Influence of Nb, Ti and Mo on Microstructure and Mechanical Properties of Vanadium Solid Solutions

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Abstract. The present study addresses the microstructural evolution and mechanical properties of three different cast V-5X (X = Nb, Ti and Mo) alloys. All alloy compositions are located in the vanadium solid solution (V SS) phase field in their respective phase diagrams. While the alloys V-5Ti and V-5Nb solidified as single-phase V SS after arc-melting, the alloy V-5Mo additionally shows some amount of molybdenum solid solution (Mo SS) in the resulting as-cast microstructure. To improve the mechanical database on vanadium-based alloys, room temperature compression tests were performed and microhardness measurements were carried out by the Vickers indentation method. The lattice parameters were determined by X-ray diffraction analysis and they were calculated using the density functional theory. By carrying out these experiments, the data available for vanadium-based alloys were extended being now available for further optimization of novel V-Si-B high temperature alloys.

1 Introduction

Vanadium base alloys as new structural lightweight materials are of interest for high temperature applications, e.g. in turbines for energy conversion, because of their promising stress-strain behavior in combination with a low density and high melting point of vanadium [1, 2]. In particular, V-Si-B alloys show outstanding mechanical properties at high temperatures, which are comparable to the state-of-the-art Ni-based superalloy CMSX-4 [3]. Therefore, and due to the similarities compared to the well-investigated Mo-Si-B system, which is also a promising candidate to replace Ni-based alloys, ternary V-Si-B alloys recently gained more scientific interest [4-9].

Comparing the isothermal sections available in the literature for the V-Si-B [10] and Mo-Si-B [11], both metal-silicon-boron (Me-Si-B; Me = V, Mo) systems show comparable three phase fields in their metal-rich corner. These fields consist of an A2 structured Me SS metal solid solution phase (V SS, Mo SS), an intermetallic A15 structured Me 3 Si phase (V 3 Si, Mo 3 Si) and a ternary Me 5 SiB 5 (V 5 SiB 2 , Mo 5 SiB 2 ) intermetallic phase with a D8 1 crystal structure [10, 12, 13]. The latter is the so called T2 phase. In context of high temperature applications and according to the literature available for Me-Si-B alloys, a microstructure consisting of a Me SS matrix with homogeneously distributed intermetallic Me 3 Si and Me 5 SiB 2 phases is expected as the desired microstructure [3, 12, 14]. The solid solution matrix may be responsible for the fracture toughness and the intermetallic phases control the high temperature strength as well as the creep and oxidation resistance of those alloys [3, 12, 14-16]. Hasemann et al. [7] recently investigated the ternary eutectics consisting of the three phases as mentioned above for the Mo-Si-B and V-Si-B systems. They determined the volume fractions in the ternary eutectic Me SS-Me 3 SiB 2 -Me 3 Si
grains to be clearly different comparing both systems. The V-Si-B eutectic consists of about 50 vol.% solid solution phase whereas the Mo-Si-B counterpart shows only 20 vol.% of the MoSS phase [7]. A study on ternary V-Si-B alloys has also shown, that the phase fraction of VSS phase truly governs the plastic deformability at room temperature in VSS-V5SiB2-V5Si alloys. Transmission electron microscopy (TEM) investigations on previously deformed compression samples proved that dislocations can only be observed in the VSS regions [6]. In 1997, Henshall et al. [17] already demonstrated that the volume fraction of the VSS phase can be used to control the fracture toughness of binary VSS-V5Si alloys. These results [6, 7, 17] allow the conclusion that for the V-Si-B system, the materials properties can rather be controlled by optimization of the solid solution phase than in the Mo-Si-B case. However, the effects of several alloying elements on the microstructure and mechanical properties of vanadium solid solutions are insufficiently examined, yet. Therefore, the present work addresses the alloying effects of various elements on vanadium-based alloys.

