First principles density functional theory calculations on the elastic properties of Mo-Si based solid solutions

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Abstract. The alloy system Mo-Si-B gained a lot of attention, as it showed superior elastic properties than currently used Ni based superalloys at elevated temperatures. In the Mo-Si-B alloy system, Mo based solid solutions play an important role as a compound and one can observe a solid solution with small amounts of Si and tiny, almost negligible, amounts of B. To improve the ductility of this alloy at higher temperatures, titanium is added and as a result Mo-Si-Ti solid solutions are formed. To get an idea of the elastic properties of new Mo based solid solutions, first principles density functional theory calculations serve as a powerful method for the prediction and qualitative, often almost quantitative results for the elastic moduli are achieved. Here we show the elastic properties like bulk, shear and Young’s modulus as well as the Vickers hardness, calculated with first principles density functional theory (DFT), of Mo-Si-Ti based solid solutions with approximated atom concentrations Mo-1 at.% Si, Mo-3 at.% Si, Mo-2 at.% Si-1 at.% Ti, Mo-3 at.% Si-1 at.% B and Mo-3 at.% Si-1 at.% Ti.

1 Introduction
To improve the thermodynamic efficiency of aircraft engines, a slight increase of the gas inlet and therefore operating temperature would result in a significant efficiency gain. So, recent advances aim to overcome state-of-the-art Ni-based superalloys which are limited in their maximum operating temperatures with new high temperature materials [1]. Promising candidates for these applications are Mo-Si-B alloys, because they offer a balanced proportion of continuously distributed Mo solid solution phase and intermetallic phases (mainly the A15 and the T2 phase), which is important to obtain good high temperature and acceptable room temperature properties [2]. However, as Mo-Si-B alloys contain both ductile solid solution and brittle intermetallic phases, the distribution, volume fractions and properties of constituents must be tailored for specific load-dependent applications. Research on the Mo solid solution phase is aimed in avoiding embrittlement by interstitial elements as well as by solid solution elements likewise. Unfortunately, significant embrittlement is given intrinsically by the alloying element Si, which is dissolved up to concentrations about 3 at.% in technical alloys [3-5]. Another drawback is that the base material Mo, although a refractory metal with a high melting point of around 2600 °C, tends to have a high density (10.22 g/cm³) [6], which is not particularly beneficial for aeronautical applications. To reduce the density and improve the ductility at higher temperature Ti is added to the Mo-Si-B alloy [7], similar to the alloying of Mo-Si-B with vanadium [8]. The effect of small amounts of Ti added to the Mo-Si solid solution was investigated recently in a study by Krüger et al. for a multi-phase Mo-Si-B-Ti alloy with a continuous Mo solid solution matrix [9]. Another study by
Schliephake et al. left out the boron and investigated the effect of large amount of Ti in the Mo-Si alloy system, where the T1 phase is formed instead of the T2 phase [10].

Density functional theory calculations on the elastic properties of the compounds in Mo-Si-B alloys were mainly focused on the intermetallic phases like MoSi$_2$, Mo$_2$Si$_3$, Mo$_3$Si, Mo$_3$SiB$_2$ and Mo$_5$B [11]. A study by Hütter et al. presented the elastic properties of bcc Mo, Mo$_3$Si and Mo$_3$SiB$_2$ [12]. DFT calculations on Ti$_3$Si$_3$ show a decrease of the bulk, shear and Young’s modulus compared with Mo$_3$Si$_3$ [11, 13] indicating an improvement in ductility at low temperatures for titanium silicides. This finding is supported by a DFT study about Nb$_{2-x}$Ti$_x$Si$_3$. With increasing amount of Ti, the bulk, shear and Young’s modulus is decreasing, improving the ductility at low temperatures [14]. Elastic properties via the DFT calculations on the quaternary T2 phase in Mo-V-Si-B alloys are available for Mo$_{3-x}$V$_x$Si$_2$B$_2$ and were presented recently by Touzani et al. They showed that the elastic properties improve with increasing amount of V [15]. Also, DFT calculations were used to explain the solid solution hardening (SSH) and weakening (SSW) effects by transition metals in bcc Mo [16-18]. It was shown that the electron concentration was the key factor to determine if alloying with a certain element would cause SSH or SSW. Also, as displayed in experiments, it was proven that SSW would only occur at low solute concentrations and with little change in the electron concentration at low temperatures ($T < 300$ K), while SSH is possible for higher solute concentration and temperatures ($T \geq 300$ K) [19]. However there is a lack of the DFT calculated intrinsic elastic properties of Mo-Si based solid solutions.

