC: ZrC: TaC: NbC: TiC = 1:1:1:1:1) and milled at 250 rpm for 6 h using a planetary ball milling system and then reactively sintered in

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vacuum at 2000 °C for 5 min under a pressure of 30 MPa. The synthesis routes of CCCs were reviewed before,⁷ which can be classified into three approaches based on the starting powders: (1) commercial metal carbide powders, (2) metallic element and carbon powders, and (3) metal oxide and carbon powders. The powder processing is followed by SPS, hot pressing, and most recently, selective laser sintering.⁸ It may be important to note that in all these reports, a high temperature of more than 1800 °C^{9,10} is required to form single-phase CCCs, which may need more thermodynamic investigations.

The reported CCCs are all MC-type carbides (M = transition metal, such as Ti, Zr, Hf, V, Nb, Ta, Mo, W), which exhibit a rock salt B1 structure (Fig. 1) with a space group $Fm\bar{3}m$, with the same structure found in most transition metal monocarbides such as ZrC and TiC. The metal elements share a face-centered-cubic (FCC) sublattice with composition disorder, while the carbon atoms occupy another FCC sublattice. This rock salt crystal structure has been confirmed by x-ray diffraction experiments on many CCCs. The neutron diffraction data of (HfZrTaNbTi)C, obtained from the VULCAN diffractometer at Oak Ridge National Laboratory, fit well with the rock salt average structure model, with the metal elements at the (1/2,1/2,1/2) site and fully disordered over the long-range scale, whereas the carbon atoms are at the (0,0,0) crystallographic site.¹¹ The main difference from transition metal monocarbides is that significant lattice distortion from the ideal rock salt structure occurs due to various atomic sizes and bonding strengths of metal elements in CCCs. However, it still needs to elucidate whether the distortion mainly occurs in the metal or carbon FCC sublattice using techniques such as the extended x-ray absorption fine structure (EXAFS) analysis, which has not been reported in CCCs yet. It is interesting to note that the EXAFS analysis of compositionally complex oxide, (MgCoNiCuZn)O, shows that metal cations are most likely distributed randomly on an FCC sublattice, while the oxygen anions are displaced from the ideal locations to accommodate the distortions in the anion FCC sublattice.¹²

Recent research on CCCs has revealed many unique physical and chemical properties, such as lower thermal conductivity, higher hardness, and improved irradiation and oxidation resistances¹³ compared to monocarbides such as ZrC or TiC. However, the fundamental mechanisms underlying these properties and relationship to their unique characteristics (e.g., compositional complexity, chemical disorder, and lattice distortion) need to be better understood. These properties indicate that CCCs may be promising candidate materials for extreme environments, such as fuel cladding or carbide-based fuels in advanced fission reactors, plasma-facing materials in fusion reactors, and strengthening phase of structural components in gas turbines.

The fundamentals of radiation damage events as well as radiation effects on microstructures and mechanical properties of materials have been explained in several textbooks^{14,15} and are briefly summarized here as an introduction. Radiation damage starts from the interaction of an energetic incident particle (e.g., neutron, ion, electron) with a lattice atom (termed as primary knock-on atom, PKA) in a solid material, which receives kinetic energy and displaces from its lattice site. This atom displacement process, accompanied by the PKA generation, results in the creation of

displacement cascade of point defects, including many pairs of vacancies and interstitials. As the point defects accumulate during irradiation, the resulting radiation damage can manifest as the formation of defect clusters (e.g., di-vacancy, di-interstitial) and extended defects (e.g., dislocation loops, voids, and stacking-fault tetrahedra), instability of phases, segregation of chemical elements, precipitation of new phases, radiation enhanced diffusion, void swelling, irradiation hardening, etc. Moreover, the kinetic energy of the incident ion is transferred to electrons and atomic nuclei simultaneously, and subsequently, much of the electronic energy deposition is transferred to the atomic structure via electron-phonon coupling, resulting in the local inelastic thermal spikes.¹⁶ The radiation damage is intricate and generally dependent on the specific material and microstructures, temperature, irradiation dose, and types of energetic incident particles.¹⁷

II. NUCLEAR APPLICATIONS AND IRRADIATION DAMAGE IN TRANSITIONAL METAL MONOCARBIDES

Refractory ceramics such as ZrC, ZrN, and SiC are used as structural and fuel matrix materials in gas-cooled fast reactors (GFRs) under regular operation and up to 1600 °C during a loss-of-coolant accident.¹⁸ Among these ceramics, ZrC is a candidate for carbide-based composite-type fuels and coating material for tri-structural-isotropic (TRISO) particle fuels, due to its high melting temperature (~ 3530 °C), thermal conductivity ($20\text{--}40\text{ W m}^{-1}\text{ K}^{-1}$),¹⁹ high fission product retention capability, low susceptibility to amorphous phase formation, and stability of the Zr sublattice.²⁰