Properties like ambient and high temperature strength, adequate oxidation behavior, a low brittle-to-ductile transition temperature (BDTT) as well as an acceptable fracture toughness and a low density are known to define the profile of requirements for high temperature materials [2, 18]. Most of these properties are related to a high melting point, thus, several alloy systems based on refractory metals are in focus of research since several years [19-21]. Therefore, the addition of refractory metals Mo and Nb were examined in the present work with respect to their effects on the VSS phase. In the context of structural materials for fusion reactors, several V-Cr-Ti alloys were investigated in the past. The literature indicates that an improvement in strengthening can also be expected by the addition of titanium. In particular, the solid solution strengthening [22-24] and the oxidation resistance can be improved by addition of Ti [25, 26]. In order to use the beneficial effects of those alloy elements (Nb, Ti, Mo) for future vanadium-based high temperature alloys, basic investigations like room temperature compression tests, microstructural investigations and hardness measurements were performed in the present study.

2 Materials and Methods

The alloys V-5Nb, V-5Ti and V-5Mo and a reference sample of plain vanadium were produced by conventional arc melting under argon atmosphere in a water cooled copper crucible with a diameter of 25 mm (Arc Melter MAM-1; Edmund Buehler GmbH). Prior to melting, the starting materials vanadium (min. 99.9 % purity; HMW-Hauner GmbH), niobium (min. 99.9 %; HMW-Hauner GmbH), titanium (min. 99.8 %; HMW-Hauner GmbH) and molybdenum (min. 99.9 %; HMW-Hauner GmbH) were carefully weighed out (10 g per alloy) according to the alloy compositions. To ensure a high degree of homogeneity over the sample size, the button-shaped samples were re-melted for five times and flipped between each melting step. The mass losses measured after melting were negligible for all samples (< 0.1 wt.%). All investigations within the present study were carried out under as-cast conditions. Inductively coupled plasma optical emission spectroscopy (ICP-OES) was used to examine the chemical alloy compositions. Sample pieces of each alloy were dissolved in HCl + HNO3 + HF and analyzed using a Thermo Scientific iCAP6500 spectrometer (measuring accuracy < 3%). The oxygen concentrations (in wt.%) were determined in accordance with the carrier gas procedure via melt extraction with subsequent infrared detection using a Bruker G8 Galileo System. Table 1 summarizes the results of the chemical analyses.

Samples for metallographic preparation were embedded in hot mounting epoxy resin (Struers Poly Fast) and subsequently ground from 180 - 2200 grit, followed by mechanical polishing with 3 μm and 1 μm diamond suspension and finished using colloidal silica. Microstructures (as-cast) were investigated using optical microscopy (OM; Zeiss Axiovert 200M) and a FEI (Thermo Fisher Scientific) Scios DualBeam scanning electron microscope (SEM). SEM images were typically performed in the backscattered electron (BSE) mode. Energy dispersive X-ray spectroscopy (EDS, EDAX) were used to measure the concentration of alloying element in the VSS (vanadium solid solution) phase. The phase analyses of V-5X (X = Nb, Ti, Mo) alloys was performed with X-ray diffraction analysis (XRD) in a 0/0 reflection geometry with a 20 range from 20° to 160° using a PANalytical X’Pert Pro Bragg-
Brentano diffractometer and Co-Kα/α₂ radiation. XRD measurements were carried out on previously ground samples. The obtained diffraction patterns were analyzed by the Rietveld technique using Topas Academic 5 program package [27] in order to determine the phase fractions in the alloys. The lattice parameters were determined by the whole powder pattern fitting (WPPF) approach with the Pawley fit of the XRD data using Topas 5 and evaluated against the values determined by the density functional theory (DFT).

To mimic the random distribution of atoms in the V-5X (X = Nb, Ti, Mo) solid solution, special quasi-random structures (SQS) [28, 29] with 128 atoms per cell made via the Monte Carlo SQS (mcsqs) code as implemented in the alloy theoretic automated toolkit (ATAT) were used [30]. The SQS and the simple unit cells of V (100% V) were then used as starting structures for the first-principles structural relaxation carried out with Quickstep [31] as implemented in the CP2K version 5.1 program package [32]. Using the Gaussian plane wave method (GPW) [33], for V, Nb, Ti and Mo the DZVP-MOLOPT-SR-GTH basis set [34] for the atomic centered Gaussian functions were chosen, while for the interatomic part the GTH-pseudopotentials were used [35-37]. Exchange and correlation in this DFT-based method were treated with the generalized gradient approximation (GGA) functional as parameterized by Perdew, Burke and Ernzerhof (PBE-GGA) [38]. Cell shape and volume variations were allowed during the structural optimization until a total energy self-consistency of 10⁻⁶ Ha and until the self-consistency for the forces and maximum geometry change of 10⁻⁵ Ha/Bohr and 10⁻⁵ Bohr, respectively, were achieved. The energy cut-off for the plane waves on the grid were 600 Ha and the k-mesh sampled via the Monkhorst-Pack algorithm [39] were 4x4x4 during the cell optimization.

