

Review

Elemental Segregation and Solute Effects on Mechanical Properties and Processing of Vanadium Alloys: A Review

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Abstract: Vanadium (V) alloys, such as V-Cr, V-Ti, and V-Cr-Ti alloys, are promising candidates for structural components in fusion energy systems because of their low activation, excellent radiation resistance, good compatibility with liquid lithium, and high ductility. Despite these advantages, the limited high-temperature strength and poor creep performances of V alloys have constrained their operating temperature range, challenging the application of these materials over the past few decades. The mechanical behavior is strongly dependent on microstructural features, including precipitates, intergranular and intragranular boundaries, dislocations, and point defects. At the same time, these features serve as preferable sites for solute or impurity atoms to segregate. The elemental segregation alters the local chemistry and stability of these defects, influencing microstructural evolutions and various materials properties that are essential for fusion energy applications. This review paper aims to provide a comprehensive overview of experimental and computational studies on elemental segregation and solute/impurity effects on the mechanical behaviors and microstructural evolution in V alloys. The conventional and advanced manufacturing processes of V alloys will be also discussed. Finally, this review will provide a concise perspective on the potential research directions of V alloys for future fusion reaction applications.

Keywords: vanadium alloys; solute effects; mechanical properties; elemental segregation; advanced manufacturing



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1. Introduction

Vanadium (V) alloys are promising structural materials for fusion blanket applications due to their low-activation properties, excellent compatibility with liquid lithium, and strong resistance to irradiation damages enabled by their body-centered cubic (BCC) crystal structure [1–9]. Unlike other low-activation materials commonly used in fusion systems, such as ferritic/martensitic steels and silicon–carbide (SiC)-based composites, V alloys stand out as the only system exhibiting both non-ferromagnetic and ductile properties [7]. These characteristics make V alloys promising candidates for advanced fusion materials capable of enduring high levels of irradiation in extreme environments. However, the limited high-temperature strength and poor creep resistance of V alloys have restricted their operating temperature, thus limiting their broader application in fusion technology over the past few decades.

In V alloys, crystal defects, including precipitates, grain boundaries (GBs), dislocations, and point defects, play significant roles in influencing the microstructural evolution and properties of these materials, particularly under extreme conditions such as high temperature, irradiation, and other harsh environments [10]. For instance, three-dimensional (3D)

defects, such as precipitates formed from excess solutes and impurities, are crucial for improving mechanical properties of V alloys [11–14]. Two-dimensional (2D) defects, such as GBs which separate adjacent grains, are the major sink of point defects in V alloys [15–18]. One-dimensional (1D) defects, like dislocations, serve as a major carrier of deformation and significantly affect the plastic behavior of V alloys [19–21]. Zero-dimensional defects (0D), such as vacancies and interstitials, are even more pervasive in V alloys, especially after irradiation, and frequently interact with solutes or impurities to form solute-vacancy complexes [10,22,23].

Due to the high Gibbs free energy of defects, solute or impurity atoms tend to interact with these defects to lower their energies [24,25]. This interaction often results in elemental segregation (a.k.a. adsorption) at defected regions, such as GB segregation [25], surface adsorption, and dislocation segregation [19]. The segregated solutes (e.g., Ti, Cr, Mn, Fe, and other transition metals) or impurities (e.g., C, O, and N elements) can significantly alter the local chemistry and structures of these defects, thereby affecting a broad range of material properties that are critical to fusion energy applications [10]. For example, in one of the most promising V alloys, V-4Cr-4Ti, extensive experimental and computational studies have revealed that Ti elements are favorable to segregate to the V GBs and sample surfaces [26–28]. These segregated Ti atoms can interact with impurities such as C, O, and N, and then form precipitates (e.g., Ti(CON)), which strengthen the V alloys and improve their radiation-resistance properties via lowering the interstitial impurities in the matrix of V alloys [29].

Elemental segregation to crystal defects does not always enhance the materials properties of V alloys. More frequently, these segregation behaviors have significant detrimental effects on the properties and performance of these materials. For instance, at high Ti concentration, a large amount of Ti segregation can cause GB embrittlement, potentially triggering catastrophic failure of V alloys [30]. Additionally, Ti atoms have been observed to segregate to the climbing dislocations [19], which subsequently degrades the mechanical properties of V alloys. In medium-entropy V-Cr-Mn alloys, Cr and Mn elements tend to segregate to the vacancy regions, forming brittle CrMn_3 precipitates that comprise the mechanical performance of these materials [31]. Therefore, understanding the segregation behavior of solute or impurity atoms to defects and how their interaction with different defects is crucial for developing next-generation V-based structural materials for advanced fusion systems.

This review provides a comprehensive overview regarding the elemental segregation to crystal defects and the effect of solute or impurities on the mechanical properties and performance of V alloys; see Figure 1. The paper is organized as follows: Section 2 discusses prior experimental and computational studies on the elemental segregation at various crystalline defects (e.g., GBs, precipitates, surfaces, and voids) in V alloys; Section 3 focuses on the effects of solutes or impurity atoms on mechanical behaviors of V alloys based on both experimental and theoretical studies; Section 4 summarizes the effects of solute or impurity atoms on the microstructural evolution of V alloys, with a particular focus on the recent experimental studies using advanced electron microscopy techniques; Section 5 discusses how different advanced manufacturing processes control the microstructures and associated properties of V alloys; finally, Section 6 offers a perspective on future experimental and computational studies aimed at developing advanced V alloys for fusion energy applications.

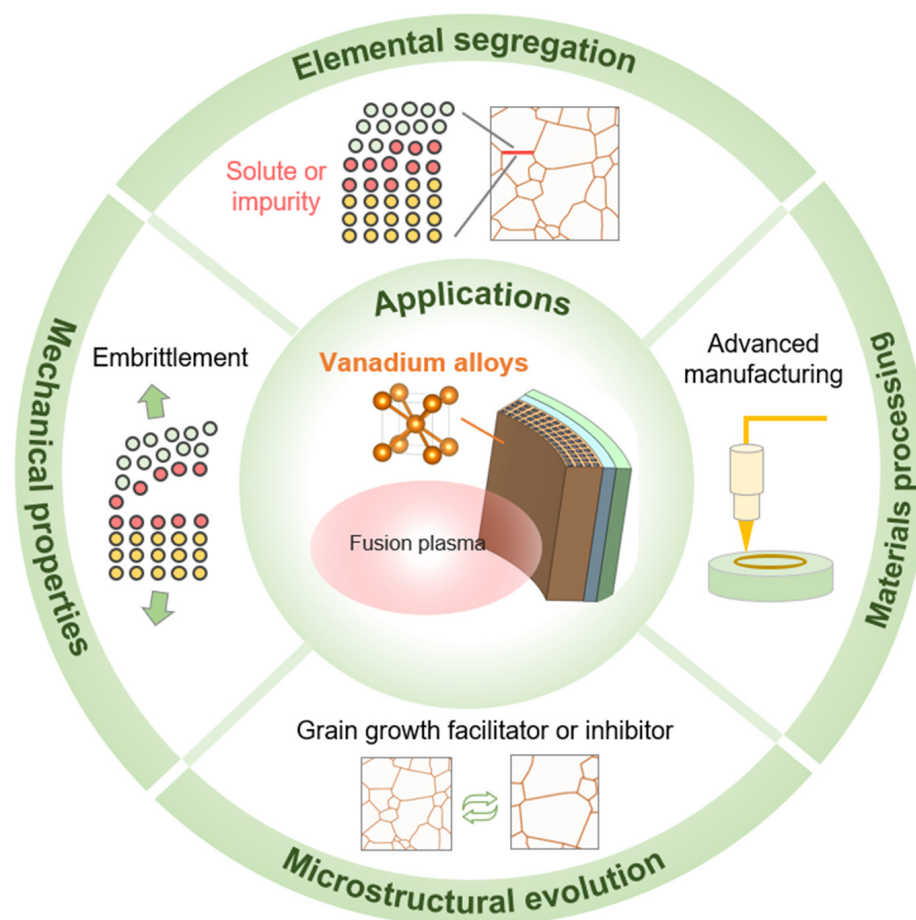


Figure 1. An overview of the element segregation to crystal defects (e.g., grain boundaries, surfaces, precipitates) and the effects of solute or impurity on the composition structure–property–processing relationships in V alloys.

2. Solute Segregation Behavior in Vanadium

The properties of V alloys are strongly influenced by the amount and type of alloying elements and interstitial impurities, and their interactions. These elements can also interact with irradiation-produced defects that diffuse along defect gradients towards defect sinks, creating strong driving forces for solute segregation, which is often referred to as irradiation-induced segregation (RIS) [17,26,27,32–34]. RIS has been widely studied in V alloys through experiments and is explained by a simple size factor theory: undersized and oversized elements tend to interact with interstitials and vacancies, respectively [35,36]. The interaction between undersize solute atoms and interstitials usually results in solute enrichment at defect sinks, such as internal and external surfaces, GBs, and dislocations, while the interaction between oversize solute atoms and vacancies leads to solute depletion at these locations. Since RIS plays a vital role in the performances such as the void swelling behavior of V alloys for fusion applications, this section will provide a thorough overview of segregation behavior of a range of solute elements to various defect sinks.

2.1. Segregation to Grain Boundaries

GBs are major sinks for irradiation-induced defects, such as vacancies. Many studies examined GB segregation in various binary and ternary V alloys under different conditions such as ion irradiation, neutron irradiation and annealing treatment [17,26,27,32–34]. Below is a summary of the GB segregation behavior of common solutes and impurities in V alloys.

Ti: In a binary alloy (V-5.3 at.% Ti) and a ternary alloy (V-14.7 at.% Cr-5.2 at.% Ti) ion irradiated to 50 dpa at 925 K, no obvious change in Ti concentration at GBs with respect to matrix was observed [26]. However, in a V-15Cr-5Ti (wt.%) neutron irradiated to 14 dpa at 600 °C, the Ti level was much higher at GBs and lower in the regions adjacent to the boundaries [27].

Cr: In a V-14.7 at.% Cr alloy ion irradiated to 50 dpa at 940 K, significant depletion of Cr at GBs was observed from EDS measurements [26]. However, the segregation behavior of Cr was influenced by the presence of other solute elements. For example, in the presence of Ti, apparent Cr enrichment was observed at GBs in a V-14.7 at.% Cr-5.2 at.% Ti alloy after ion irradiation to 50 dpa at 925 K. Similar observation of Cr enrichment at GBs was found in a V-15Cr-5Ti (wt.%) alloy under neutron irradiation to 14 dpa at 600 °C [27]. In contrast, in a V-Cr-Fe-Zr quaternary system after ion irradiation, Cr depletion was observed at V GBs [26].

Fe: Takeyama et al. [34] performed energy dispersive X-ray spectroscopy (EDS) measurements on a V-3 at.% Fe neutron irradiated to a fluence of 1×10^{25} n/m² at 740 K. They observed Fe enrichment at GBs and Fe depletion in the areas adjacent to GBs for distances up to ~250 nm. GB segregation of Fe was also observed by Loomis et al. [26] in a V-9.6 at.% Cr-3.1 at.% Fe-0.7 at.% Zr alloy ion irradiated to 50 dpa at 925 K.

Ni: Ohnuki et al. [19] observed segregation of Ni at GBs in a V-1 at.% Ni system neutron irradiated to 17.7 dpa at 400 °C. In addition, the Ni segregation resulted in a Cr depletion at vanadium GBs.