There is extensive literature on irradiation defects in ZrC. In the neutron-irradiated ZrC_{0.87}, displacement damage colloquially called “black dots” (<2 nm) occurred at 670 °C, which matured to faulted Frank loops at 1280 °C and transitioned to large prismatic loops at 1496 °C.²¹ The proton-irradiation-induced microstructures in ZrC mainly consist of a high density (in the order of 10^{23} m^{-3}) of faulted Frank loops (~ 5 nm), while no irradiation-induced amorphization, voids, or precipitates were observed after irradiation with a 2.6 MeV proton beam at 800 °C to doses of 0.7 and 1.5 displacements per atom (dpa).²² Similarly, faulted Frank loops (~ 7 nm) at a high density ($4.2 \times 10^{22}\text{ m}^{-3}$) were observed after proton irradiation at 800 °C to 1.8 dpa.¹⁸ Under Kr ion irradiation, the evolution of irradiation defect clusters in ZrC_{0.8} and ZrC_{0.9} was studied using *in situ* irradiation experiments at the Intermediate Voltage Electron Microscope-Tandem facility with 1 MeV Kr²⁺ ions up to 12.8 dpa at 20–1073 K.²³ The “black dots” were observed at temperatures below 27 °C, while visible defects did not migrate but interacted with the neighboring defects resulting in coarsening of defect clusters at temperatures above 600 °C. In addition, the stoichiometry of ZrC has shown a significant effect on the irradiation-induced microstructure such as the size and density of dislocation loops.^{24,25} The kinetics of point defects, including the migration of point defects and recombination of Frenkel pairs, in ZrC, was studied using the *ab initio* methods.²⁰ The calculations showed that the Zr and C interstitials have lower migration barriers than vacancies, and the recombination of Zr Frenkel pairs has a low barrier. These theoretical predictions are consistent with the

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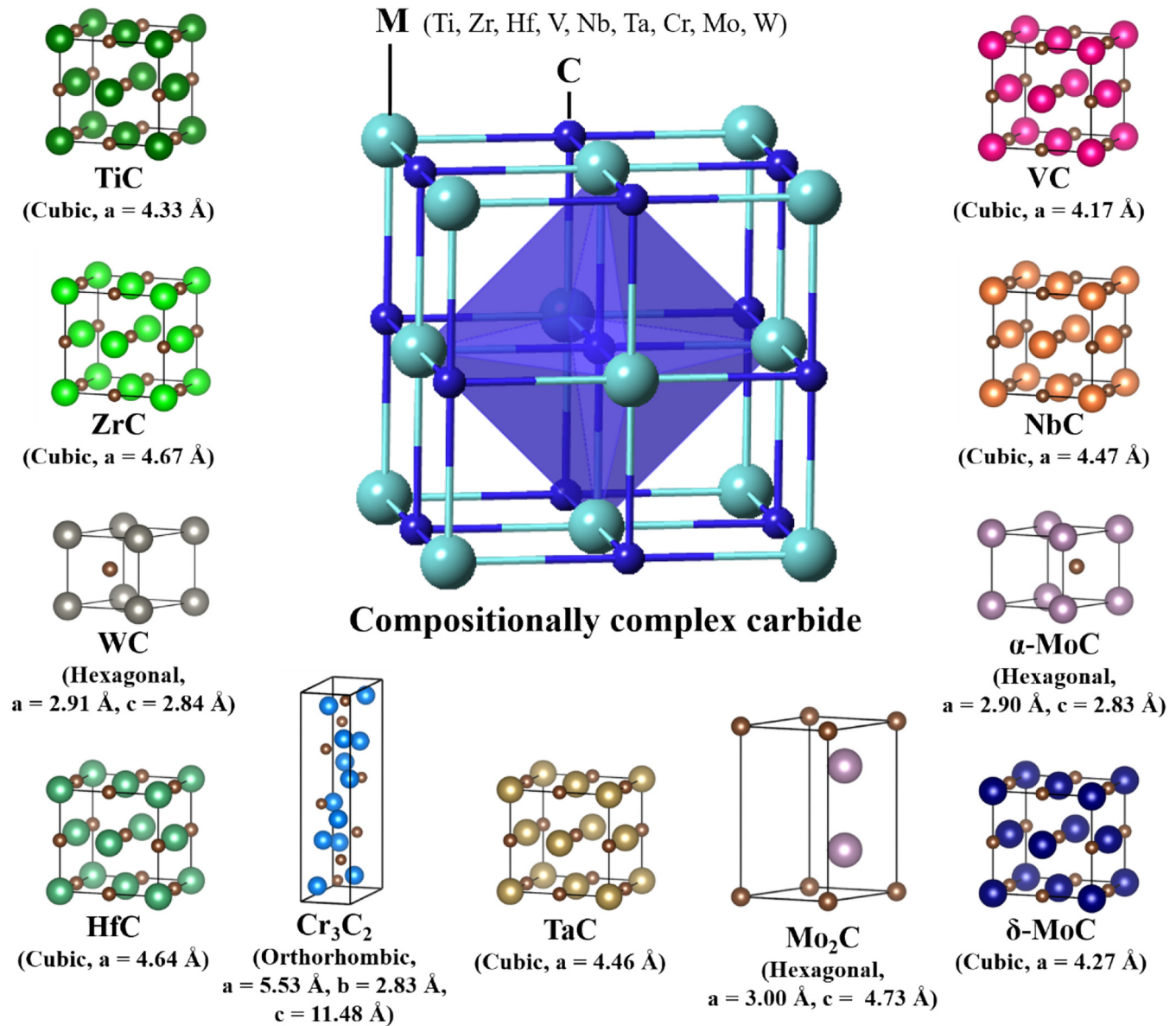


FIG. 1. Crystal structures of compositionally complex carbides (CCCs) and transition metal monocarbides.

easy defect recombination and high amorphization resistance in ZrC.