Therefore, in this work DFT calculations of the isotropic and anisotropic bulk, shear and Young’s moduli as well as the Vickers hardness of Mo based solid solutions at 0 K will be presented. For this purpose models of the Mo-Si-B-Ti solid solutions Mo-0.781 at.% Si, Mo-3.125 at.% Si, Mo-2.344 at.% Si-0.781 at.% Ti, Mo-3.125 at.% Si-0.781 at.% B, Ti and Mo-3.125 at.% Si-0.781 at.% Ti will be investigated.

2 Experimental procedure

To mimic the random distribution of atoms in the Mo-Si based solid solutions Mo-0.781 at.% Si, Mo-3.125 at.% Si, Mo-2.344 at.% Si-0.781 at.% Ti, Mo-3.125 at.% Si-0.781 at.% B, Ti and Mo-3.125 at.% Si-0.781 at.% Ti special quasirandom structures (SQS) [20,21] with 128 atoms (129 for Mo-3.125 at.% Si-0.781 at.% B) per 4x4x4 bcc supercell made via the Monte Carlo SQS (mcsqs) code as implemented in the Alloy Theoretic Automated Toolkit (ATAT) [22] were used (see Figure 1). The SQS unit cells were then used as starting structures for further calculations. The first-principles calculation were carried out with Quantum ESPRESSO [23, 24] for the structural relaxation of solid Mo and the Mo-Si based solid solutions using PAW pseudopotentials [25] from the PSLibrary version 1.0.0 [26]. The kinetic energy cut-off of the plane waves were set to 100 Ry, while the cut-off for the charge density and potential was set to 400 Ry. The structural relaxation stopped until a total energy convergence of $10^{-5}$ Ry and a force convergence of $10^{-4}$ Ry/\(a_0\) was reached. The Marzari-Vanderbilt cold smearing [27] and a Gaussian spreading of 0.01 Ry were chosen to account for the Brillouin-zone integration in metals. The k-mesh was divided by 4x4x4 for the Mo-Si solid solutions using the Monkhorst-Pack algorithm [28]. Exchange and correlation in this density functional theory (DFT) based method were treated with the generalized gradient approximation (GGA) functional as parameterized by Perdew, Burke and Ernzerhof (PBE-GGA) [29]. The elastic properties were determined with thermo_pw [30], a Fortran program using Quantum ESPRESSO routines as the underlying engine. In order to get the Voight-Reuss-Hill [31-33] approximated bulk, shear and Young’s modulus, the standard algorithm and frozen ions were used. To calculate the Vickers hardness, Tian et al’s formula [34] was used. In this work the isotropic and anisotropic elastic moduli will be presented. It is worth noting though that Tian’s formula works best for solid state materials with an experimental Vickers hardness above 5 GPa [34].

For the sake of simplicity and to improve the readability in the following paragraphs Mo-0.781 at.% Si, Mo-3.125 at.% Si, Mo-2.344 at.% Si-0.781 at.% Ti, Mo-3.125 at.% Si-0.781 at.% B, and Mo-3.125 at.% Si-0.781 at.% Ti will be called Mo-1Si, Mo-3Si, Mo-2Si-1Ti, “Mo-3Si-1B” and “Mo-3Si-1Ti”, respectively. The latter two are only hypothetical (hence the “”) and were not experimentally discovered and described yet.
3 Results and Discussion

3.1 Structural relaxation

First, the results of the structural relaxation will be discussed (See Table 1).