Mo: Mo was reported to be slightly depleted at GBs for a V-2.5 at.% Mo alloy ion irradiated to 50 dpa at 900–970 K [26].

W: Slight W depletions at GBs were observed from EDS measurements of a V-2.5 at.% W alloy ion irradiated to 50 dpa at temperatures ranging from 900 to 970 K [26]. However, the W segregation was inconclusive since the presence of impurities including Si and S might affect the results [26].

Impurity (C, N, O, S, P): Impurity elements have a strong effect on mechanical behavior and irradiation resistance of vanadium alloys. Kurtz et al. [17] examined the effect of different heat treatments on the GB chemistry of fractured surfaces of a production-scale heat (No. 832665) of V-4Cr-4Ti (wt.%) from Charpy impact testing. Comparison between intergranular and cleavage facets revealed that C, N, S, P segregated to GBs for all heat treatments, with C segregation being less than that of the other elements. However, O depletion at GBs was observed for all conditions. Kameda et al. [16] also observed segregation of P and S in a V-20 wt.% Ti system, but the segregation depended on treatment conditions as detailed below. Three treatment conditions were employed, including unirradiated and unaged, aged but without irradiation, and neutron irradiated.

Intergranular S segregation was promoted by thermal aging. However, neutron irradiation resulted in S desegregation [16]. Intergranular segregation of P was enhanced by both thermal aging and neutron irradiation. The irradiation reduced the GB segregation of C and O, while thermal aging increased segregation of both elements. The authors pointed out that both the coupling effect of defect and impurity fluxes and the impurity solubility play a role in affecting the GB composition during irradiation. When no other solute element presents, Jo et al. [32] observed no obvious segregation of O or N in V; see Figure 2. Yet, a clear enrichment of S and P elements at V GBs was observed using scanning transmission electron microscopy (STEM) combined with EDS mapping (see Figure 2).

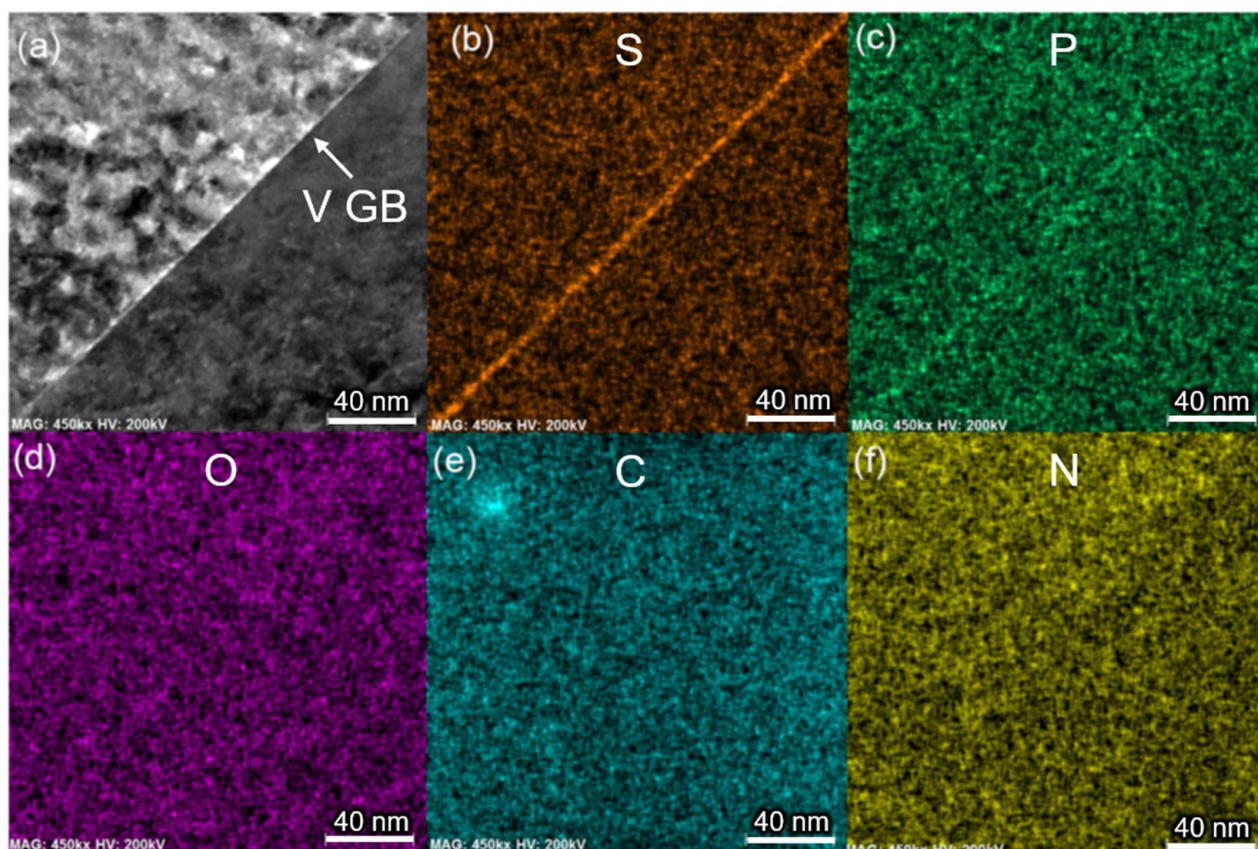


Figure 2. (a) HAADF micrograph of a GB in a V-5N alloy. EDS mapping of (b) S, (c) P, (d) O, (e) C, and (f) N showing segregation of S and P elements at this GB, while O, C, and N do not exhibit enrichment. Reprinted with permission from Ref. [32]. 2024 Elsevier.

2.2. Segregation to Sample Surfaces

Another major sink for irradiation-induced defects is sample surfaces, and therefore, solute concentration at these surfaces may exhibit a dramatic change compared to that in the matrix due to the defect-solute interaction. To examine solute content at surfaces, Auger Electron Spectroscopy (AES) is a widely adopted technique. The segregation of solute atoms to V surfaces are summarized below.

S: Bajaj and Gold [37] observed significant S segregation to the transgranular cleavage fracture surface of V-15Cr-5Ti (wt.%) in both unirradiated and neutron-irradiated condition. The AES results showed S levels on the order of 3–35 wt.%, although no S was reported in the bulk chemical analysis of the alloy. However, in follow-on experiments on the duplicate nonirradiated samples with an average bulk content of S about 5 wppm [37], no S was detected on the transgranular fracture surface regions, while every high level of S on the order of 10 wt.% was detected on the intergranular regions. Further examinations of S segregation were performed on other heats of unirradiated V-15Cr-5Ti (wt.%), V-20Ti (wt.%), and VANSTAR-7[®] (V-9.7Cr-3.4Fe-1.3Zr, wt.%) with bulk S content in the range of 35–50 wppm [38]. S enrichment at fracture surfaces was only observed for one annealed V-20Ti sample and a cold-worked VANSTAR-7[®] sample [20]. Therefore, S segregation at sample or fracture surfaces is still inconclusive.

Cr: Loomis et al. [26] performed AES measurement of a V-14.7 at.% Cr alloy ion irradiated to 50 dpa at 900 K and observed a significant Cr enrichment in the near-surface layer, whereas a significant Cr depletion at the surface was observed as the irradiation temperature increased to 940 K, suggesting that Cr concentration at surfaces may reduce with increasing irradiation temperature. However, Rehn et al. [39] reported that a maximum

of Cr segregation (~25 at.%) to near-surface layers in a V-14.7%Cr alloy occurred after irradiation under 950 K and 24 dpa. This discrepancy in RIS of Cr in V was attributed to impurities including Si and S, which affect the segregation behavior of Cr.

Agarwal et al. [40] also studied the Cr segregation in a V-15 wt.%Cr ion irradiated to 5–60 dpa at 650 °C using AES, and observed a surface layer ~200 Å thick that has been significantly enriched in Cr and a depleted subsurface region which extends to a depth of ~1000 Å. Moreover, the first few atom layers at the irradiated surface contain ~50 wt.% Cr. The observed enrichment of Cr at the surface, which serves as a sink for both interstitial- and vacancy-type defects, is consistent with the size-effect prediction of Okamoto and Wiedersich [35].

Although most previous studies pointed to segregation of Cr to sample surfaces, the behavior can be influenced by the presence of other solute elements. For example, in a quaternary system of V-9.6Cr-3.1Fe-0.7Zr (at.%) irradiated at 925 K to 50 dpa, obvious Cr depletion was observed at near-surface layers, while Fe was clearly enriched in these regions. This suggests that when multiple solute elements with different segregation tendencies coexist, they may compete for segregation sites, resulting in the depletion of solutes with weaker segregation tendencies.

Ti: Both binary V-5.3 at.% Ti and ternary V-5.2 at.% Ti-14.7 at.% Cr exhibited a substantial enrichment of Ti in the near-surface region after ion irradiation [26]. In addition, the presence of Ti enrichment resulted in Cr depletion in the near-surface region to a depth of 2.5 nm in the ternary V-5.2 at.% Ti-14.7 at.% Cr alloy.

Fe: AES analysis of a quaternary system, i.e., V-9.6 at.% Cr-3.1 at.% Fe-0.7 at.% Zr alloy ion irradiated to 50 dpa at 925 K, showed an enhanced Fe concentration to ~6 at.% in the near-surface layer [26]. Similar to the Ti effect on Cr segregation, the Fe enrichment resulted in Cr depletion in the near-surface region for this quaternary alloy.

Ni: AES measurement of a V-8 at.% Ni sample ion irradiated to 50 dpa at temperatures ranging from 925 K and 970 K showed an enrichment of Ni in the near-surface layers [26].

Mo: For a V-2.5 at.% Mo alloy ion irradiated to 50 dpa at 935 K, a depletion of Mo in the near-surface layer was observed from AES experiments [26].

W: For a V-2.5 at.% W alloy ion irradiated to 50 dpa at 935 K, a depletion of W in the near-surface layer was observed. However, the W depletion may be affected by the presence of impurities including Si and S, both of which were highly enriched in the near-surface layers [26].

2.3. Segregation to Voids

Segregation of both substitutional and interstitial solute elements around voids have been observed, and it was proposed that radiation-induced segregation is an important factor for void suppression. For interstitial impurities such as C and O, they interact with radiation-induced point defects and give a strong influence on the nucleation of voids and/or segregation around voids [35]. Therefore, in this section, segregation behavior of solute elements as well as their effects on void formation will be reviewed.

Si: In a V-3.2 at.% Ti-1.8 at.% Si alloy ion irradiated to 50 dpa at 925 K, voids with an average diameter of 74 nm and a number density of $1.6 \times 10^{19} \text{ m}^{-3}$ were formed. In addition, these voids were surrounded by an ~100 nm zone devoid of precipitates. EDS analysis showed that the zones devoid of precipitates were enriched with 3.5 at.% Si, while the precipitates were strongly enriched with Ti. It is worth noting that Ti was shown to effectively suppress void formation in many V alloy systems [22,41–43]. As a result, V alloys with Ti usually exhibit none or very few voids.