### Table 1. Chemical compositions of as-cast V-5X alloys measured by ICP-OES and melt extraction.

| Nominal composition | Nb [at.%] | Ti [at.%] | Mo [at.%] | Oxygen [wt.ppm] | Nitrogen [wt.ppm] |
|---------------------|-----------|-----------|-----------|-----------------|------------------|
| V-5Nb               | 4.96      | -         | -         | 1080 ± 90       | 13 ± 1           |
| V-5Ti               | -         | 4.96      | -         | 1150 ± 130      | 4 ± 2            |
| V-5Mo               | -         | -         | 4.80      | 1000 ± 90       | 6 ± 2            |
| V                   | -         | -         | -         | 830 ± 150       | 7 ± 3            |

Mechanical properties of the alloys were investigated using compression tests and microhardness measurements. Compression samples with a typical length of 3 mm and a diameter of 1.6 mm were cut via electrical discharge machining (EDM). Compression tests were performed at room temperature using a Zwick/Roell Z100 electro-mechanical universal testing machine at an initial (engineering) strain rate of \( \dot{\varepsilon} = 10^{-3} \text{s}^{-1} \). Five samples per alloy were tested. The yield stresses were determined by the 0.2% offset method (\( \sigma_{0.2} \)). Microhardness measurements referred to DIN EN ISO 4516:2002 were performed by generating a series of 30 indents set within the grains at well-defined intervals. The tests were performed by indenting a Vickers pyramid with a force of 1 N (HV 0.1) and a hold period of 10 s in the solid solution alloys.

### 3 Results and Discussion

#### 3.1 Microstructural Investigations

The as-cast microstructures of the V-5X (Nb, Ti, Mo) alloys and the reference sample consisting of arc melted vanadium are illustrated in Figure 1. In accordance to the respective binary phase diagrams of V-Nb [40], V-Ti [41] and V-Mo [42], all alloys solidified within the V₃S phase region. Thin deformation scales evidently formed during the metallographic polishing process which can be assumed from the irregularities obtained in the SEM/OM images. Rietveld analysis performed on the measured XRD
patterns (Figure 2) demonstrate, that the alloys V-5Nb, V-5Ti as well as vanadium are single phased consisting of only the VSS phase. Reflexes of molybdenum, however, can be observed in the patterns of alloy V-5Mo. Results of the Rietveld analysis show a small part of ~ 1 vol.% Mo or low-concentrated MoSS in the microstructure. However, larger Mo phase regions have not be detected in the SEM analysis, which suggests that the Mo-rich phase is homogenously distributed. In order to verify the dissolved amount of alloying elements in the VSS phase, EDS spot analyses were conducted. The alloy V-5Mo shows two regions of VSS phases. There are grains/regions with around 5.2 at.% Mo and the others with only 1.8 at.% Mo. It cannot be explained, yet, how these deviations may be evolved during solidification. However, there are calculated results on the binary Mo-V system that show a miscibility gap at lower temperatures, which may explain the present observation [43, 44]. In case of Nb and Ti-containing alloys EDS results showed that almost 5 at.% of Nb/Ti were dissolved in the VSS phase, which corresponds to the results of the ICP-OES measurements.

![Figure 1](image-url) Figure 1. Micrographs of the as-cast microstructures for the alloys a) V, b) V-5Mo, c) V-5Nb, d) V-5Ti.