Void swelling may occur in irradiated materials (i.e., most metals such as stainless steels) at elevated temperatures when vacancies have a high mobility. Voids were not reported in irradiation-induced microstructures in most reports of transitional metal monocarbides such as ZrC and TiC.²⁶ Small voids ($\sim 5 \text{ nm}$) were only observed after neutron irradiation at extremely high temperatures and dose (1496°C , $5.8 \times 10^{25} \text{ N/m}^2$, $E > 0.1 \text{ MeV}$), but the

number density of these voids was extremely low. The absence of void swelling in ZrC may be explained by the *ab initio* calculations that suggested that Zr and C vacancies have high migration energy barriers resulting in a low mobility of vacancies.²⁰

The lattice parameter expansion occurs in transition metal monocarbides after neutron, proton, and ion irradiation. After fast neutron irradiation, the lattice expansions in TiC, ZrC, and NbC were 0.23%–0.46% at $300\text{--}700^\circ\text{C}$ at a neutron dose of $1\text{--}2 \times 10^{21} \text{ cm}^{-2}$.²⁷ Under proton irradiation, the lattice expansion of

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ZrC was reported to be 0.09% and 0.11% at 0.7 and 1.5 dpa, respectively, after irradiation by 2.6 MeV proton at 800 °C.²² Under heavy ion irradiation, the lattice expansions were reported to be 0.23% after 1.2 MeV Au⁺ ion irradiation at 25 °C,²⁸ 0.13% after 4 MeV Au ion irradiation to 7 dpa at 25 °C,²⁹ and 0.7% and 0.9% after 1 MeV Kr ion irradiation to 10 and 30 dpa at 27 °C, respectively.³⁰ It is suggested that irradiation-induced interstitial defects mainly contribute to the expansion in lattice parameters in transition metal monocarbides.³⁰

III. IRRADIATION DAMAGE IN COMPOSITIONALLY COMPLEX CARBIDES

The first report of irradiation damage research of CCCs was in 2019 for the 120 keV helium ion irradiation of (HfZrTaNbTi)C samples.³¹ Since then, there has been a growing interest in understanding the irradiation damage behavior of CCCs using ion irradiation experiments. The transformative “multi-principal component” concept is expected to be used to design and develop new ceramic materials for extreme environments encountered in the next-generation fission and fusion energy systems, such as high temperature and irradiation dose. It is generally hypothesized that the irradiation resistance of compositionally complex alloys and ceramics can be improved due to the potential slow energy dissipation that may positively affect the defect recombination dynamics and delay the damage accumulations.^{32,33} Particularly, chemical complexity, in which different metal elements with various atomic sizes and bonding lengths may result in a complex energy landscape favoring the point defect recombination as well as possibly slowing down the interdiffusion of irradiation-induced defects. Moreover, the chemical short-range order structures induced by the preferential atomic bonding in compositionally complex systems might also have a positive effect in hindering the diffusion of point defects, slowing down the evolution of defect clusters.³⁴ To provide an overview of the current state of knowledge, this review critically examines the existing literature on the irradiation behaviors of CCCs. The literature data encompass ion irradiation utilizing various sources (including Zr, C, Xe, and He ions), spanning temperatures from 25 to 800 °C, and irradiation doses ranging from 0 to 22 dpa.

A. Phase stability

Due to the shallow (typically less than 2 μm) damage depth of ion irradiation, grazing incidence x-ray diffraction (GIXRD) measurements have been performed to analyze the crystal structure modification in the near-surface irradiated region of CCC samples. In all the literature, various CCC samples [including (ZrNbTaTi)C, (HfZrTaNbTi)C, (WTiVNbTa)C, (ZrTiNbTaW)C, and (CrNbTaTiW)C] have been reported to maintain their original single-phase rock salt crystal structures in the all the irradiation temperature and dose ranges. This indicates the superior stability of the rock salt crystal structure and the unique resistance to the amorphization of CCCs. This is in contrast to many other ceramics, such as A₂Ti₂O₇ (A = Yb, Er, Y, Gd)³⁵ and Ti₃(Si, Al)C₂,³⁶ in which the ion irradiation can disrupt the chemical short-range order, leading to the formation of amorphous phases that gradually increases with the irradiation dose.