Cr: The solute element of Cr usually gives rise to a significant increase in void swelling in V. For example, the addition of 14.7 at.% Cr to V results in an increase in the void

swelling from <2.2% to >13% on ion irradiation to 50 dpa at 940–970 K [26]. The voids in the microstructure irradiated at 940 K have a disc shape with an average diameter of 190 nm and were believed to be composed of a high density ($\sim 10^{22} \text{ m}^{-3}$) of ~ 10 nm diameter voids. EDS results showed a significant depletion of Cr at the void surfaces at 940 K. However, in neutron-irradiated V-Cr binary alloys, Cr segregation to voids or cavities was observed or strongly indicated. For example, Matsui et al. [44] observed a significant segregation of Cr around cavities in a V-5 at.% Cr alloy irradiated to 4.5–15 dpa at temperatures ranging from 400 °C to 600 °C. In another study on a V-10Cr alloy irradiated to 14 dpa at 870 K, faceted voids with sizes from 5 to 100 nm were uniformly distributed, and the faceted morphology was attributed to Cr segregation to void surfaces [19].

Fe: Takeyama et al. [34] examined the microstructure of a V-3 at.% Fe sample fast neutron irradiated to $1 \times 10^{25} \text{ n/m}^2$ at 740 K, which included voids with different sizes. Large-void areas were observed with Fe strongly segregated to these areas. Therefore, a void formation mechanism was proposed: after the formation and growth of dislocation loops, RIS occurs preferentially on them, and voids are formed initially near the dislocations. Then, voids continue to grow with an increase in irradiation dose, while RIS occurs near the voids and new voids would be nucleated in a different area.

Ni: Ni segregation to void surfaces was suggested from a study by Gelles and Stubbins [21], where V-1Ni alloy was fast neutron irradiated to 31 dpa at 500 °C. A wide variation in void shape was observed as the voids are cuboidal with dodecahedral truncation. The degree of truncation on the specific truncation planes varies widely from void to void, suggesting segregation of Ni to the voids.

Nb: In a V-3 at.% Nb alloy neutron irradiated to $1 \times 10^{25} \text{ n/m}^2$ at 740 K [34], voids formed in clusters, surrounded by void-depleted area. Nb depletion was observed in regions with clustered voids, while areas without voids showed higher Nb concentration and relatively low dislocation density. The proposed mechanism for this behavior is as follows: dislocation loops initially form and grow with increasing irradiation dose, eventually leading to loop entanglement. This process causes Nb depletion near dislocation. In areas with higher high solute concentration, the mutual recombination of defects will be enhanced so that void nucleation and growth are retarded. On the other hand, in the tangled dislocation areas, voids will be formed by the effect of the dislocation bias. Thus, the colonial void distribution seems to appear.

Mo: The presence of Mo resulted in a decrease in void swelling of V [26]. The microstructure of ion irradiated a V-2.5 at.% Mo alloy showed no visible voids and an absence of irradiation-induced precipitates. EDS measurements indicated a slight depletion of Mo at void surfaces.

W: The addition of W reduces void swelling in V [26]. The microstructure of ion irradiated a V-2.5 at.% W alloy showed no voids or irradiation-induced precipitates. EDS measurements indicated a slight depletion of W at void surfaces. However, the segregation behavior of W may be affected by the presence of impurities of Si and S. In another study of a V-8.6W system neutron irradiated to a dose of 14 dpa at 870 K, a low density of voids was reported [19]. The voids showed two morphologies: small spherical voids and larger cuboidal voids, with the largest ones reaching about 50 nm. The cuboidal shape suggests solute coatings on these voids.

Finally, we summarized the segregation behavior of the most commonly studied solute or impurity atoms in V alloys in the Table 1.

Table 1. A summary of solute or impurity segregation tendency in V alloys with different radiation sources.

Elements	Grain Boundary (GB)	Sample Surface	Void Surface	Refs.
Ti	- No obvious GB segregation under ion irradiation - Obvious Ti enrichment at GBs under neutron irradiation	Enrichment of Ti at sample surfaces under ion irradiation	N/A	[26,27]
Cr	Both GB segregation and depletion of Cr were reported	- Enrichment of Cr was observed under ion irradiation - Transition to depletion at higher irradiation temperature	- Depletion of Cr at void surfaces under ion irradiation - Cr segregation to voids under neutron irradiation	[19,26,27,40,44]
Fe	No obvious GB segregation under ion irradiation	Fe enrichment at sample surfaces under ion irradiation	Strong Fe segregation to void surfaces under neutron irradiation	[26,34]
Ni	GB segregation of Ni under neutron irradiation	Ni enrichment at sample surfaces under ion irradiation	Ni segregation to void surfaces under neutron irradiation	[21,26,34]
Nb	N/A	N/A	Nb depletion in colonial void areas under neutron irradiation	[34]
Mo	Slight Mo depletion at GBs under ion irradiation	Mo depletion at sample surfaces under ion irradiation	Slight Mo depletion at void surfaces after ion irradiation.	[26]
W	Slight W depletion at GBs under ion irradiation	W depletion at sample surfaces under ion irradiation	Inconclusive: slight W depletion at void surfaces after ion irradiation, while W enrichment occurred after neutron irradiation	[19,26]
C	C enrichment at GBs under heat treatment	N/A	N/A	[17]
N	N enrichment at GBs after heat treatment	N/A	N/A	[17]
O	O depletion at GBs after heat treatment	N/A	N/A	[17]
Si	N/A	N/A	Si enrichment in areas surrounding voids in a V-Ti-Si alloy under ion irradiation	[17]
P	P enrichment at GBs after heat treatment	N/A	N/A	[17]
S	S enrichment at GBs after heat treatment	Inconclusive: both strong segregation and no segregation were reported for heat treated and irradiated conditions	N/A	[17,32,37,38]

2.4. Theoretical Calculations on Segregation Behavior

To complement experimental studies, theoretical calculations are always carried out to elucidate the fundamental mechanisms of elemental segregation in V alloys. Prior theoretical studies on segregation in V alloys have primarily relied on the first-principles density functional theory (DFT) calculations [10,28,45–49] and phenomenological models such as the diffusion model [50]. Although the RIS process is always difficult to model in these simulations, the segregation tendency of solute or impurity atoms in V alloys and associated mechanisms obtained from theoretical calculations at zero K still offers valuable information. In this review, we will primarily focus on discussing the prior DFT studies of solute segregation at V GBs.

The segregation tendency of solute or impurity segregation in V GBs can be evaluated by calculating their segregation energy, E_{Seg} , which can be simply calculated by $E_{\text{Seg}} = E_{\text{GB}}^{\text{X}} - E_{\text{Bulk}}^{\text{X}}$, where E_{GB}^{X} is the total energy of one solute (X) segregated at GB and $E_{\text{Bulk}}^{\text{X}}$ is the total energy of this solute located in the bulk region [51–53]. Based on this definition, a negative E_{Seg} value indicates a favorable segregation tendency of solute atoms to the GBs, while a positive E_{Seg} value suggests an unfavorable segregation tendency. The GB sites with positive E_{Seg} are also referred to as anti-segregation [51–53].

In addition to E_{Seg} , another physical quantity used to quantify the segregation tendency of solute atoms is segregation tendency energy, denoted as $E_{\text{Seg}}^{\text{T}}$ [28]. This quantity is calculated based on the average binding energies between solute atoms and GB sites. In this case, a positive $E_{\text{Seg}}^{\text{T}}$ represents a favorable segregation tendency, while a negative value suggests an unfavorable tendency. A comprehensive DFT study by Ko et al. [28] calculated $E_{\text{Seg}}^{\text{T}}$ for a wide range of metallic and nonmetallic elements across the periodic table based on the averaged values from $\Sigma 3(111)$ twin and $\Sigma 9(114)$ symmetric-tilt GBs. To better illustrate these results, we have extracted the $E_{\text{Seg}}^{\text{T}}$ values and presented them as a color map on the periodic table in Figure 3. Next, we will review and discuss the segregation behavior based on the $E_{\text{Seg}}^{\text{T}}$ map, along with other DFT studies on E_{Seg} , for all potential solute or impurity atoms in V alloys.

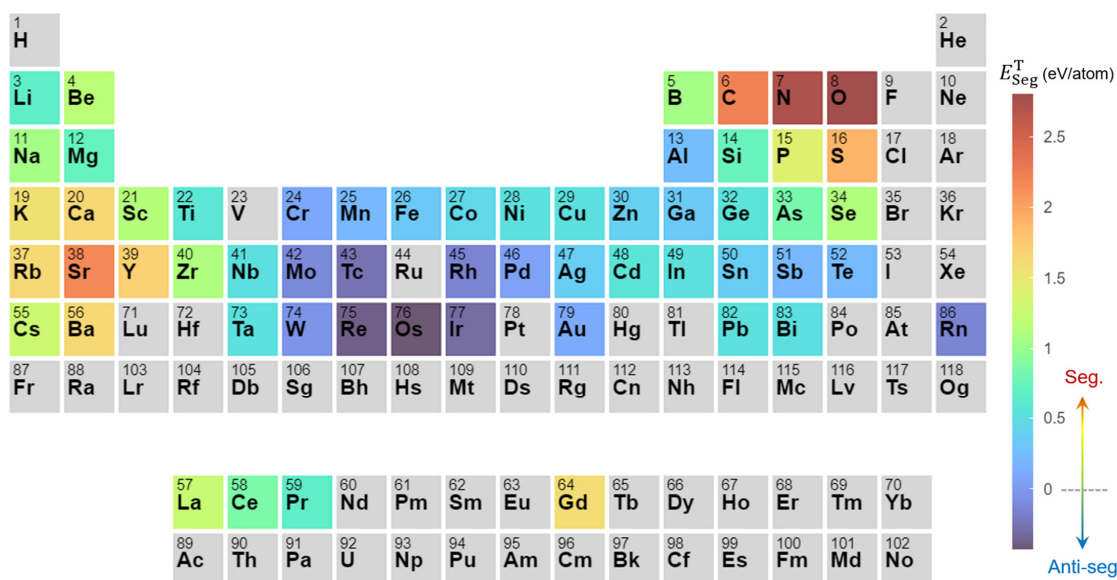


Figure 3. DFT-calculated segregation tendency energy, $E_{\text{Seg}}^{\text{T}}$, map for commonly studied metallic and nonmetallic elements across the periodic table at GB. The positive $E_{\text{Seg}}^{\text{T}}$ indicates a favorable segregation tendency, while negative values suggest an unfavorable segregation tendency. The $E_{\text{Seg}}^{\text{T}}$ values for most of the elements were reprinted with permission from Ref. [28], 2024 Elsevier, and the $E_{\text{Seg}}^{\text{T}}$ of B, C, N, and O were adapted from Ref. [46]. The atoms without available $E_{\text{Seg}}^{\text{T}}$ values are colored grey.

Hydrogen, helium, and alkali metals: Many theoretical studies have indicated that H or He elements have a strong tendency to segregate or diffuse to V GBs [54–58]. For instance, DFT calculations by Zhou et al. [54] have shown that the E_{Seg} of H and He at the interstitial sites in V $\Sigma 5(310)$ GBs are -0.29 eV/atom and -0.27 eV/atom, respectively. The negative E_{Seg} suggests that both atoms are favorable to segregate at the interstitial sites at V GBs. This behavior can be simply understood by the fact that GBs can provide more free volume, allowing these small atoms to be accommodated more easily compared to the bulk phases. Similarly, alkali metals such as Li, Na, K, Rb, and Cs exhibit an energetically favorable tendency to segregate at V GBs, as indicated by the positive $E_{\text{Seg}}^{\text{T}}$ values shown in Figure 3. Generally, $E_{\text{Seg}}^{\text{T}}$ tends to increase with the atomic numbers of alkali metals, with particularly large $E_{\text{Seg}}^{\text{T}}$ values observed for the Cs and K elements (>1.5 eV/atom).