The lattice parameters of the as-cast alloys were determined in order to achieve additional information about the solid solution phase as well as to identify possible effects concerning the resulting mechanical properties of the alloys. The lattice parameters were calculated using the density functional theory as explained in section 2 and measured by X-ray diffraction combined with WPPF analysis. The results for both methods including their respective deviation (in brackets) compared to vanadium are displayed in Figure 2 (right side). In general, the lattice parameters of vanadium increased for all alloys by adding Ti, Nb or Mo. Due to the small amount of non-dissolved Mo in the alloy V-5Mo, the measured deviation in the lattice parameters differs by 0.1 % compared to the DFT calculations. Compared to the DFT values, the deviation of the lattice parameters measured with XRD are compared to the arc-melted
vanadium sample and thus, the values slightly differ compared to the model-based vanadium. Differences are explained by the amount of oxygen and nitrogen (see Table 1) as well as possible impurities in the as-received starting materials used for the alloy manufacturing.

All alloying elements lead to an increase of the lattice parameter. However, the qualitative increase in the lattice parameters are comparable for both techniques and can be ranked in decreasing order for Nb > Ti > Mo. Compared to V, the lattice parameter for alloy V-5Nb is increased by 0.59 %, for alloy V-5Ti by 0.43 % and for alloys V-5Mo by 0.16 %.

The DFT method seems to be promising in order to estimate lattice constants without performing elaborate experiments. Since the change in lattice parameter is known as a crucial factor in the theory of solid solution hardening [45, 46], DFT analyses can help to estimate reliable values in the future.

### Table 1: Lattice Parameter

|                  | DFT [Å] | XRD [Å] |
|------------------|---------|---------|
| V                | 2.9948  | 3.0318  |
| V-5Nb            | 3.0119  | 3.0498  |
| ( + 0.57 %)      | (+ 0.59 %) |
| V-5Ti            | 3.0073  | 3.0447  |
| ( + 0.42 %)      | (+ 0.43 %) |
| V-5Mo            | 3.0026  | 3.0365  |
| ( + 0.26 %)      | (+ 0.16 %) |

**Figure 2.** XRD patterns of different V-5X alloys (left) and lattice parameter with the respective deviation compared to vanadium (right). Lattice parameter were calculated via DFT and measured via XRD combined with Rietveld analysis.

### 3.2 Mechanical Properties

The mechanical properties of the alloys were investigated using room temperature compression tests as well as microindentation (Vickers) tests. In the engineering stress vs. strain diagram in Figure 3, the results of the compression tests are shown. For reasons of clarity, only three out of five test curves per alloy were plotted. Figure 4 displays the yield stresses, maximum compressive stresses and total compressive strains measured in compression tests. It cannot be excluded that mechanical properties in the present work were influenced by the oxygen/nitrogen content of the alloys (VSS + O/N) since oxygen and nitrogen are known to embrittle V already at comparably minor portions [47]. However, the compressive strains do not indicate significant embrittlement. All binary alloys show high deformability up to 26 % total compressive strain at room temperature which is comparable to the vanadium sample. This observation is in good agreement with recently published results for different V-based alloys [4, 6]. Taking into account the compressive yield stresses (σ₀.2), alloying vanadium with 5 at.% Nb leads to the lowest values of 250 ± 70 MPa followed by 5 at.% Ti with 300 ± 50 MPa and 5 at.% Mo, which results in the highest yield strength of 310 ± 50 MPa. The arc-melted vanadium sample results in σ₀.2 of 140 ± 25 MPa. The strengthening effects of the different alloying elements can therefore be ranked in decreasing order as follows: Mo > Ti > Nb. This result is quite unexpected when taking into account the change of lattice parameter measured for alloys in this study (Figure 2). The increase in strength shows a contrary course compared to the lattice constant and contradicts the theory presented in [45] and [46].
The tendency is contrary to the mechanical data on V-based alloys already available in the literature. Harrod and Gold [48] published a comprehensive compilation and review on the mechanical properties of several V-based alloys in the 1980s. They report the alloying effects of Mo, Ti and Nb on the room temperature yield strength of vanadium in decreasing order as follows: Nb > Mo > Ti. It has to be noted that they obtained their data from various sources. Sample fabrication and purity as well as test parameters were not comprehensively reported. However, the results of tensile tests on V-10X sheet samples (X = Nb, Mo, Ti) by Rajala and van Thyne [49] show the same tendency with regard to the effect of the alloying elements on the yield strength (Nb > Mo > Ti) as reported in [48]. A final ranking with respect to the strength contributions of the respective alloying elements (Mo, Ti and Nb), however, does not seem to be expedient due to the equality of compression data measured in the present work (Figure 4).