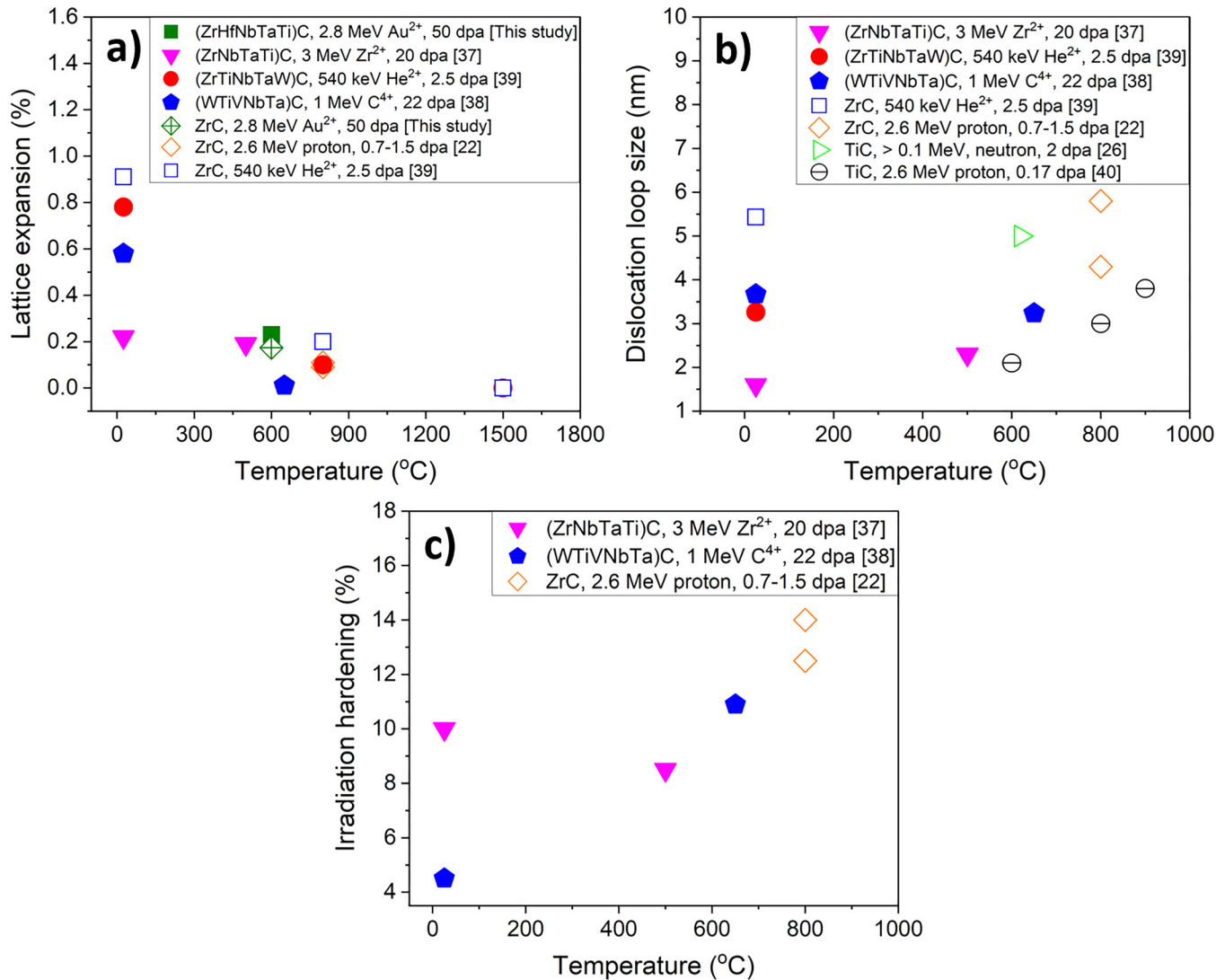
GIXRD patterns of ion-irradiated CCC samples typically exhibit a slight peak shift to lower 2θ angles, indicating the lattice parameter expansion according to Bragg's law. For example, (ZrNbTaTi)C irradiated with 3 MeV Zr²⁺ at room temperature with a dose of 20 dpa shows an approximately 0.22% increase in lattice parameters.³⁷ Similarly, (WTiVNbTa)C exhibits a 0.58% lattice parameter expansion when irradiated with 1.0 MeV C ions at a dose of approximately 22 dpa at room temperature.³⁸ However, irradiation of 540 keV He²⁺ ions on (ZrTiNbTaW)C at about 2.5 dpa at room temperature leads to lattice parameter expansion of up to 0.78%.³⁹ Figure 2(a) is a summary of the literature data on the lattice parameter expansion of ion-irradiated CCCs compared with the monocarbides such as ZrC and TiC. Generally, the increasing irradiation temperature results in less lattice parameter expansion while the relationship between the irradiation dose and lattice expansion appears to be weak.