Alkaline earth metals: The segregation behavior of alkaline earth elements at V GBs are typically seldom studied by experiments as these elements are either typically difficult to form alloys with V or difficult to be observed in experiments. Based on the DFT-calculated $E_{\text{Seg}}^{\text{T}}$ map shown in Figure 3, we can see that $E_{\text{Seg}}^{\text{T}}$ values of these elements are always positive, suggesting they are also highly favorable to segregate to V GBs. Among these elements, Sr has the strongest segregation tendency with a large $E_{\text{Seg}}^{\text{T}}$ value of 2.16 eV/atom, while Mg has the weakest segregation tendency with a low $E_{\text{Seg}}^{\text{T}}$ value of 0.74 eV/atom.

Transition metals: These metallic elements are typically from groups III to XII, and their segregation behaviors have been widely studied in V alloys through both experimental and computational modeling. As shown in Figure 3, the color map of $E_{\text{Seg}}^{\text{T}}$ shifts to green and blue within the transition metal regions, indicating a decreased segregation tendency compared to the elements from the first two groups (I and II). Yet, most of the transition metals are still favorable to segregate to V GBs due to their positive $E_{\text{Seg}}^{\text{T}}$. For instance, group III metals, such as Sc and Y, have large $E_{\text{Seg}}^{\text{T}}$ values of 1.12 eV/atom and 1.69 eV/atom, indicating their strong segregation tendency to V GBs. Furthermore, group IV and V elements also exhibit positive $E_{\text{Seg}}^{\text{T}}$, which implies that they are also favorable to segregate at V GBs. These DFT predictions perfectly align well with prior experimental observations, as summarized in Table 1. For instance, SEM experiments by Loomis et al. have shown that Ti segregation are commonly observed at the free surfaces and GBs [26], as well as other low-energy boundaries like twin boundaries in V-Ti alloys [59].

In addition, Figure 3 illustrates that DFT-calculated $E_{\text{Seg}}^{\text{T}}$ for group VI elements significantly decreases and even becomes negative for Mo (-0.11 eV/atom) and W (-0.04 eV/atom). These negative $E_{\text{Seg}}^{\text{T}}$ values suggest these elements are not energetically favorable to segregate at V GBs, which are in perfect agreement with experimental observations. For instance, Loomis et al. found no segregation of Mo and W at either free surfaces or GBs in V alloys [26]. Although W is unfavorable to segregate to GB, it is reported that W can segregate to dislocations, thereby changing the plastic behavior of V alloys. One explanation for their anti-segregation behavior at V GBs is their similar chemical properties to V, which likely causes these atoms to form a solid solution with the V matrix instead of segregating at V GBs. The low $E_{\text{Seg}}^{\text{T}}$ value for Cr atoms (~ 0.096 eV/atom) indicates its weak segregation tendency to V GBs, which is probably due to the similar chemical properties of Cr and V. This finding also aligns with prior experimental observations, where both enrichment or depletion of Cr at V GBs are both observed [26].

As we continue examining the $E_{\text{Seg}}^{\text{T}}$ map to the right within the transition metal regions in Figure 3, groups VII to VIII elements tend to display dark blue colors, which indicates a large negative value of their $E_{\text{Seg}}^{\text{T}}$. Thus, the transition metals from groups VII to VIII, such as Tc, Re, Os, and others, are highly unfavorable for segregation at V GBs. Interestingly,

within these groups, transition metals in the same period as V atoms, such as Mn and Fe, always have relatively higher segregation tendency (see Figure 3). Yet, the underlying mechanisms driving the different segregation pathways of Mn and Fe are still unclear, thus motivating future studies. Finally, transition metals from groups X to XII (e.g., Ni, Cu, Zn, and Ag) generally have positive $E_{\text{Seg}}^{\text{T}}$ values from around 0.3 to 0.5 eV/atom, suggesting a favorable tendency to segregate at the boundaries in V alloys.

Nonmetallic elements: The interfacial segregation of nonmetallic elements at V GBs has been extensively studied [16,26,48], as these elements often occur as impurities in V alloys. Generally, most nonmetallic elements show a strong tendency to segregate to V GBs, as illustrated in Figure 3. Among them, C, N, O, and S always exhibit very high DFT-calculated $E_{\text{Seg}}^{\text{T}}$ values [46], consistent with STEM observation in Figure 2. Instead of segregating into matrix sites of host element V, these nonmetallic elements are typically more likely to segregate into the interstitial sites at V GBs [10,45].

3. Solute or Impurity Effects on Mechanical Behaviors of Vanadium Alloys

Understanding the effects of solute or impurity atoms on the mechanical behavior of V alloys is important to optimize their properties for fusion applications. As we discussed in the prior section, the segregation of solute atoms or impurity atoms to defects changes the local chemistry and thermodynamics of these defects. Such interactions will significantly change the deformation and mechanical behavior of V alloys, such as strength, ductility, and hardness, as well as high-temperature creep behaviors. In addition, alloying elements can directly change the energy landscape of binary alloys, and thus alternating the mechanical behaviors. Section 3 primarily reviews the prior experimental and computational studies on the solute/impurity atoms and their interactions with other defects (e.g., GBs, precipitates) on mechanical behaviors of V alloys.

3.1. Strength and Hardness of Vanadiums Alloys

Ti: With the well-established development of Ti-Al-V alloys, particularly Ti-6Al-4Al, and their widespread lightweight applications in aerospace industries due to their excellent mechanical properties both at ambient and high temperature [60,61], there has been significant interests in studying the influence of the Ti element on the mechanical properties of V alloys. Consequently, the effect of Ti addition on the mechanical properties of V alloys has been widely investigated. It is typically found that increasing Ti additions enhances the ultimate tensile strength (UTS) and yield strength (YS) of V (Figure 4a) [29], while some studies show that the strength decreases and then increases with increasing Ti at higher Ti concentrations (1~3 wt.%) [62]. The observed result was attributed to the combined effects of precipitation, solid solution strengthening, and scavenging effects, and their contributions to the YS were theoretically estimated in high-purity V-4Cr-based alloys, as shown in Figure 4b [29]. Solid solution strengthening is found to be the predominant contributor, followed by GB strengthening and precipitation strengthening (Figure 4b). Particularly, Ti can scavenge the impurities in the V alloy matrix, such as C, O, and N, by forming Ti(CON) precipitates. It is found that a low concentration of Ti addition (1 wt.%) is sufficient to scavenge the impurities, while further increasing the Ti concentration does not significantly affect the precipitation strengthening.

Nb: Nb atoms always act as a strong solid solution strengthener for V [63]. V-Nb alloys show a classic solid solution behavior, though an unexplained ductility minimum occurs around 10% Nb. Similar strengthening behavior was also observed at low temperatures down to $-196\text{ }^{\circ}\text{C}$ [63]. In addition, twinning behavior in V-Nb alloys occurs in two regimes: low temperatures below $-196\text{ }^{\circ}\text{C}$ and high temperatures around $400\text{--}600\text{ }^{\circ}\text{C}$ due to dynamic strain aging, which elevates the UTS above the critical twinning stress

($\sim 690 \text{ MNm}^{-2}$). For Nb > 45%, twinning after large strains contributes to high ductility at -196°C , but ductility decreases with temperature, reaching a minimum at 900°C [63].

Other solute elements: In addition to Ti, the effects of various substitutional solutes (Nb, Cr, Mo, W, Ta, Fe, Ni, Zr, Hf, Al, Si, Y, and rare earths) have been evaluated [62]. All elements appear to act as effective strengtheners in V, with Ta, Fe, and Ni being the most effective and Cr being the least effective [62]. The effect of Ti seems to saturate at low levels, as has been discussed earlier. It is noted, however, that the database is not sufficient to define the hardening rate and saturation concentration for all the solutes. The spread in results also highlights the importance of investigating the microstructure and other variables, such as interstitial impurities, in the alloys.

Impurities (B, C, N, O, S, P): Due to its high affinity for interstitial impurities, the plasticity of V is highly sensitive to impurities like O and N. These impurities can strengthen V through solid solution strengthening while reducing the ductility at high concentrations [8,62,64–66]. The hardness of V is found to increase linearly with the O and N concentrations except at high O and N concentrations (4536 wppm of N or 9092 ppm of O) [32]. It is also found that the N element is two to three times more effective than O in strengthening V [32].

C atoms in solid solution can also enhance the strength of V; however, this effect diminishes at higher C concentrations due to the precipitation of V_2C [62]. Due to the relatively low solubility of C in V, the overall strengthening effect remains limited [62].

B elements are effective in grain refinement and enhancing the strength of V. Their impact is significantly strong at very low temperature (e.g., -196°C), but weakens at room temperature [62].

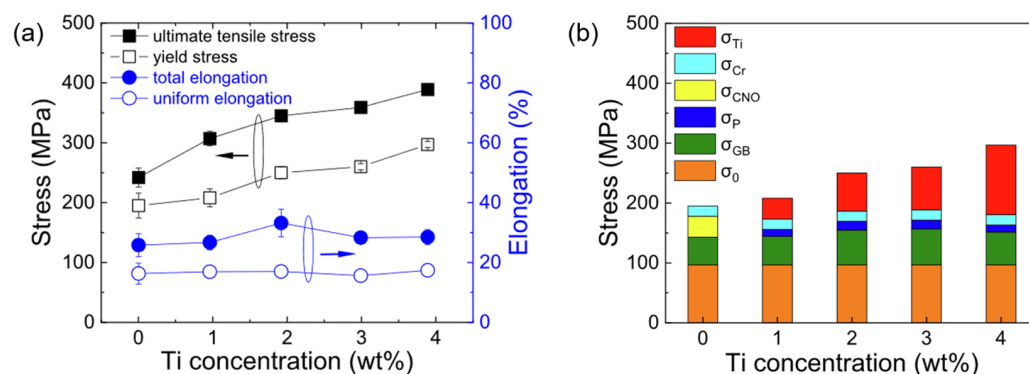


Figure 4. (a) Room temperature tensile properties of high-purity V-Cr-based alloys as a function of Ti concentration. (b) Strengthening contributions from different strengthening mechanisms. σ_0 : friction stress of single crystal vanadium, σ_{CNO} , σ_{Cr} , σ_{Ti} : solid solution strengthening, σ_{GB} : GB strengthening, and σ_P : precipitation strengthening. Panels (a,b) were reprinted with permission from Ref. [29]. 2024 Elsevier.

3.2. Ductility of Vanadiums Alloys

Alloying elements: The effects of Ti on the ductility of V are varied. At low Ti additions (<0.5%), ductility decreases [62]. Shen et al. reported that increasing Ti content (1–4 wt.%) increases the UTS of high-purity V-4Cr-based alloys but does not have a strong impact on elongation [29]. At higher Ti concentrations (10–40 wt.%), V-Ti alloys exhibit high ductility, and the Ti content has been found to have equal or less influence on ductility compared to the effects of heat treatment [62]. However, Ti additions can enhance the ductility of V alloys that initially exhibit very low ductility, such as hot-forged V [62]. This improvement is attributed to the scavenging effects of Ti, which (i) reduce the content of interstitial impurities in solid solutions and (ii) modify the distribution and morphology of precipitates [62].

Babitzke reported that the room temperature ductility of V-Nb alloys reaches a minimum at 10 at.% of Nb, although the reason for this behavior is unclear [67]. In contrast, Rajala and Van Thyne found that the ductility minimum of V occurs at 50 at.% Nb [68]. At high Nb concentrations, the ductility of V increases at $-196\text{ }^{\circ}\text{C}$ by promoting deformation twinning [63].

