# DFT study of the Phase Stability and Electronic structure properties of O-Phase Ti2AlX (X= Nb, V, Ta, W, Mo) alloys

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## Introduction

**First Principles Study of Ti2AlX (X= Nb, V, Ta, W, Mo) alloy**

- We work on TiAl alloys for mechanically loaded high-temperature applications. O-Phase Ti2AlX can form in some of those alloys. Thus, its properties and especially its stability and how this is influenced by alloying elements is interesting.
- Electronic Density of States (DOS) provides information about bonding conditions in the phase and can be related to experimental Electron Energy Loss Spectroscopy (EELS) spectra. By searching for similar structures in DOS and EELS bonding conditions and alloying effects can be determined.

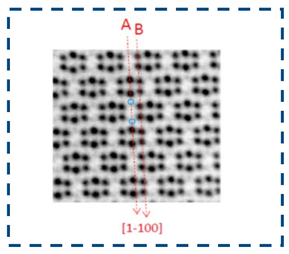



**FIG.1.** STEM micrograph of Ti-42Al-8.5Nb alloy [1].

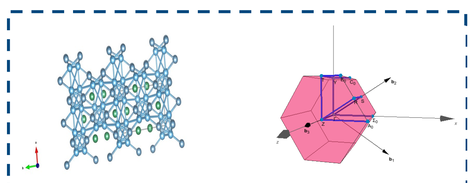


**FIG.2.** Optimized geometric structure of Ti2AlNb. The blue circles are Ti atoms, the gray circles are Al atoms, the green circles are Nb atoms. Brilloum zone planes Ti2AlX.

### Challenges to their further development

- The formation of O-Phase Ti2AlX in other systems than Ti-Al-Nb is only scarcely investigated experimentally as well as theoretically.
- The presence of O-Phase in parts may have detrimental effects on their properties or could be utilized to optimize the material if its formation and properties are well understood.

## Project Goals and Methods

### Project Goals

- Understand role of alloying elements (X) on Ti2AlX stability and properties.
- Explain and characterize bonding type.

### Density functional theory (DFT)

- DFT is a first-principles computational modeling method (based on quantum mechanics rather than classical mechanics or empirical data).
- Calculates ground-state properties of a system.
- Less than 1,000 atoms in DFT modeled systems [2].
- We used the Vienna Ab initio Simulation Package (VASP) to implement DFT.

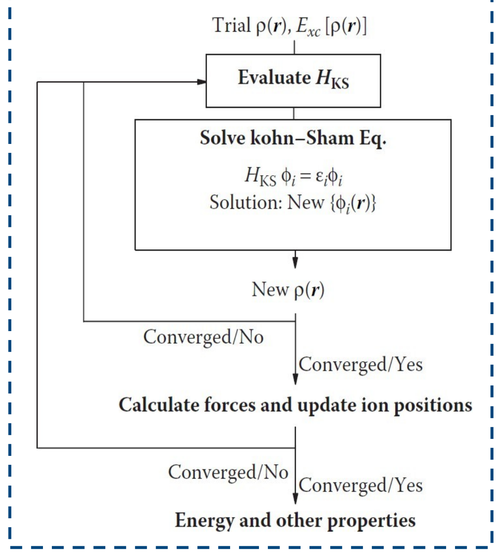



**FIG.3.** Flow of DFT calculations [2].

## Results and discussion

### Computational details Analysis

**Table1.** Calculated formation Energy of the Ti2AlX alloys by VASP.

| Alloys O-Phase | | Method | | |
|---|---|---|---|---|
| | pot | VASP | | |
| | PAW-PBE | En.tot (eV) | En./atom (eV) | En./formation (eV) |
| | | Calc. | Calc. | Calc. |
| Ti2AlV | Ti_pv, V | -116.11081 | -7.256925625 | -0.205905 |
| Ti2AlNb | Ti_pv, Nb_pv | -122.26434 | -7.64152125 | -0.27771325 |
| Ti2AlMo | Ti, Mo | -126.22181828 | -7.888863642 | -0.33269775 |
| Ti2AlW | Ti, W | -133.29317157 | -8.330823223 | -0.256904 |
| Ti2AlTa | Ti, Ta | -128.45432243 | -8.028395152 | -0.307366451 |