Recent research on irradiation damage in other families of compositionally complex ceramics, including oxides, MAX phases, borides, and nitrides, has also indicated an enhanced irradiation resistance compared to conventional ceramics. However, CCCs appear to have superior phase stability and resistance to amorphization and lattice expansion compared to the other compositionally complex ceramic families. For instance, (LuYEuGd)₂Ti₂O₇ compositionally complex pyrochlore oxide⁴¹ and (TiVNbZrHf)₂SnC MAX phase⁴² irradiated with 800 keV Kr²⁺ at room temperature exhibited amorphization at the critical dose of 0.26 and 0.87 dpa, respectively. Similarly, the (AlCrMoNbZr)N thin film irradiated with 400 keV He⁺ with a peak dose of 2.7 dpa presented a mixture of crystalline and amorphous regions compared to the as-deposited film.⁴³ In contrast, CCCs such as (ZrNbTaTi)C³⁷ and (WTiVNbTa)C³⁸ retain their structural crystallinity after being irradiated with heavy ions for all the irradiation conditions reported in the literature (from 25 to 800 °C, 0 to 50 dpa). A recent study showed that the crystalline structure of (HfNbTaTiZr)B₂ remained stable after 10 MeV Au⁺ irradiation at 0.44 dpa at room temperature.⁴⁴ However, this compositionally complex boride underwent a volume expansion up to 1.98% in comparison with only 0.66% volume swelling, calculated from 0.22% lattice expansion in (ZrNbTaTi)C after 3 MeV Zr²⁺ to 20 dpa at room temperature.³⁷ These comparisons suggest that CCCs may possess a better irradiation resistance than other compositionally complex ceramics such as oxides, nitrides, or borides, rendering them the preferred choice of irradiation-resistant ceramic materials for further investigations.

B. Radiation-induced defect clusters and gas bubbles

Like those in transition metal monocarbides, dislocation loops are the primary defect clusters caused by heavy ion irradiation in CCCs. These loops can be categorized as perfect and faulted Frank loops. Frank loops are generated from the collapse and condensation of vacancy or interstitial shells on the close-packed plane, which are sessile (immobile) and typically occur in FCC lattices.¹⁴ In contrast, perfect dislocation loops are glissile (mobile). Using the classical *g·b* conditions in the transmission electron microscopy (TEM) characterizations, Wang *et al.*³⁷ identified the Burgers vectors of *b* = *a*/2<1 1 0> for perfect loops and *b* = *a*/3<1 1 1> for faulted Frank loops in 3 MeV Zr²⁺ irradiated (ZrNbTaTi)C at 25,

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FIG. 2. Summary of the literature data for the quantitative evaluation of the irradiation damage in the CCC: (a) lattice parameter expansion; (b) dislocation loop diameter; and (c) irradiation-induced hardness increase as a function of irradiation temperature and dose.^{22,26,37–40} The filled symbols are for CCC, while the open symbols are for monocarbides.

300, and 500 °C. The edge-on Frank loops on the {1 1 1} habit planes were also observed in 1.0 MeV C-ion irradiated (WTiVNbTa)C at room temperature and 650 °C.³⁸ These Burgers vectors of dislocation loops are the same as those in the FCC structure, which indicates that the dislocation loops are likely formed in the FCC sublattice of either metal or carbon in the rock salt structure of CCCs. Generally, the irradiation-induced defects transform from dislocation loops to dislocation networks at higher radiation doses. At a given radiation dose, the loop size changes with irradiation temperature. Figure 2(b) presents the quantitative literature data of dislocation loop diameter in the ion-irradiated CCCs compared with that in monocarbides. It is generally observed that the

loop size in ion-irradiated CCCs, such as (WTiVNbTa)C and (ZrTiNbTaW)C, remains a few nanometers that are significantly smaller than those in monocarbides under the same irradiation temperature and dose.^{38,39} This sluggish growth of dislocation loop size in the CCC may be related to the atomic-level inhomogeneity in the metal sublattice that may pin the point defects to delay the damage accumulations. However, higher temperatures may facilitate the mobility of point defects, leading to a slight growth of dislocation loop size along with a decrease in its number density.

The formation of voids in irradiated materials is driven by the supersaturation of vacancies.¹⁴ Voids have not been observed in CCCs in the range of irradiation conditions reported in the existing

literature. This is another benefit of CCCs because volumetric swelling occurs when voids form and grow at elevated temperatures. The absence of voids may indicate the high migration energy of metal and carbon vacancies. Zhao calculated the migration energies of a single C vacancy in (TaZr)C, (NbTaZr)C, and (NbTaTiZr)C using the *ab initio* simulation based on density functional theory (DFT), which are in the range of 2.5–6.0 eV.³² These are generally higher than those of monocarbides such as ZrC (4.0 eV) and TiC (3.9 eV),³² suggesting that void formation may be delayed in CCCs.

In the fusion reactor environment, helium and hydrogen isotopes are introduced into first-wall materials by direct implantation or nuclear transmutation reactions during neutron irradiation. High helium concentrations result in the formation of helium bubbles, which can enhance void swelling, produce surface blistering, and cause high-temperature intergranular embrittlement.⁴⁵ Gas bubble formation has been observed after inert gas ion [e.g., helium (He) or xenon (Xe)] irradiation in CCCs. Wang *et al.* first observed small He bubbles with a diameter of 1 nm after 120 keV He ion irradiation of (HfZrTaNbTi)C samples at room temperature.³¹ Later, Xin *et al.* conducted a similar study of helium bubbles in (ZrTiNbTaW)C compared with those ZrC after 540 keV He ion irradiation at room temperature and subsequent annealing. The initial helium bubbles were also tiny (~1 nm) after irradiation, while after annealing at 1500 °C, the diameter of He bubbles in (ZrNbTaTiW)C grew to approximately 3.5 nm, which is smaller than those in ZrC (5.5 nm) under the same conditions.³⁹ Xe bubbles (~2.1 nm) were observed in (CrNbTaTiW)C after 300 keV Xe⁺ irradiation at 300 °C for 10 dpa, which are much smaller than those observed in nuclear fuel ceramics such as UO₂ or U₃Si₂.⁴⁶