Similar to the effects of Ti, Zr increases the ductility of hot-forged V [62].

Cr, Mo, W, Hf, and Ta have been reported to reduce the ductility of V [62]. But the dataset on the effect of these alloying elements is limited.

In addition, Si, Al, and Y addition enhances the ductility of V-Ti-Cr alloys at irradiation temperatures around $400\text{ }^{\circ}\text{C}$ [69]. Si (up to 0.08 at.%) or Al (up to 0.3 at.%) have no obvious effect on V ductility at room temperature.

Impurities (B, H, C, N, O, S, P): V metals with low interstitial content are highly ductile at almost all temperatures [62]. Interstitial elements are the most important factor in determining the ductility of V. O and N elements have been found to decrease the ductility of V at and above room temperature [32], with a similar effect observed for B atoms [62]. At elevated temperatures, the maximum reduction in ductility was observed in the temperature range that promotes strain aging ($\sim 200\text{--}500\text{ }^{\circ}\text{C}$) [62]. Impurity elements also have substantial effects on the ductility of V at low temperatures. Dissolved H, C, O, and N at relatively low concentrations can raise the ductile-to-brittle transition temperature (DBTT) of unalloyed V to above room temperature, as discussed in the next session. H leads to catastrophic loss in ductility within an intermediate range of temperatures, which seems to be correlated to the hydride plate formation temperature [70]. When the temperature falls below from approximately $-75\text{ }^{\circ}\text{C}$ to $-100\text{ }^{\circ}\text{C}$, the ductility improves as the temperature drops and can become comparable to that of a material without hydrogen [71].

3.3. Ductile-to-Brittle Transition Behaviors in Vanadiums Alloys

The ductile-to-brittle transition behavior of V alloys is highly sensitive to the thermo-mechanical processing routes [17,72]. This sensitivity has been attributed to several factors: (1) incorporation of interstitial impurities such as O, N, and C, (2) precipitation processes that remove impurities from the solid solution, (3) impurity segregation at grain boundaries, and (4) the resulting grain size of the material [17].

Alloying elements: As observed in V, V-Ti, V-Ti-Si, and V-Cr-Ti systems, increasing Cr and Ti contents increases the DBTT [73]. V alloys with a total Cr and Ti content less than 10 wt.% do not exhibit ductile-to-brittle transition behavior above $-196\text{ }^{\circ}\text{C}$ [73]. With a high Cr content, V-15Cr-5Ti with higher Si content shows higher DBTT.

Impurities (H, C, N, O, S, P): The tensile stress-strain behavior of V demonstrates temperature-dependent ductile-to-brittle transition behavior, similar to that of other BCC metals [62]. Impurities, particularly O and H elements, can increase the ductile-to-brittle transition temperature (DBTT) of V [62,74]. Hydrogen concentration as low as 6 ppm effectively increases the DBTT of V [62]. In BCC metals, the segregation of light elements (C, O, H) to the core of screw dislocations increases the Peierls stresses, reducing dislocation mobility and contributing to embrittlement [75]. In addition, O solutes can interact with point defects in BCC metals and form ordered O-vacancy complexes that are highly stable [76]. The DBTT is found to be $20\text{ }^{\circ}\text{C}$ for pure V (99.95% purity) using small-punch test [74]. This transition temperature rises significantly with increasing O concentration, reaching $40\text{ }^{\circ}\text{C}$, $65\text{ }^{\circ}\text{C}$, and $135\text{ }^{\circ}\text{C}$ at $\sim 0.5\text{ at.}$, 1 at. , and 1.5 at. O, respectively [74]. Through detailed deformation microstructure characterization and in situ compression tests, Wang et al. found that an increase in O concentration increases the density of V-O complexes, which substantially reduce the density and mobility of screw dislocations [74]. This immobilization of dislocations below the DBTT leads to embrittlement. Conversely, the interaction

between V-O complexes and dislocations enhances high-temperature toughness above the DBTT, contributing to improved mechanical performance at elevated temperatures [74].

Segregation of impurities to GBs during thermo-mechanical processing influences the ductile to brittle transition behavior. Kurtz et al. [17] investigated the GB chemistry and Charpy impact properties of V-4Cr-Ti after different heat treatments. The results show that heat treatment at 1125 °C for 1 h resulted in measurable increases in S concentration at GBs and an increased DBTT. Subsequent aging at 890 °C for 24 h can restore toughness of V alloys by reducing S concentration at GBs and lowering interstitial solid solution levels through the formation of precipitates [17].

3.4. Creep Properties of Vanadiums Alloys

Alloying elements: Creep resistance is essential for V alloys in nuclear reactor systems operating, and their creep behaviors have been studied at elevated temperatures, typically from 300 °C to 1200 °C [77]. Compared to HT-9 and 316 stainless steels, the V-4Cr-4Ti alloy exhibits a higher creep strength, particularly at higher Larsen–Miller parameters (i.e., at high temperatures and/or long service times) [77]. In V-Ti binary alloys, increasing Ti content typically decreases the creep strength [62]. Work by Bohm and co-workers shows that, although the ultimate tensile strength continuously increases with increasing Ti content, the creep strength of V-Ti alloys increases up to 3 wt.% of Ti before declining with further Ti addition [62]. They also found that, at high Ti levels, the creep ductility becomes more sensitive to the test duration [62]. In addition, Cr can improve the creep strength of V alloys [9]. Co-addition of Zr and C significantly reduces the creep rate. Ternary V alloys containing Zr and C, such as VANSTAR-7, VANSTAR-8, and VANSTAR-9, are some of the most promising candidates for superior creep resistance.

Impurities (C, N, O, S, P): The creep properties of V and its alloys are sensitive to impurities, especially dissolved O atoms [77]. The creep rate shows significant changes, decreasing by 4–5 orders of magnitude as the O content increases from 220 to 750 ppm at 650 °C [62]. Purification of the V-4Cr-4Ti alloy by Zr-treatment decreases the creep strength and ultimate tensile strength and suppresses the effect of dynamic strain aging [78]. Precipitates containing interstitial impurities contribute to the high-temperature creep strength of V alloys with high O levels [78]. Increasing Cr content can offset the loss of creep strength due to high purification but increases the radiation-induced DBTT [78].

3.5. Mechanical Performance Under Irradiation

Although V alloys generally exhibit promising irradiation resistance at elevated temperatures, irradiation at low temperatures (200–400 °C) can lead to significant hardening and embrittlement, as shown in Figure 5 [69]. Recent studies have focused on understanding these mechanisms to improve alloy performance, emphasizing the control of impurities and optimizing alloy compositions to enhance irradiation tolerance [15]. Si, Al, and Y addition enhances the ductility of V-Ti-Cr alloys at irradiation temperatures around 400 °C (Figure 5) [69]. The reduction in elongation after low-temperature irradiation are primarily attributed to radiation-induced defect accumulation and the formation of precipitates enriched with interstitial impurities [69,78,79]. It is typically found that an increase in interstitial impurity level, particularly O concentration, decreases the uniform elongation after irradiation at 400 °C or lower [69].

In nuclear applications, V alloys are exposed to high-energy neutron fluxes, which leads to the generation of He within the alloy matrix. Understanding the influence of He on the mechanical degradation of vanadium alloys is critical for their viability in advanced nuclear technologies [7]. He element is also known to affect the mechanical properties of V alloys [69]. By investigating the tensile properties of pure V and V-based binary alloys

(V-Si, V-Ti, V-Cr, V-Fe, V-Nb and V-Mo) with and without He charging, Tanaka and Matsui found a strong correlation between He-induced embrittlement and apparent solid solution hardening, and atomic size factors of solute atoms [69]. He-induced apparent solid solution hardening is largest for alloys with strongly under-sized solutes (e.g., Fe, Si, Cr) and is lowest for pure V or alloys with weakly over-sized solutes (e.g., Mo, Ti). The dependence of reduction in ductility by He on atomic size factor shows a similar trend. V alloys with Ti showed maximum He embrittlement and a completely brittle failure behavior through transgranular fracture. Although He-induced dislocation loops and bubbles contribute to the observed hardening, the major source of hardening is believed to be He clusters. The observed effects of atomic size factor on hardening and ductility loss suggest that under-sized solutes have a stronger binding energy with He, resulting in high He cluster density in the matrix and a lower He population of GBs.

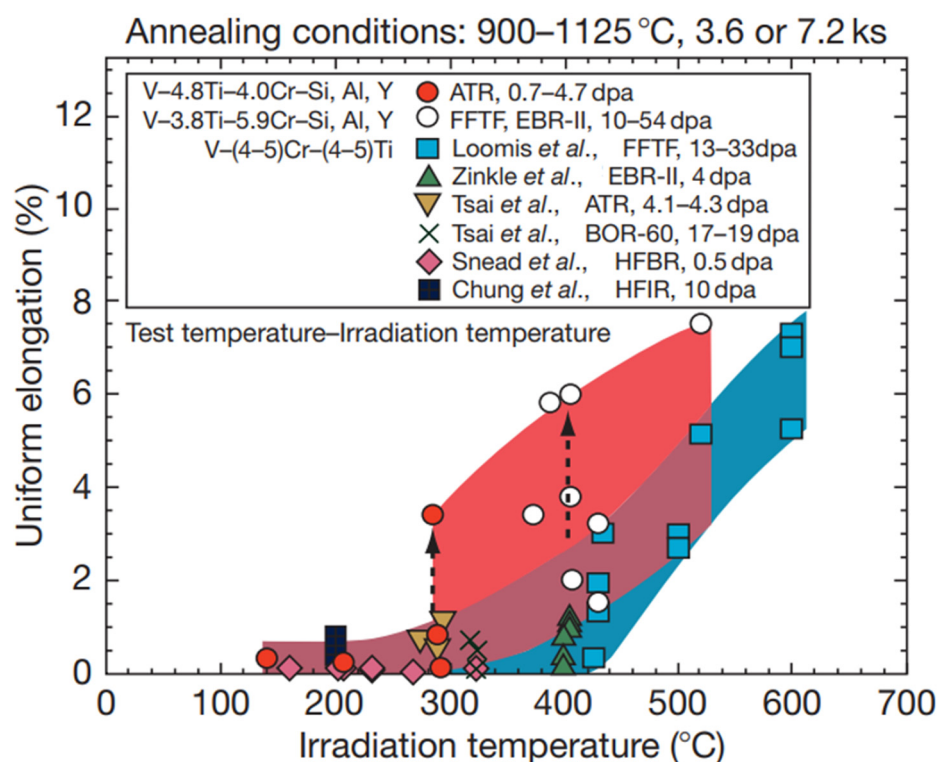


Figure 5. Uniform elongation of V alloys under different irradiation temperatures for V-Cr-Ti alloys (Reprinted with permission from Ref. [69], 2024 Elsevier). This reproduced figure was also extracted from Ref. [7] with permission.

Several recent studies [80,81] showed that irradiation enhances the hardening behavior of V-Cr-Ti alloys with a small addition of Ti elements. Further analysis based on TEM/APT experiments revealed that this improvement is attributed to the formation of irradiation-induced Ti(CON) precipitates [80,81], which is also supported by dispersed barrier-hardening theory.

3.6. Theoretical Calculations of Solute or Impurity Effects on Mechanical Behavior of Vanadium

Many theoretical studies have been carried out to understand the fundamental mechanisms by which solute or impurity atoms change the mechanical behaviors of V alloys. As discussed in prior sections, the segregation of solute or impurity atoms to GBs and sample surfaces is a pervasive phenomenon in V alloys and plays a significant role in controlling their mechanical properties. In a nice review paper by Zhang *et al.* [10], the solute-defect interactions in V and its alloys are thoroughly discussed, with a particular focus on solute

interaction with defects in the bulk phase of V. In this Review, we will primarily focus on the theoretical studies regarding how interfacial segregation of solute or impurity affects the mechanical properties of GBs in V alloys.