**FIG. 4.** Total energy vs volume per formula unit of a)Ti2AlNb, b)Ti2AlTa, c)Ti2AlMo, d)Ti2AlV. The symbols denote the calculated energies while the lines show the fitted Murnaghan equation of state. E = E0 + B0 * vol / BP * (((V0 / vol)**BP) / (BP - 1) + 1) - V0 * B0 / (BP – 1.0).

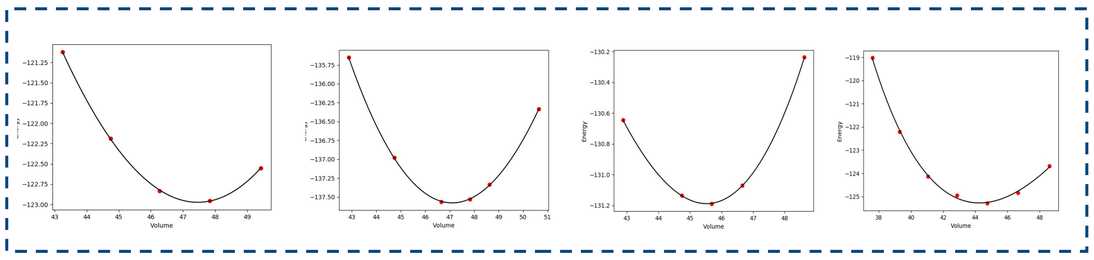
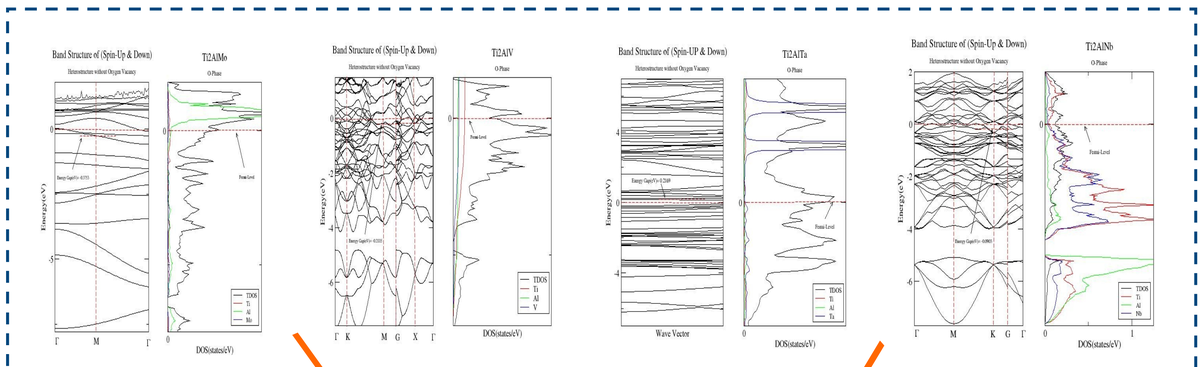