C. Influence of grain boundaries

Irradiation at elevated temperatures may cause spatial redistribution of solute and impurity elements, leading to the enrichment or depletion of alloying elements in regions near grain boundaries. The most famous example of radiation-induced segregation (RIS) is the depletion of chromium at grain boundaries of the irradiated 300 series stainless steels.⁴⁷ RIS is not observed in CCCs in the range of irradiation conditions reports in the existing literature. For instance, the chemical compositions of metal elements still show a uniform distribution across the grain boundaries in 3 MeV Zr²⁺ irradiated (ZrNbTaTi)C at 25, 300, and 500 °C³⁷ as well as 300 keV Xe⁺ irradiated (CrNbTaTiW)C at 300 °C according to energy dispersive spectrometry (EDS) analysis.⁴⁶ Nevertheless, these RIS studies were conducted with heavy ions to emulate the irradiation damage caused by neutrons in the actual reactors. Due to differences in displacement efficiencies between neutrons and heavy ions,⁴⁸ additional studies may be needed to evaluate the RIS resistance in the CCC under neutron irradiation. Recently, electron energy loss spectroscopy (EELS) study has revealed an enrichment of carbon atoms at the grain boundary at 300 °C, diminishing at 600 °C in 3.15 MeV C⁴⁺ irradiated SiC.⁴⁹ It may need more investigations of RIS in CCCs by EELS analysis. If the element segregation occurs in a few tens of nanometers near grain boundaries, it may be difficult to reveal it using EDS.

On the other hand, grain boundaries may act as sinks for the absorption and annihilation of irradiation defects. In many metals

such as Fe and Cu, the fundamental mechanisms involve the biased absorption of interstitials over vacancies during collision cascades and strong interactions with vacancies in interstitial-loaded boundaries.^{50,51} As a result, nanocrystalline materials containing a large fraction of grain boundaries, such as stainless steels,⁵² ZrO₂,⁵³ and MgGa₂O₄,⁵⁴ have shown improved radiation resistance compared with their polycrystalline counterparts. It is also observed that the nanocrystalline (CrNbTaTiW)C with a grain size of 9.8 nm exhibits no dislocation loops after irradiation with 300 keV Xe⁺ ions at 300 °C.⁴⁶ However, grain growth may also occur in the nanocrystalline CCC at elevated temperatures, as shown in nanocrystalline (CrNbTaTiW)C.

D. Irradiation hardening

Figure 2(c) presents the quantitative literature data of the hardness increase in the ion-irradiated CCC compared with that in monocarbides. Due to the shallow damage depth of ion irradiation in these ceramics, nanoindentation tests need to be used and the indentation depth needs to be within 1/10 of the irradiated layer thickness to avoid the influence of the unirradiated regions underneath the irradiated layer.³⁷ The experimental results from Wang *et al.*³⁷ in 3 MeV Zr²⁺ irradiation on (ZrNbTaTi)C at 25, 300, and 500 °C as well as Zhu *et al.*³⁸ in 1.0 MeV C⁴⁺ irradiation on (WTiVNbTa)C at room temperature suggest that the irradiation hardening effect increases with increasing defect size and density. The source of irradiation hardening is primarily radiation-induced point defects and dislocation loops that hinder the slip behavior during the nanoindentations. Thus, the irradiation hardening effect can be affected by the evolution of defect structures as functions of temperature and irradiation dose. When the transformation from a combination of “black dots” and tangled dislocations into primary “black dot” defects in (WTiVNbTa)C occurs at 650 °C, the relative change of hardness is reduced from 10.9% to 4.5%.³⁸

E. Thermal conductivity

Since the discovery of CCCs in 2018, their thermal diffusivity and conductivity have been reported to be significantly lower than the constitute monocarbides at room temperature.⁵ The suppressed thermal conductivity has been generally explained by the scattering of phonons induced by the chemical disorder and lattice distortion in CCCs. However, the relative partitioning of thermal carriers (electrons and phonons) in CCCs depends sensitively on the temperature and stoichiometry.⁵⁵ Irradiation generates extrinsic lattice defects, which can further alter the thermal transport in CCCs and affect their nuclear applications as fuel cladding, carbide-based fuels, or plasma-facing materials. It is important to note that although there are many thermal conductivity measurement approaches (e.g., laser flash), a high spatial resolution method is needed to measure the local thermal conductivity in the shallow irradiation damage layer near the surface of ion-irradiated samples. Dennett *et al.*⁵⁶ first measured the thermal conductivity of 3 MeV Zr²⁺ irradiated (ZrNbTaTi)C at 25, 300, and 500 °C using a spatial domain thermal reflectance (SDTR) method. By applying a multi-layer thermal transport model, it was determined that the reduction in thermal conductivity is greatest in (ZrNbTaTi)C irradiated at 25 °C, suggesting that the dislocation loops may contribute less to