Hydrogen, helium, and alkali metals: Due to small atomic sizes, H and He elements are well-known segregators to the interstitial site in the GBs of V alloys [54–58], as discussed in Section 3.5. The segregation of H and He elements to GBs plays significant roles in altering the GB mechanical behaviors of V alloys. For instance, DFT calculations indicate that H segregation reduces the GB strength of V, and lowers its fracture energy by weakening the strengths of interfacial V–V bonds, thereby degrading the mechanical performance of V GBs [54]. Similarly, the segregation of He embrittles V GBs by weakening the interfacial bonding strength based on DFT calculations [58]. Furthermore, He segregation can also increase the sliding energy barrier of V GBs, thus inhibiting their migration ability [55]. For alkali elements, such as Li, Na, K, Rb, and Cs, they are favorable to segregation to V GBs due to their small volume, but their effects on GB strength are still less explored, which motivates future studies.

Transition metals: The effects of transition metals segregation on the mechanical behaviors of V GBs are complex and can vary depending on the specific solute atoms and GB structures. DFT cohesion energy calculations show that group III to V elements, such as Ti, Zr, Hf, Nb, and Ta tend to enhance the GB cohesion of both $\Sigma 3(111)$ twin and $\Sigma 5(210)$ symmetric-tilt GBs [47,48]. Group VI to X elements, including Cr, Mn, Fe, Co, and Ni, often have detrimental effects on the GB strength of $\Sigma 3(111)$ twin boundaries, but can positively improve the GB cohesion in $\Sigma 5(210)$ symmetric-tilt GB [47,48]. Mo and W, which exhibit negative E_{Seg}^T (Figure 3), are generally identified as GB embrittlers. This is because the larger atomic radius of these atoms leads to significant lattice mismatch and GB volume expansions once they segregated at V GBs. Although some experimental studies have suggested that Cr elements are not favorable for enhancing the ductile behavior of V [62], a DFT study by Pan et al. indicated that Cr and Fe can improve V ductility by contributing more electrons to form metallic bonds with V atoms [82].

Nonmetallic elements: Nonmetallic elements, such as O, N, B, S and others, typically have substantial impact on the mechanical behavior of V GBs. For instance, the segregation of O and S atoms at V GBs can reduce GB strength, thereby leading to GB embrittlement [46]. Similarly, Si is favorable to segregate to V GBs, but it has a relatively weaker tendency to embrittle V GBs compared to the O and S atoms [46]. In contrast, DFT calculations have shown that other nonmetallic elements, such as C, N, and B, play as GB cohesion in V alloys [46,82]. The GB strengthening by solute can be clearly seen in the DFT-calculated stress–strain curves as shown in Figure 6a, although such effects become weak in relaxed GB (Figure 6b). One explanation is that their unique chemical bonding, which exhibits both covalent and ionic characteristics, contributes to high stiffness and enhanced resistance to shear deformation in V alloys. Yet, a downside of these elements is their tendency to reduce the ductility of V alloys.

The effect of elemental segregation on the mechanical behavior of V GBs also depends on the specific atomic sites where solute or impurity atoms segregated at GBs. Ko et al. [28] performed a DFT-based tensile test and studied the deformation of the V twin boundary with different solute atoms at different atomic sites. As shown in Figure 6c,d, the segregation of the solute atom at site 2 at the V twin boundary is typically favorable to enhance GB strength, but segregation to site 1 is detrimental to GB strength. This finding suggests that the precise control of segregation structure at GBs could be an effective engineering strategy for enhancing interfacial strength of V alloys.

By examining Figure 6a–d, a clear difference in the stress–strain curves is observed, even for pristine V metals without any solutes. Such a difference is probably due to the

use of different GB bicrystal models in these studies. Specifically, twin boundaries with different thickness exhibit different deformation behavior (e.g., strain) for a given loading distance. Furthermore, GB thickness can change the strength of GBs due to the boundary interactions, particularly for the DFT calculations that use a relatively small simulation cell with periodic boundary conditions. These factors may account for the different stress–strain curves observed in Figure 6a–d.

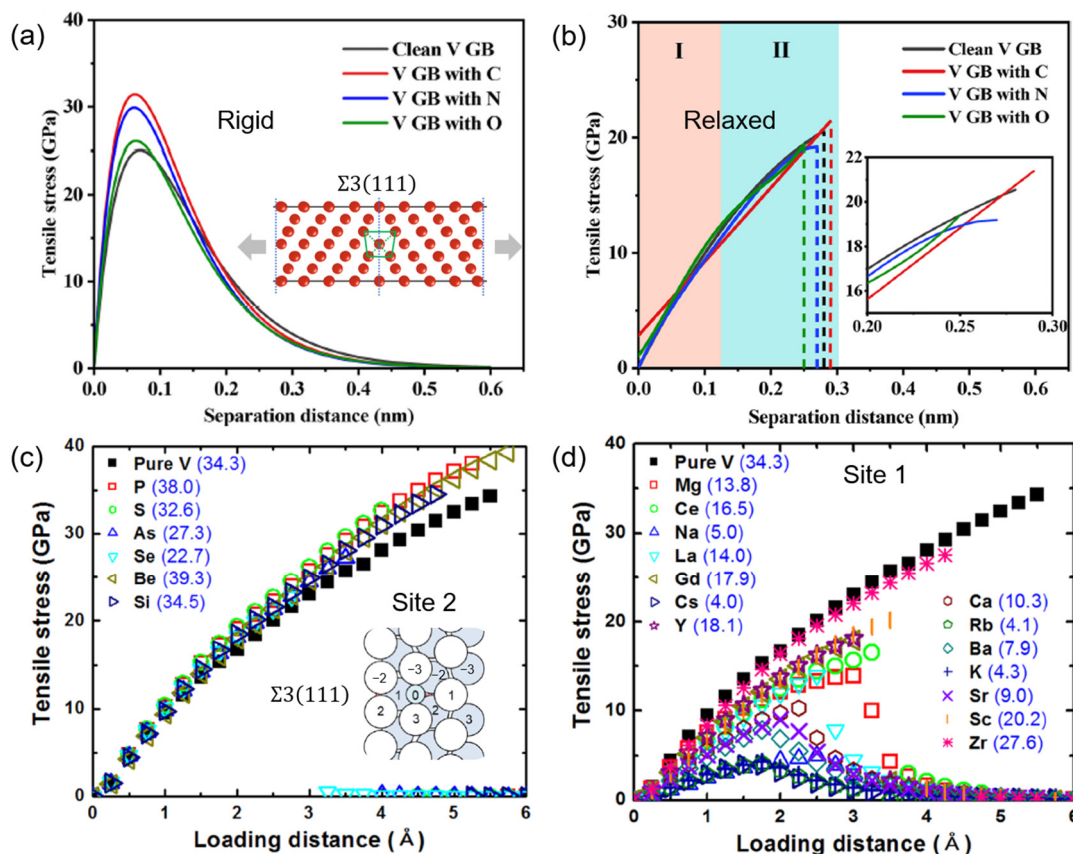


Figure 6. DFT tensile test of $\Sigma 3(111)$ twin with various solute segregation at (a) rigid GB and (b) relaxed GB. In panel (b), regions I and II represent different stage of tensile simulation, and dashed lines indicate fracture regions. DFT tensile tests of the same twin boundary with different solute or impurity atoms segregated at (c) site 2 position and (d) site 1 position. Panels (a,b) were reprinted with permission from Ref. [82], 2024 Elsevier and panels (c,d) were reprinted with permission from Ref. [28], 2024 Elsevier.

4. Solute or Impurity Effects on Microstructure Evolution of Vanadium Alloys

Section 3 discusses the effects of solute and impurity atoms on the mechanical behaviors of V alloys. Beyond the atomistic-level mechanisms of these effects, changes in the mechanical properties (e.g., strength, hardness, ductility, and other) are also closely related to the microstructure resulting from the presence of solute or impurity atoms. In this section, we will briefly review the effects of solute or impurity atoms on the microstructural evolutionary behaviors of V alloys.

4.1. Grain Growth Inhibition

One notable effect of solutes or impurities on the microstructural evolution of V alloys is the inhibition of grain growth through several mechanisms. The first mechanism involves the formation of precipitates, where excess solute atoms combine with impurities (e.g., C, O, N atoms) to form secondary phase particles that hinder grain growth in V alloys. For

instance, in V-Cr-Ti alloys, a graduate increase in Ti content reduces the grain size of V alloys due to the formation of Ti-rich precipitates; see Figure 7a–c [29]. Similar phenomena have been observed with the addition of Y [83–85] and La elements [86]. The second mechanism relates to GB segregation, where segregated solutes or impurities can retard GB migration and reduce their free energies, thereby inhibiting grain growth. This phenomenon has been widely studied in nanocrystalline alloys [87–89]. However, to the best of our knowledge, few studies have specifically examined the impact of solute or impurity segregation on GB migration in nanocrystalline V alloys.

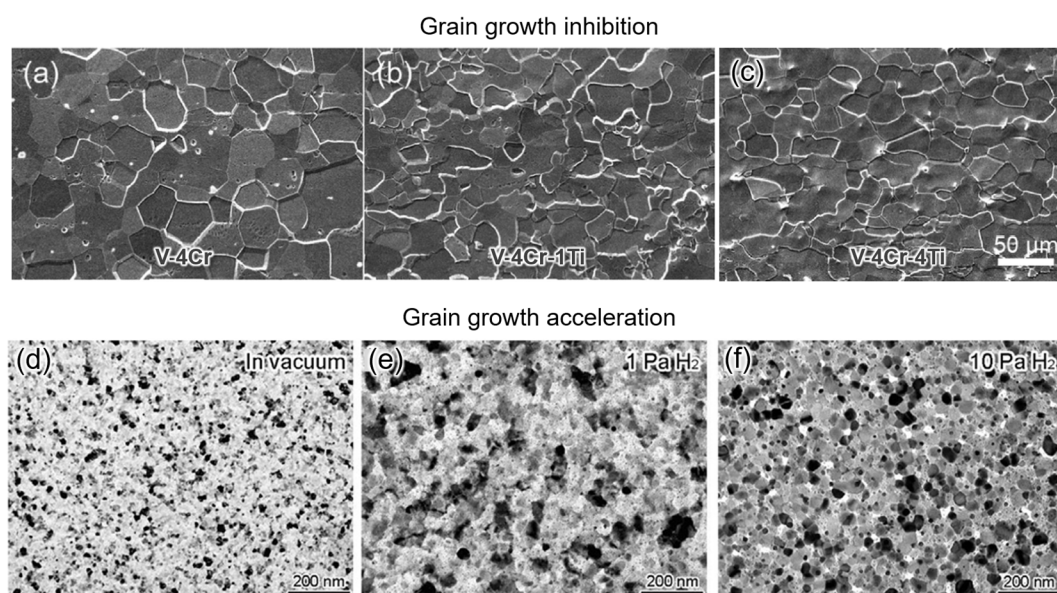


Figure 7. SEM images of microstructures of three V-Cr-Ti alloys: (a) V-4Cr, (b) V-4Cr-1Ti, and (c) V-4Cr-4Ti. TEM images of grain growth in vanadium thin films with different H₂ gas pressure: (d) in vacuum, (e) 1 Pa H₂, and (f) 10 Pa H₂. Panels (a–c) were reprinted with permission from Ref. [29], 2024 Elsevier, panels (d–f) were reprinted with permission from Ref. [90], 2024 Elsevier.