For the element molybdenum in the solid state the lattice parameter is 3.1610 Å. In the study by Sturm et al. [5] the experimental lattice parameter was reported to be 3.1478 Å. So the lattice parameter from our DFT calculation is in good agreement with the experiment. As the radius of the Si atom in crystals is smaller (Mo: 145 pm, Si: 110 pm), one expects a smaller lattice parameter with increasing Si concentration. This is indeed true as the lattice parameter of Mo-1Si and Mo-3Si are 3.1588 Å and 3.1537 Å, respectively. For Mo-2Si-1Ti the situation is a bit different. The radius of the Ti atom (140 pm) is about the same as of Mo, the lattice parameter should be between the ones of Mo-1Si and Mo-3Si as the concentration of Si is higher than in Mo-1Si, but lower than in Mo-3Si. In fact, the lattice parameter is 3.1554 Å, which is right between the lattice parameters mentioned above. The lattice parameter for the hypothetical “Mo-3Si-1B” (3.1592 Å) is larger than the lattice parameter of Mo-3Si (3.1537 Å) as expected due to the occupation of an interstitial site by the boron atom. However, the lattice parameter of the hypothetical “Mo-3Si-1Ti” is expected to be similar to the lattice parameter of Mo-3Si, as Mo is substituted by Ti. This is true, because the lattice parameter is 3.1536 Å while the lattice parameter of Mo-3Si is 3.1537 Å.

| Compound          | \(a\) (Å) | \(B\) (GPa) | \(G\) (GPa) | \(E\) (GPa) | \(H^p\) (GPa) |
|-------------------|-----------|-------------|-------------|-------------|-------------|
| Mo                | 3.1610    | 258.7       | 117.1       | 305.1       | 10.88       |
| Mo-1Si            | 3.1588    | 260.1       | 116.8       | 304.8       | 10.77       |
| Mo-3Si            | 3.1537    | 258.0       | 113.1       | 296.0       | 10.23       |
| Mo-2Si-1Ti        | 3.1554    | 257.4       | 113.2       | 296.2       | 10.29       |
| “Mo-3Si-1B”       | 3.1592    | 256.9       | 112.5       | 294.5       | 10.19       |
| “Mo-3Si-1Ti”      | 3.1536    | 256.7       | 112.4       | 294.1       | 10.17       |
3.2 Elastic properties

In the next two paragraphs the DFT calculated isotropic and anisotropic elastic properties will be presented and discussed.

3.2.1 Isotropic elastic properties. In this paragraph the isotropic elastic properties e.g. bulk, shear, Young’s moduli and Vickers hardness of Mo, Mo-1Si, Mo-3Si, Mo-2Si-1Ti, “Mo-3Si-1B” and “Mo-3Si-1Ti” (see also Table 1) will be discussed. The isotropic bulk moduli of Mo, Mo-1Si, Mo-3Si, Mo-2Si-1Si, “Mo-3Si-1B” and “Mo-3Si-1Ti” are very similar: 258.7 GPa, 260.1 GPa, 258.0 GPa, 257.4 GPa 256.9 GPa and 256.7 GPa, respectively. A slightly different situation is apparent for the shear and Young’s moduli. Regarding these properties, it is possible to divide the six compounds into three groups of two: For Mo and Mo-1Si the isotropic shear moduli are 117.1 GPa and 116.8 GPa, respectively, and therefore very similar to each other. Lower shear moduli are found for Mo-3Si and Mo-2Si-1Ti as they are 113.1 GPa and 113.2 GPa, respectively, and therefore almost the same. A similar situation is present for the shear moduli of Mo-3Si-1B” and “Mo-3Si-1Ti”. The shear moduli of these hypothetical compounds are 112.5 GPa and 112.4 GPa and very close to each other. The isotropic Young’s moduli of Mo, Mo-1Si, Mo-3Si, Mo-2Si-1Ti, “Mo-3Si-1B” and “Mo-3Si-1Ti” are 305.1 GPa, 304.8 GPa, 296.0 GPa, 296.2 GPa, 294.5 GPa respectively. The isotropic Vickers hardness are 10.88 GPa, 10.77 GPa, 10.23 GPa, 10.29 GPa and 10.17 GPa for Mo, Mo-1Si, Mo-3Si, Mo-2Si-1Ti, “Mo-3Si-1B” and “Mo-3Si-1Ti”, respectively. The Vickers hardness of Mo-3Si and “Mo-3Si-1B” are very similar to each other (10.23 GPa, 10.19 GPa) and could be sign that interstitial atoms at low concentration do not have a large influence on the isotropic Vickers hardness of Mo-Si based solid solutions. Interestingly, “Mo-3Si-1B” (10.19 GPa) and “Mo-3Si-1Ti” (10.17 GPa) have similar Vickers hardness, despite a different mechanism of doping (interstitial site vs transition metal substitution).