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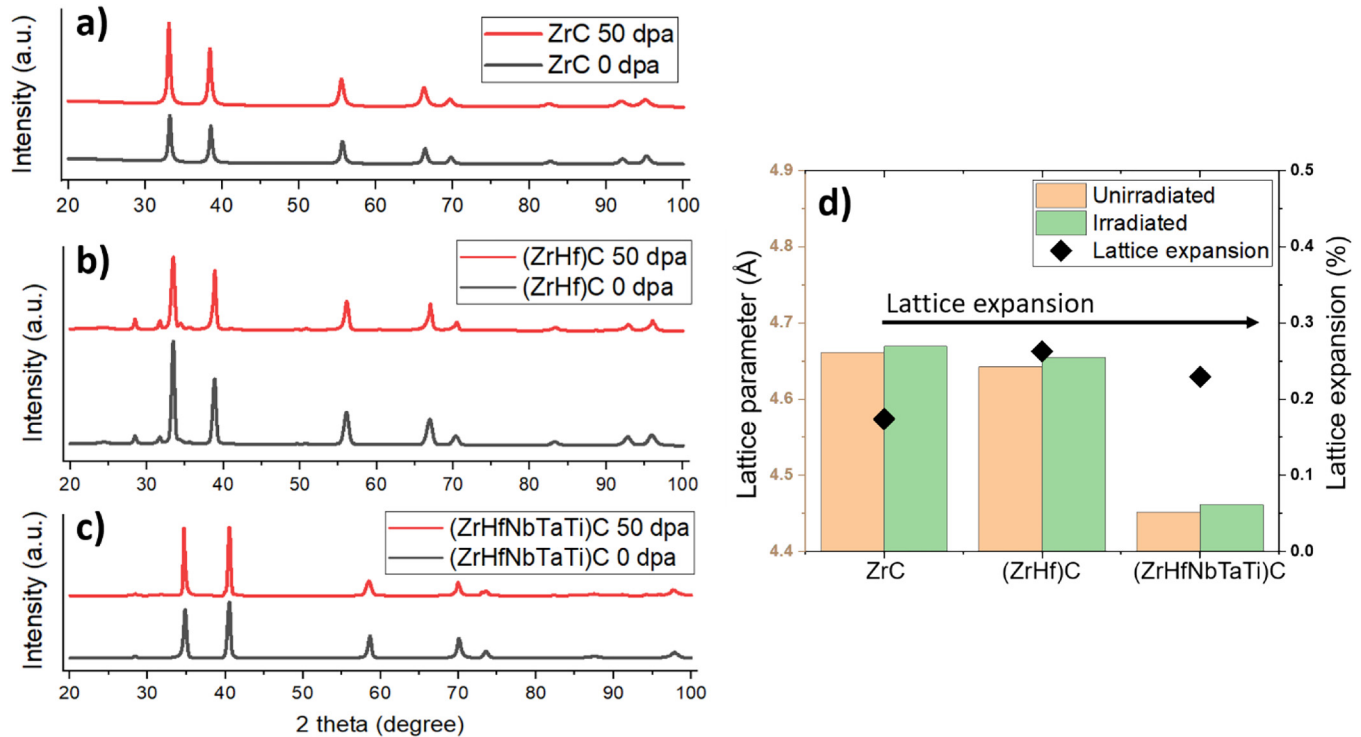


FIG. 3. Grazing incident x-ray diffraction (GIXRD) patterns of (a) ZrC, (b) (ZrHf)C, (c) (ZrHfNbTaTi)C before and after irradiated with 2.8 MeV Au²⁺ at 600 °C to 50 dpa, (d) lattice parameter before and after irradiation and the percentage of lattice expansion.

phonon scattering, likely due to the suppression of their long-range strain fields, than the extrinsic nanoscale defects (i.e., point defects and small clusters below TEM resolution).

IV. PERSPECTIVE FOR FUTURE RESEARCH

Compared to the existing materials for nuclear applications (including stainless steels, nickel alloys, ZrC, SiC, and potentially high-entropy alloys), CCCs appear to be more resistant to amorphization, growth of irradiation defect clusters, and void swelling. Nevertheless, it is noted that the irradiation conditions in the limited literature only cover the ion irradiation (including Zr, C, Xe, and He ions), the temperature from 25 to 800 °C, and the irradiation dose from 0 to 22 dpa. The next-generation fission and fusion reactors aim to provide enhanced fuel-to-energy conversion efficiency, resulting in more extreme operating conditions, such as higher temperatures (700 to above 1300 °C), higher radiation levels (50–200 dpa),⁵⁷ and corrosive coolants (e.g., molten salts, liquid sodium). In this context, our recent experiments are conducted on (ZrHfNbTaTi)C with 2.8 MeV Au²⁺ irradiation at 600 °C to a maximum fluence of 7.1×10^{11} ions/cm that is equivalent to a peak irradiation dose of 50 dpa (Fig. 3). GIXRD analysis shows that in this more extreme irradiation environment, (ZrHfNbTaTi)C still retains its original single-phase rock salt crystal structure, without phase transformation or amorphization although further

selected-area electron diffraction analysis may be needed to verify no local amorphization. The lattice parameter expansion of (ZrHfNbTaTi)C, ZrC, and (ZrHf)C was comparable (~0.2%), in which (ZrHf)C is a binary metal carbide solid solution. These new data on lattice parameter expansion have been added to Fig. 2(a).