4.2. Grain Growth Acceleration

Although solutes or impurities typically hinder the grain growth of V alloys, they can, in some cases, accelerate it. For instance, unlike typical solute or impurity atoms, H is always treated as an interstitial solute due to its small atomic sizes. This unique feature causes H elements to behave quite differently in V alloy. An interesting study by Martin et al. [90] found that the V alloys exhibit enhanced grain growth behaviors in the presence of an H environment and finally stabilize at high H content; see Figure 7d–f. They further explained that the increased GB mobility is ascribed to the reduced formation energy of ledges or steps by the H element, rather than GB segregation.

4.3. Precipitation Morphology with Solute or Impurity

Solute or impurity atoms can significantly influence the morphology of microstructural features, especially precipitates in V alloys. With the advancement of electron microscopic techniques, atomistic details of the local structure and chemical composition of these precipitates can be clearly characterized. In this section, we discuss recent TEM/STEM studies on exploring the nanostructures of precipitates in V alloys.

Ti-rich precipitates typically exhibit a long, needle-like morphology [86], and Figure 8a shows STEM images and EDS mapping of representative precipitates with an elongated shape in a V-4Cr-4Ti alloy. When La was introduced to this alloy system, these Ti-rich precipitates became smaller, and were barely visible when the weight fraction of La is equal to or higher than 0.5% [86]. In addition to La, other solute elements can affect the

morphology and/or elemental distribution of precipitates in V alloys. For instance, in V-Cr-Ti alloys with Y addition, STEM experiments indicated the formation of nanoprecipitates with a core-shell structure; see Figure 8b. In this case, the precipitate interior is enriched with Y, while Ti atoms are favorable to segregate to the interfacial region between the Y-rich precipitate and V matrix [84] (Figure 8b).

In a cold-rolled V-Ni alloy followed by thermal annealing, Ni dendritic segregation gives rise to formation of dendrite-like precipitates [91], which affect the deformation behaviors of V alloys. However, Ni dendrite precipitates are not observed in V-Cr-Ti-Ni alloy [92]. Instead, Ni forms spherical nanoparticles in the VCr-rich phases [92]; see Figure 8c. Another interesting microstructure is found in V-4(Al-5Ti-B) alloys, where slender, needle-like TiB precipitates have been pervasively observed (Figure 8d).

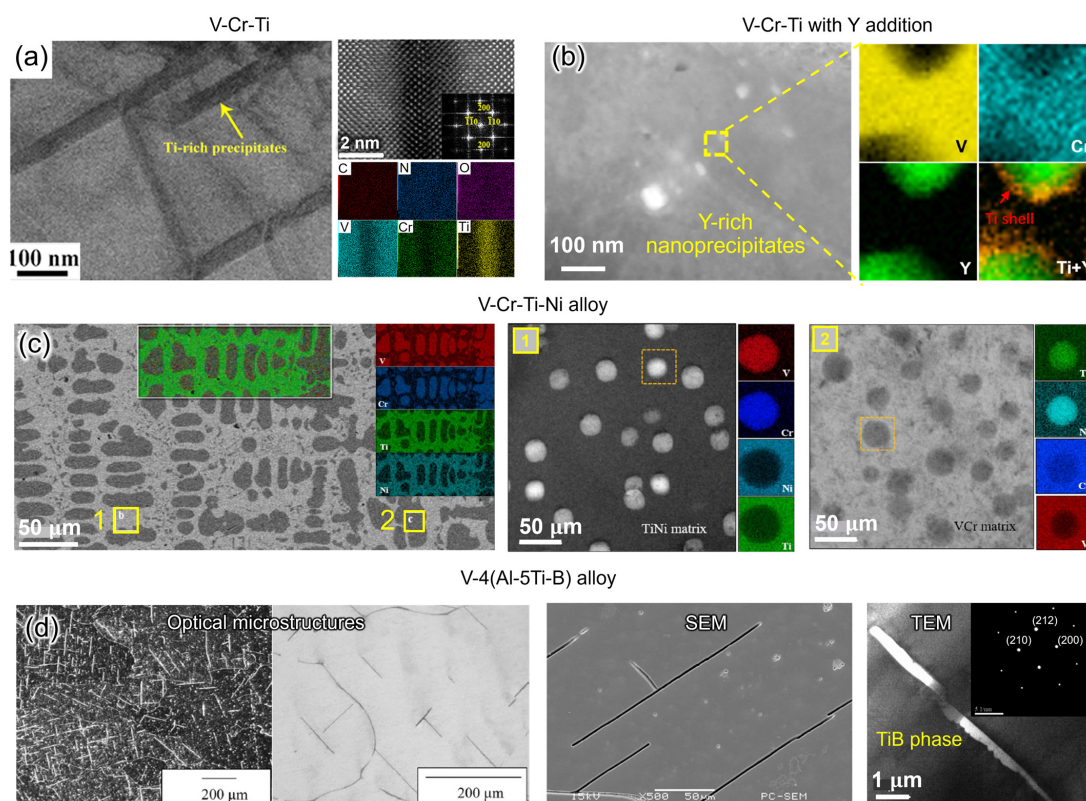


Figure 8. Precipitate morphology with solute or impurity effects: (a) Ti-rich precipitates in a V-Cr-Ti-La system [86], (b) nanoprecipitates with a core-shell structure where the interior is Y-rich and Ti segregates at precipitates/matrix interfaces [84], (c) Spherical nanoparticles in VCr-rich phases in V-Cr-Ti-Ni alloy [92]. The yellow boxes, labelled 1 and 2, respectively represent the TiNi matrix and VCr matrix, and their corresponding zoom-in SEM images with EDX mapping are shown in right panels, (d) optical microstructure of V-4(Al-5Ti-B) alloy with slender needle-like TiB precipitates characterized by SEM and TEM images [93]. Panel (a) was reprinted with permission from Ref. [86], 2024 Elsevier; panel (b) was reprinted from Ref. [84]; panel (c) was reprinted with permission from Ref. [92], 2024 Elsevier; panel (d) was reprinted with permission from Ref. [93], 2024 Elsevier.

5. Manufacturing of Vanadium Alloys

The microstructures of V and its alloys are closely controlled by the manufacturing process through the process-structure link. To achieve the designed microstructures and properties, both conventional alloy processing methods and advanced manufacturing techniques can be employed. This review will briefly discuss the current status and challenges for existing manufacturing processes for fabricating V alloys, as shown in Figure 9.

5.1. Conventional Manufacturing of Vanadium Alloys

The manufacturing constraints of V alloys have significantly limited the wide application of V alloys in fusion reactors. Historically, from the late 1990s until early 2010s, major efforts of V alloys manufacturing were focused on scale-up production through a conventional casting and forging approach [2], while the focus has shifted towards the advanced manufacturing, aiming at rapid prototyping, high materials usage, and low cost [94].

Ingots metallurgical process: One of the most employed metallurgical processes for V alloys is casting. In this process, the V sample is electron-beam melted and casted into ingots and then subjected to post-processes in various temperature or atmospheres to improve homogeneity [95–97]. The critical issues for casting are the impurities introduced during fabrication processes, such as O and N [32]. As discussed in Section 3, O and N elements are highly favorable to interact and segregate to the defects, thus these impurities are typically detrimental to V alloys' properties. Specifically, N was found to increase the hardness of V alloy threefold compared to O, as described by Jo's finding [32]. Ductility or elongation reduced while increasing O and N. Therefore, to mitigate the O and N absorption, the fabrication process should be protected under a vacuum. For instance, the high purification of NIFS-HEAT-2 [98] significantly enhanced weldability, workability, and low-activation characteristics, while maintaining comparable high-temperature creep properties under service stresses.

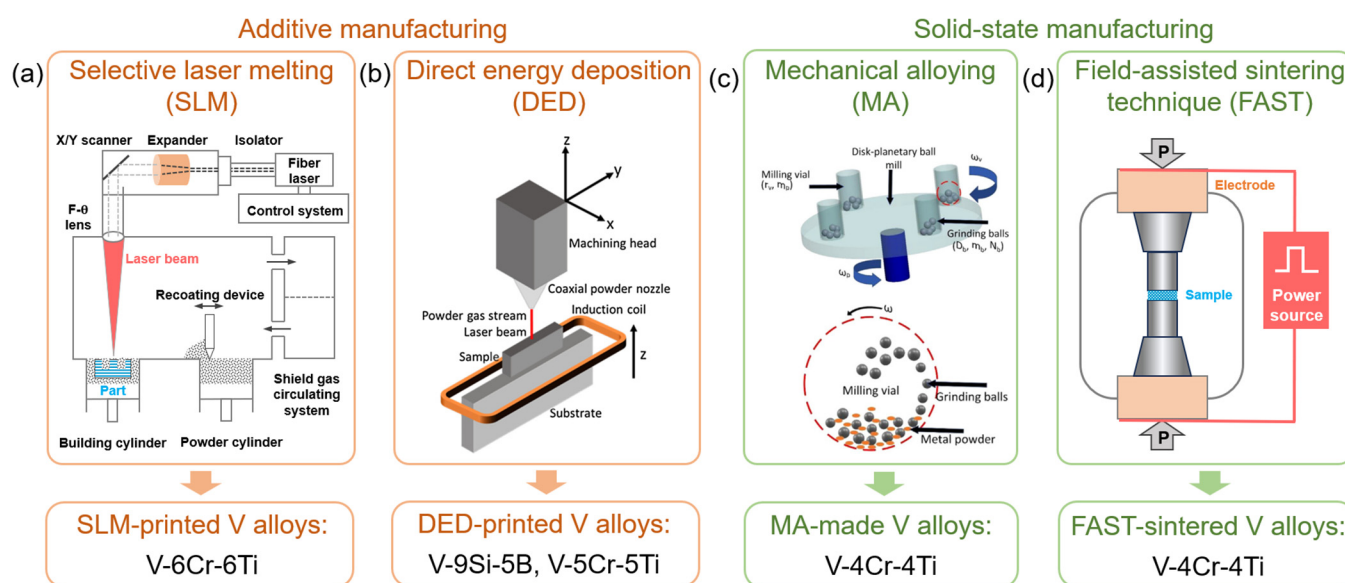


Figure 9. Additive manufacturing (AM) of V alloys. (a) Schematic of selective laser melting (SLM) AM, which has been adopted for printing V-6Cr-6Ti alloy. (b) Schematic of direct energy deposition (DED) AM, which has been used to print V-9Si-5B alloys. Solid-state manufacturing of V alloys. (c) Schematic of mechanical alloying (MA) [99] for fabricating fine powders of V alloys for AM and other sintering techniques. (d) Schematic of field-assisted sintering technique (FAST), which can rapidly sinter V alloys such as V-4Cr-4Ti [100]. Panel (a) was reprinted with permission from Ref. [101], 2024 Elsevier, and panels (b,c) were reprinted with permission from Refs. [102,103], 2024 Elsevier.

Post-processing: Relatively few studies have explored the microstructure evolution during post-processing steps of V alloys. Li et al. [104] investigated the microstructure and properties of V-5Cr-5Ti alloy after hot forging, observing that the forging process broke the alloy's microstructure into axial grains with an average grain size of 80 μm through deformation strain and dynamic recrystallization. Additionally, acicular or flake precipitates were transformed to short strips or elliptical-shaped $(\text{VTi})_2(\text{CON})$ precipitates. Fan studied the microstructure and mechanical properties of V-5Cr-5Ti alloy after high-

pressure torsion. It was determined that the subgrain size of the V alloy decreases with shear deformation until a certain value and no further reduction is observed [105].