The bulk, shear and Young’s modulus of Mo according by a DFT study by Hütter et al. using LDA are 302 GPa, 135 GPa and 352 GPa, respectively [12]. The Vickers hardness using Tian et al’s formula is 11.87 GPa. The calculated elastic properties are therefore higher than in our DFT study, which might be due to the well-known “overbinding” problem of LDA, overestimating the strength of chemical bonding.

3.2.2 Anisotropic elastic properties. In this paragraph the anisotropic shear, Young’s moduli and Vickers hardness of Mo, Mo-1Si, Mo-3Si, Mo-2Si-1Ti, “Mo-3Si-1B” and “Mo-3Si-1Ti” (“see also Figures 2-4) are discussed. Due to the cubic crystal structure, the bulk moduli of all the compounds are isotropic and were already described in the paragraph above. As the crystal structure of the Mo based solid solution compounds is very similar, the minimum and maximum of the other elastic properties shear moduli, Young’s moduli and Vickers hardness are along the same crystallographic directions.

![Figure 2. Anisotropic shear moduli of Mo (red), Mo-1Si (orange), Mo-3Si (dark blue), Mo-2Si-1Ti (light blue), “Mo-3Si-1B” (cyan) and “Mo-3Si-1Ti” (black).](image)
The shear moduli of the Mo-based solid solutions (Figure 2) show their maximum along the vicinity of the [111] direction, while the minimum can be seen along the [100] direction. The shear moduli of Mo and Mo-1Si along the [110] direction are 119.2 GPa and 119.1 GPa, respectively and therefore very similar. The shear moduli of Mo-3Si, Mo-2Si-1Ti, “Mo-3Si-1B” and “Mo-3Si-1Ti” along the same direction are 115.5 GPa, 115.8 GPa, 115.3 GPa, 114.8 GPa, respectively, and very similar for these four compounds. The maxima of the shear moduli of Mo, Mo-1Si, Mo-3Si, Mo-2Si-1Ti, “Mo-3Si-1B” and “Mo-3Si-1Ti” are 129.4 GPa, 126.4 GPa, 121.6 GPa, 122.0 GPa, 120.9 GPa, and 121.0 GPa. The minima of the shear moduli are 96.4 GPa, 101.6 GPa, 99.3 GPa, 99.0 GPa, 97.9 GPa and 98.9 GPa for Mo, Mo-1Si, Mo-3Si, Mo-2Si-1Ti, “Mo-3Si-1B” and “Mo-3Si-1Ti”, respectively. Unlike the isotropic shear moduli the maxima and minima of the anisotropic shear moduli of Mo and Mo-1Si differ from each other and more so for the shear moduli of Mo-3Si, Mo-2Si-1Ti, “Mo-3Si-1B” and “Mo-3Si-1Ti”, which are very similar to each other. The anisotropic behavior of the shear moduli in general is very similar for Mo-3Si, Mo-2Si-1Ti, “Mo-3Si-1B” and “Mo-3Si-1Ti”. Experimental values of the shear moduli are present for Mo and Mo-0.34 at.% Si [5]. The latter might be qualitatively compared to Mo-1Si of our DFT calculation. The shear moduli of Mo and Mo-0.34 at.% Si are 117.4 GPa and 119.9 GPa, respectively. These values are just between the maxima (129.4 GPa and 126.4 GPa) and minima (96.4 GPa and 101.6 GPa) of Mo and Mo-1Si, respectively. Unfortunately, the crystallographic directions during the experimental shear moduli measurements are unknown, making a valid comparison difficult. According to the study by Sturm et al. [5] the shear modulus seems to decrease with increasing Si concentration above 0.34 at.%.