While significant progress has been made in understanding irradiation damage in the emerging materials of CCCs, several fundamental and engineering issues need to be addressed in future research.

A. Neutron irradiation

Because the literature data are limited to ion irradiation studies, future research needs to employ proton and neutron irradiation sources to further evaluate their irradiation resistance. Since the 1960s, ion irradiation has been successfully employed to simulate neutron damage in materials, offering advantages such as a rapid dose rate and no radioactive effects.¹⁴ However, there are concerns regarding establishing an equivalence between ion and neutron irradiation due to distinct energetic characteristics and displacement efficiency.⁴⁸ Although ion irradiation can be used as a fast-screening tool to down-select the promising chemical compositions of CCCs, it will be essential to conduct neutron irradiation experiments in the next stage to validate their irradiation resistance.

B. New compositions and microstructural design

While tens of CCCs have been successfully synthesized, only a limited number of them [including (ZrNbTaTi)C, (ZrHfNbTaTi)C, (WTiVNbTa)C, (CrNbTaTiW)C, and (ZrTiNbTaW)C] have been used for studying radiation damage behavior, which restricts our knowledge and assessment of irradiation resistance of carbides with complex chemical compositions. Carbides of refractory transition metals from groups IV, V, VI (Ti, V, Cr, Zr, Nb, Mo, Ta, W) exhibit outstanding physical and chemical properties, rendering them highly desirable for the advancement of structural materials under extreme conditions. Moreover, most of these refractory carbides demonstrate considerable mutual solubility, facilitating the solid solution formation of CCCs. However, for neutronic considerations, metal elements with neutron-absorbing properties, such as hafnium (Hf), may not be a suitable component of the CCC for nuclear reactor applications. Moreover, high-throughput computational and experimental tools may be needed to accelerate the evaluation of irradiation damage behavior from a large number of chemical compositions to down-select the promising CCC with maximum irradiation resistance. Furthermore, it will also need the design of “sinks” in their microstructures for the absorption and annihilation of irradiation defects, which may include the specific grain boundaries (e.g., incoherent twin boundaries⁵⁸) and nano-scale interfaces (e.g., metal/carbide⁵⁹ or carbide/oxide interfaces⁶⁰).

C. Computational modeling and machine learning

In the context of radiation damage in materials, computational modeling such as molecular dynamics (MD) has been conducted to explore the multiscale physics involved in irradiation effects of structural materials.⁶¹ Recently, Zhao⁶² has proposed three machine learning (ML) approaches for predicting irradiation response in high-entropy alloys, developing interatomic potentials, and analyzing defect evolution. Among them, the ML-based interatomic potentials may be the most attractive ML tool for CCCs. Although the traditional method of DFT calculations can provide quantum mechanical accuracy of interatomic potentials, it is limited by the time and spatial scale of the simulation that can be performed. The ML models, such as Gaussian approximation⁶³ or deep learning potentials,⁶⁴ may become a universal tool to model interatomic interactions in CCCs, where the empirical formula may be insufficient to describe the complex interactions due to chemical complexity.

D. Mechanical properties

At present, studies of mechanical properties of the irradiated CCC are only limited to irradiation hardening by nanoindentation tests. It will need various types of mechanical tests to determine the effect of irradiation damage on the strength, fracture toughness, and creep behavior of CCCs. The flexural strength of carbide ceramics can be measured by 3-point or 4-point bending tests, while fracture toughness can be measured by single-edge notched beam, chevron notch beam, or indentation-induced crack methods.⁷ Irradiation creep of carbides can be examined by bending or compression experiments.⁶⁵ However, a significant technical challenge is that the shallow irradiation damage layer near

the surface of ion-irradiated samples and, thus, neutron-irradiated samples might be more appropriate for these macroscopic mechanical tests.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose

Author Contributions

Lanh Trinh: Data curation (equal); Investigation (equal); Methodology (equal); Writing – original draft (lead). **Fei Wang:** Investigation (equal); Methodology (equal); Validation (equal). **Kaustubh Bawane:** Funding acquisition (supporting); Resources (equal); Validation (equal). **Khalid Hattar:** Resources (equal); Writing – review & editing (supporting). **Zilong Hua:** Validation (equal); Writing – review & editing (supporting). **Linu Malakkal:** Resources (equal); Writing – review & editing (supporting). **Lingfeng He:** Resources (equal); Writing – review & editing (supporting). **Luke Wadle:** Formal analysis (equal). **Yongfeng Lu:** Supervision (equal); Writing – review & editing (supporting). **Bai Cui:** Conceptualization (lead); Funding acquisition (lead); Supervision (lead); Writing – review & editing (lead).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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