Welding: Welding for V alloys is highly challenging due to the possible contamination, and precautions and shielding are needed, with some initial trials been investigated on V alloys. Successful welding of V alloys has been achieved through gas tungsten arc (GTA) [106,107] and it has been found that reducing O and N levels can decrease the DBTT, through groove box or O getter [108]. Laser welding [109,110] was tested through bead-on-plate welds, indicating comparable impact absorption energy in the weld metal and the base metal, and successful laser welding has been performed [111] on V-4Cr-4Ti alloy. Electron beam welding [112] was applied to V-4Ti-4Cr alloys (NIFS-HEAT-2) and CEA-J57, resulting in weld metal superior impact properties compared with base metals, demonstrating ductile modes of fracture. Dissimilar metal bonding by hot isostatic pressing (HIP) [113] was used to bond dissimilar metals, joining carbide-dispersion strengthened V alloy with the conventional V-4Cr-4Ti alloy, showing good bonding property with sound strength and ductility. Further systematic investigation on welding without contamination will be needed for the manufacturing of V alloys.

5.2. Advanced Manufacturing of Vanadium Alloys

In addition to the conventional wrought alloy manufacturing process, advanced manufacturing has attracted attention for fabricating V alloys, particularly due to the severe challenges associated with their production and manufacturing. This section briefly summarizes the research efforts in melting-based additive manufacturing and solid-state manufacturing approaches for V alloy in the last decade.

Additive manufacturing (AM): AM has been booming in the last decade due to its advantages of rapid prototyping and materials efficiency [114]. To date, V alloys have been fabricated by various AM techniques, including selective laser melting (SLM) [114], direct energy deposition (DED) [115], and laser melting deposition (LMD) [116]. We will briefly discuss the AM studies on V alloys below.

SLM, also known as laser powder bed fusion (L-PBF), is one of the most widely studied metal AM processes. It uses a high power-density laser to rapidly melt and fuse power particles together; see Figure 9a. Liu et al. [117] studied the manufacturing feasibility and forming properties of V-6Cr-6Ti alloy by SLM, and found that the SML was able to produce relatively high density vanadium alloys with an irregular power particle shape and a wide range of particle size. Yang and Li compared the feedstock preparation methods, including dry grinding, wet grinding, and mechanical milling for SLM of V₅Cr₅Ti alloy [94,118], and found that the dry grinding method is superior in producing spherical powder among three methods. Using the same high-energy ball milling approach, Yang [94] achieved pre-alloy V-6Cr-6Ti powders with near-sphere morphology and an average size of 20 µm, and successfully printed this V alloy through SLM. The AM-printed V alloy exhibited a strong texture feature with ultrafine grain size and a complete alloy reaction among V, Cr, and Ti elements. These features significantly improve the mechanical properties of AM-printed V alloy more than conventionally processed V alloys.

Despite the advantages mentioned above, SLM of V alloys can introduce additional impurity elements, such as O and N, during the printing process, as already observed in other alloy systems [119,120]. However, comprehensive measurements of these impurity levels are still lacking, thus worthy for future studies.

Different from SLM, DED uses their unique power distribution system to print parts on melting materials as they are being deposited [115]; see Figure 9b. Schmelzer et al. [102] investigated the printability and microstructure evolution of another class of V alloy, the near-eutectic three-phase V-9Si-5B alloy, through DED. The powder feedstock was success-

fully produced via argon gas atomization from non-pre-alloyed solid raw materials. With optimized printing parameters, cracking-free samples were printed, resulting in a very fine ternary eutectic microstructure. After appropriate heat treatment, the microstructure exhibited balanced properties by forming a solid solution BCC V matrix with homogeneously distributed V_3Si and V_5SiB_2 phases, achieving a room temperature hardness of 754 ± 40 HV 0.1, and comparable creep performance at 900 °C, with slightly higher steady-state creep rate compared to ingot metallurgy or powder metallurgy produced V-9Si-13B alloys and superalloy CMSX-4. Yet, Zr contamination, suspected to originate from the crucible during gas atomization, was observed [102].

LMD is one of the branches of DED, which combines laser and powder processing to enhance materials utilization [116]. Bai et al. [15] studied the grain morphologies and microstructures for LMD-fabricated V-5Cr-5Ti thin wall from powders prepared via plasma rotating electrode process, which yields sphere shapes with an approximate 200 μm powder size. The impurity level in the samples remains similar before and after the LMD process, except for increased contents of Fe and C from residual steel powder, and O from the atmosphere. LMD-printed samples exhibited a dense structure without obvious pores or cracks. Both columnar dendrites and equiaxed grains were observed within the thin wall samples, and their proportion, morphologies, and textures can be altered by adjusting the scanning strategy, laser power, and deposition duration, all of which influenced the solidification mode and heat flux direction. Chai et al. [12] demonstrated that a uniform solid solution can be achieved by solution treating the LMD-AM deposited V-5Cr-5Ti alloy at 1560 °C for 1 h, and precipitate could form during follow-on annealing heat treatment from 800 °C to 1200 °C, resulting in improved hardness.

Solid-state fabrication: Solid-state fabrication of metals can be broadly classified into two categories: mechanical alloys (MA) and field-assisted sintering techniques (FAST), both of which have been applied to V alloys. MA is an effective approach to control the grain morphology of a V matrix by incorporating additional particles; Figure 9c [121–124]. This method is widely used to produce feedstock powder for various AM processes, such as SLM, DED, and LMD [94,99,117,118]. Moreover, the additional particles mixed into V alloys can significantly influence the properties of V alloys. For instance, Zheng et al. [99] systematically studied the hardening effects of three carbide nanoparticles (e.g., TiC, SiC, and Ti_3SiC_2) on V-4Cr-4Ti alloys with Y through a combinatorial process of MA, HIP, and high-temperature annealing. While these particles are not completely dissolved during the MA process, Ti_3SiC_2 is the most effective hardening particle for V alloys.

FAST is another solid-state manufacturing process which applies electric fields/currents to rapidly heat specimens and produce highly dense materials with minimal grain growth and clean GBs [125–127]; see Figure 9d. This method is advantageous for fabricating V alloys with improved high-temperature mechanical properties. Krishnan and Sinnaeruvadi [100] adopted FAST to sinter V-4Cr-4Ti alloys at 1050 °C and 1100 °C, using both unmilled and milled powders. The relative densities range from 88% to 100% for unmilled powder and from 93% to 100% for milled powder. The resulting relative densities were very well corrected with increasing sintering time and sintering temperature, while the hardness of sintered specimens, ranging from 535 Hv to 585 Hv, also increases with sintering time, temperature, and relative density. It is also noted that unmilled powder results in V-4Cr-4Ti composite (V matrix with Cr and Ti particles) after sintering, and single-phase V alloys were achieved with milled powder, indicating that ball milling is an essential step for alloying the elements in V alloys.

6. Future Perspectives

6.1. Experimental Studies on Vanadium Alloys

- **Nanocrystalline vanadium alloys:** Nanocrystalline alloys always exhibit excellent thermal stability [87–89]. Since YS is inversely dependent on grain sizes, developing V alloys with nanosized grains can give rise to much stronger materials. Furthermore, segregation of certain solute elements to GBs can effectively stabilize the nanocrystalline structure due to thermodynamic and/or kinetic stabilization effects. As a result, the high-temperature strength of V alloys can be significantly improved, allowing a much wider operating window for fusion reactor applications.
- **Mechanical performance in extreme environments:** Thermal creep performance, helium embrittlement, and irradiation embrittlement are critical issues that dictate the operational temperature limits of V-based alloys, particularly in nuclear applications. Further investigation is necessary to understand these phenomena under extreme environments, supported by the fast development of materials testing and characterization techniques, and explore the potential for expanding operational temperature ranges through the development of improved alloys.
- **High-entropy (HE) vanadium alloys:** Due to the large compositional space, high-entropy alloys (HEAs) appear to exhibit exceptional mechanical properties and performance [128–130]. Designing V-based HEAs may be a new design strategy to overcome the current issues of V alloys for fusion energy applications [30,131–134].
- **Advanced manufacturing (AM) of vanadium alloys:** Owing to the rapid prototyping capability of AM, there is an increase in research interests in applying AM techniques to fabricate existing or develop novel V alloys. More research is needed to investigate the resulting microstructure and performance of V alloys compared to those produced by conventional electron-beam melting and wrought approaches and optimize the best procedure.

6.2. Theoretical and Computational Studies on Vanadium Alloys

- **First-principles calculations:** DFT calculations are extensively used to investigate the fundamental mechanisms of solute effects on mechanical properties and their segregation behaviors. For GB segregation, most prior DFT studies calculated the E_{Seg} of solute atoms based on highly simplified boundary structures, such as $\Sigma 3(111)$ twin boundary and $\Sigma 5(210)$ or (310) symmetric-tilt GBs [28,46,47,54,82]. However, in real polycrystalline V alloys, the majority of GBs are asymmetric and randomly distributed. Therefore, future computational research should focus on the segregation behaviors at random and general GBs, such as asymmetric boundaries.
- **Atomistic simulations:** Although DFT calculations can predict the segregation tendencies of solute or impurity atoms to defect regions, such as GBs, they are typically performed at zero (0) K and in the dilute limit. Moreover, the high computational cost of DFT calculations restrict simulation to small cells, containing only tens to a few hundreds of atoms. To investigate segregation behavior at more realistic conditions (e.g., 700 °C in fusion reactors), atomistic simulations using hybrid Monte Carlo/molecular dynamic (MC/MD) simulations at NVT or NPT ensembles are highly necessary for studying segregation behaviors at random GBs.
- **Machine learning/artificial intelligence (ML/AI):** For MD simulations, accurate interatomic potentials (IAPs) are essential. However, there are not many existing IAPs for V-related systems on the NIST website [135,136]. The classical IAPs, such as the embedded atom method (EAM) and modified EAM (MEAM), may not be sufficiently accurate for predicting materials properties of V alloys. Therefore, developing ML-

based IAPs, such as SNAP, MTP, and DLP, is a promising research direction for future atomistic modeling of V alloys.

- ML/AI techniques can be also applied to predict convoluted structure–property–processing relationships in V alloys, especially in multicomponent (e.g., high-entropy) V alloys with large compositional spaces [137]. Since a high-fidelity materials database is the foundation of any ML study, developing high-throughput computational frameworks for DFT and MD simulations is necessary.
- **CALPHAD and ICME approach:** CALPHAD is one of the most widely used theoretical methods for alloy design. With the advances of integrated computational materials engineering (ICME) [138], the multiscale materials simulations method can be integrated to CALPHAD to accelerate the development of advanced V alloys with improved interfacial properties and decipher the structure–property–processing relationships in V alloys [139].
- **Defect phase diagram:** Understanding solute–defect interactions is important for designing novel V alloys with improved properties for fusion applications. A highly effective method to studying these interactions is to construct “defect phase diagrams” [140–144]. Similar to traditional bulk phase diagrams, defect states can also be mapped as a function of bulk composition and temperatures under various thermodynamic conditions. Since defect phase diagrams are increasingly recognized as fundamental materials tools for bulk phase diagrams, developing these defect diagrams for V alloys could potentially be an emergent area for future research.

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