![Figure 3](image)

**Figure 3.** Anisotropic Young’s moduli of Mo (red), Mo-1Si (orange), Mo-3Si (dark blue), Mo-2Si-1Ti (light blue), “Mo-3Si-1B” (cyan) and “Mo-3Si-1Ti” (black).

A different behavior for the anisotropic Young’s moduli is observed (see Figure 3). The maxima are along the [100] direction, while the minima are in the vicinity of the [111] direction. Along the [110] direction the Young’s moduli of Mo-1Si, is 288.4 GPa and therefore larger than the Young’s moduli of other five compounds Mo (281.2 GPa), Mo-3Si (278.8 GPa), Mo-2Si-1Ti (279.5 GPa), “Mo-3Si-1B” (276.7 GPa) and “Mo-3Si-1Ti” (278.5 GPa), which are very similar. The maxima of the Young modulus of Mo, Mo-1Si, Mo-3Si, Mo-2Si-1Ti, “Mo-3Si-1B” and “Mo-3Si-1Ti” are 390.0 GPa, 364.6 GPa, 348.3 GPa, 351.2 GPa, 347.5 GPa and 346.7 GPa, respectively. The minima of the Young’s moduli are 257.2 GPa, 269.6 GPa, 264.7 GPa, 263.7 GPa, 263.5 GPa and 262.4 GPa for Mo, Mo-1Si, Mo-3Si, Mo-2Si-1Ti, “Mo-3Si-1B” and “Mo-3Si-1Ti”, respectively. Similar to the shear moduli and unlike the isotropic Young’s moduli, the minima and maxima of the Young’s moduli of Mo and Mo-1Si differ from each other, while the anisotropic behavior as well as the minima and maxima of the Young’s moduli of Mo-3Si, Mo-2Si-1Ti, “Mo-3Si-1B” and “Mo-3Si-1Ti” are very similar to each other. The experimental Young’s moduli for Mo and Mo-0.34 at.% Si are 302.6 GPa and 307.5 GPa, respectively and lie between the maxima (390.0 GPa and 364.6 GPa) and minima (257.2 GPa and
269.6 GPa) of the DFT calculated anisotropic Young’s moduli. Again, the crystallographic directions during the experimental Young’s moduli measurements are unknown. Similar to the shear moduli the experimental Young’s modulus seems to decrease with increasing Si concentration above 0.34 at.% [5].

![Anisotropic Vickers hardness of Mo, Mo-1Si, Mo-3Si, Mo-2Si-1Ti, Mo-3Si-1B and Mo-3Si-1Ti](image)

**Figure 4.** Anisotropic Vickers hardness of Mo (red), Mo-1Si (orange), Mo-3Si (dark blue), Mo-2Si-1Ti (light blue), “Mo-3Si-1B” (cyan) and “Mo-3Si-1Ti” (black).