![Figure 3. Compressive engineering stress vs. strain curves at room temperature of alloys V-5Nb, V-5Ti, V-5Mo and arc-melted vanadium.](image)

The hardness values obtained from Vickers microindentation tests are summarized in Table 2. The vanadium sample has a microhardness of 93 HV0.1. For the V-5X samples, alloy V-5Ti has the highest hardness value with 190 ± 7 HV0.1 followed by V-5Nb with 180 ± 3 HV0.1 and V-5Mo with 174 ± 5 HV0.1. As was also apparent from the results of the compression tests, none of the alloying elements (Mo, Ti and Nb) can particularly be recommended regarding their potential to optimize the room temperature mechanical properties of the \( \text{V}_{58} \) phase. All alloying elements have led to a significant increase in strength and hardness.

**Table 2. Microhardness (HV0.1) values for V-5X alloys compared to vanadium.**

| Nominal composition | Microhardness HV0.1 |
|---------------------|---------------------|
| V-5Nb               | 180 ± 3             |
| V-5Ti               | 190 ± 7             |
| V-5Mo               | 174 ± 5             |
| V                   | 93 ± 1              |
Figure 4. Comparison of the yield stress ($\sigma_{0.2}$), maximum compressive stress ($\sigma_{\text{max}}$) and total compressive strain ($\varepsilon_{\text{max}}$) for V and V-5X alloys (X = Nb, Ti, Mo); all data were generated at room temperature.

In context of the promising V-Si-B alloys, it has to be noted that the strengths measured for alloys in this study are significantly lower than those of a comparably fabricated V-5Si sample. Hasemann et al. [6] recently published compression strength data for arc-melted binary as-cast V-Si alloys. The V-5Si sample in their study reached a yield stress ($\sigma_{0.2}$) of $580 \pm 78$ MPa [6], which is about 250 MPa higher than stresses measured for alloys in the present work (Figure 4). However, alloying with 5 at.% Si exceeds the solubility limit at room temperature, which will result in a certain amount of V$_3$Si and therefore, this effect has to be considered in order to maintain balanced strength and ductility in technical alloys [2, 5, 6]. Data in the present paper showed that additions of 5 at.% Nb, Ti or Mo increase the room temperature strengths and does not lead to a decrease of deformability. Thus, they may help to optimize the V$_{SS}$ phase in future V-Si-B alloys. However, a more detailed description can be made when the influence on Nb, Mo and Ti on the microstructure formation and the liquidus projection (cooling paths) in the respective V-Si-B-X systems has been studied more intensively.

4 Summary and Conclusions
The alloying effects in three different V-5X (X = Nb, Ti, Mo) vanadium-based alloys were investigated in order to estimate their opportunity to optimize novel V-Si-B high temperature alloys. All alloys are located in the V$_{SS}$ phase region in their respective phase diagrams. However, while V-5Nb and V-5Ti solidified as single phase alloys, the alloy V-5Mo includes different solid solution phases. The present study reports on mechanical data of the as-cast alloys determined by room temperature compression tests and microhardness measurements. Additions of 5 at.% Nb, Ti or Mo lead to an increase of the compression strengths compared to arc-melted vanadium and does not cause any embrittlement. All alloys showed a high ductility up to 26 % total compressive strain in room temperature compression tests. XRD analysis and calculations using the density functional theory (DFT) were used to examine the alloys lattice parameters. All alloying elements increased the lattice parameter, compared to plain vanadium. A comparison between XRD and DFT values showed that the deviation of the lattice
parameters with respect to vanadium is approximately the same for both methods. It can therefore be concluded that the DFT calculation provides reliable values and can minimize experimental effort to estimate the lattice constants. Based on these experimental results, the data available for V-based alloys were clearly extended.

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