As the Vickers hardness according to Tian et al. [34] is proportional to the shear modulus, a similar anisotropic behavior of the Vickers hardness and the shear modulus is expected. Indeed, the maxima of the Vickers hardness is along the vicinity of the [111] direction, while the minima are along the [100] direction (see Figure 4). The Vickers hardness along the [110] direction of Mo, and Mo-1Si are 11.25 GPa and 11.16 GPa, respectively, and very similar. For Mo-3Si, Mo-2Si-1Ti, “Mo-3Si-1B” and “Mo-3Si-1Ti” the Vickers hardness along [110] is lower and within the same range: 10.67 GPa, 10.75 GPa, 10.68 GPa and 10.61 GPa, respectively. The maxima of the Vickers hardness of Mo, Mo-1Si, Mo-3Si, Mo-2Si-1Ti, “Mo-3Si-1B” and “Mo-3Si-1Ti” are 13.09 GPa, 12.45 GPa, 11.71 GPa, 11.81 GPa, 11.64 GPa and 11.66 GPa, respectively. The minima for Mo, Mo-1Si, Mo-3Si, Mo-2Si-1Ti, “Mo-3Si-1B” and “Mo-3Si-1Ti” are 7.60 GPa, 8.32 GPa, 8.18 GPa, 8.08 GPa, 8.08 GPa and 8.02 GPa, respectively. Similar to the other elastic moduli, the anisotropic behavior of Mo-3Si, Mo-2Si-1Ti, “Mo-3Si-1B” and “Mo-3Si-1Ti” for the Vickers hardness is very akin. However, one must take the results of the Vickers hardness calculations of Mo and Mo-1Si with a pinch of salt. The experimental Vickers hardness was reported to be 2.61 GPa [35] and 4.12 GPa [3], respectively, which is below 5 GPa and Tian et al’s formula might be inaccurate in this case. Also it was shown in Ref. [19] that temperatures above 0 K will cause a decrease of the Vickers hardness in bcc Mo solid solutions, while DFT calculations consider only the ground state properties at 0 K. The experimental Vickers hardness at room temperature of Mo-2.8 at.% Si and Mo-1.8 at.% Si-0.6 at.%Ti are 8.51 GPa and 7.76 GPa, which are close to the results of the qualitative similar solid solutions Mo-3Si and Mo-2Si-1Ti used in the DFT calculations presented here (8.18 GPa and 8.08 GPa, respectively). The small disagreement might be due to the solid solution hardening (SSH) effect which might take place at room temperature or higher temperatures [19] and the DFT calculations do not include the SSH effect appropriately as mentioned above. Also, another reason for the deviation is the fact that the crystallographic directions during the experimental Vickers hardness measurements are unknown. The qualitative change of the Vickers hardness, however, is observable and displays in accordance with the experiment, the increase in hardness with increasing Si content and electron concentration. On the other hand, increasing the silicon concentration from Mo-2Si-1Ti to “Mo-3Si-1Ti” seems to lower not only the isotropic Vickers hardness but the anisotropic Vickers hardness, from 11.81 GPa/11.66 GPa to 8.08 GPa/8.02 GPa, respectively, as silicon is a substitute for molybdenum. Investigating the influence of interstitial atoms, “Mo-3Si-1B” shows a similar anisotropic Vickers hardness to Mo-3Si (Maxima: 11.71 GPa and
11.64 GPa, minima: 8.18 GPa and 8.18 GPa). This might be another sign, that interstitial atoms have only little influence on the Vickers hardness at low concentrations as already observed for the isotropic Vickers hardness. The same is true for the substitution of Si with Ti for Mo-3Si to Mo-2Si-1Ti as the anisotropic behavior of the Vickers hardness is very similar (Minima: 8.18 GPa/8.08 GPa, maxima: 11.71 GPa/11.81 GPa, respectively).

Interestingly, Mo shows the most anisotropic behavior in terms of the elastic moduli as its maxima and minima of the shear modulus, Young’s modulus and Vickers hardness are the highest and the lowest, respectively, compared to Mo-1Si, Mo-3Si, Mo-2Si1Ti, “Mo-3Si1B” and “Mo-3Si-1Ti” according to our DFT calculations.

4 Conclusions
DFT calculations to explain the elastic behavior of Mo solid solutions were performed using experimental and hypothetical alloy compositions including the elements Si, B and Ti. The calculated isotropic bulk, shear and Young’s moduli as well as the Vickers hardness of Mo-Si-B-Ti solid solutions are within the groups of Mo/Mo-1Si, Mo-3Si/Mo-2Si-1Ti and “Mo-3Si1B”/“Mo-3Si-1Ti” very similar and in decreasing order. However, the DFT calculations of the anisotropic elastic properties of these compounds show that the shear and Young’s moduli as well as the Vickers hardness of Mo and Mo-1Si differ more than expected, while the anisotropic shear and Young’s moduli as well as the Vickers hardness for Mo-3Si, Mo-2Si-1Si, “Mo-3Si-1B” and “Mo-3Si-1Ti” are very similar. In general, the Young’s moduli of all the compounds investigated here are very anisotropic, while the shear moduli and Vickers hardness show less anisotropic behavior. However and quite surprisingly, Mo show the highest anisotropic behavior for all elastic moduli presented here.

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