**Table 2.** The calculated structural properties for Ti2(Al, xM) Alloys via VASP.

| O-Phase Alloys | | Calculation type or Experiment Method | | Method | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | VASP | | Lattice constant/ Angstrom calc. | | | | | | |
| | Pot | Atoms | a (Å) | b (Å) | c (Å) | c/a (Å) | | | | |
| | PAW-PBE | | Calc. | Calc. | Calc. | Calc. | K*xx* | K*yy* | Kzz | EnCut |
| Ti2AlV | Ti, V | 16 | 5.8843941272924845 | 9.3372394782140891 | 4.5378384308587316 | 0.757377049 | 11 | 9 | 7 | 600 |
| Ti2AlMo | Ti, Mo | 16 | 6.1674013277279496 | 9.1982542189344052 | 4.4910511184175448 | 0.728191807 | 11 | 9 | 7 | 600 |
| Ti2AlTa | Ti, Ta | 16 | 6.0646126009253356 | 9.4623228729721429 | 4.6584297315838130 | 0,768133109 | 11 | 9 | 7 | 600 |
| Ti2AlNb | Ti_pv, Nb_pv | 16 | 6.0633844589243937 | 9.5359655160819283 | 4.6790461841898860 | 0.771688851 | 11 | 9 | 7 | 600 |
| Ti2AlW | Ti,W | 16 | 6.1371482820065575 | 9.2324433069801053 | 4.5126365136325797 | 0.735298596 | 11 | 9 | 7 | 600 |

**FIG.5.** Electronics band structure and corresponding DOS of Ti2AlMo, Ti2AlV, Ti2AlTa and Ti2AlNb. The Fermi-level is set at zero.




According to the Partial Density of State the most pronounced peak in the occupied states is caused by electrons of 3d of Titanium, and the most pronounced peak of unoccupied states stems from 3d orbitals of X and 2p orbitals of Al.

According to total DOS Ti2AlX is a semiconductor alloy.

**FIG 6.** The calculated formation energy change of Ti2AlX; as a function of the Fermi level at the chemical potential point P and as a function of the elemental chemical potentials.

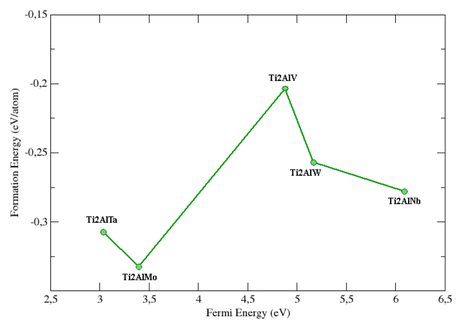



**Table 3.** DOS and Band structure properties of Ti2(Al,TM) alloys.

| Alloys | POT | Method: DFT / Structure: O-Phase | |
|---|---|---|---|
| | | Band structure & DOS/ Calc. | |
| | | Band Gap (eV) | Fermi Energy (eV) |
| Ti2AlNb | Ti_pv,Nb_pv | -0.0903 | 6.089562 |
| Ti2AlV | Ti_pv, V | -0.2115 | 4.881557 |
| Ti2AlMo | Ti_pv,Mo_pv | -0.3753 | 3.397468 |
| Ti2AlTa | Ti_pv, Ta_pv | 0.2169 | 3.037392 |
| Ti2AlW | Ti, W | -0.004 | 5.169282 |

## Analysis

### Increasing the lattice constant:

**Ta>W>Mo>V>Nb>>Ti (VASP)**
**Ta>>W>Mo>Nb>V>>Ti (CASTEP)**

### DOS & Band structure properties:

**Ti2TaAl>>Ti2NbAl>Ti2VAl>Ti2AlMo>> Ti2WAl (Width of Band Gap En.)**
**Ti2WAl>Ti2NbAl>Ti2VAl>Ti2AlMo>Ti2TaAl (Fermi En.)**

The calculations of density of states indicate that the strength of the p-d and d-d covalent bond inTi2AlX changes in the order

**Ti2AlV<Ti2WAl<Ti2AlNb<Ti2AlTa<Ti2AlMo**

## Conclusions/Future Work

### Conclusion

The Formation energies, geometry, band structure and DOS of the Ti2AlX (X= Nb, Ta, V, W, Mo ) were investigated with DFT. The calculated lattice constants are in good agreement with the available experimental values with less than 3% difference. According to the analysis of the DOS and PDOS of the four alloys, it was concluded that the conduction band of Ti2AlX is formed by the Ta, Mo, and V s-orbitals and the valence bands of the Ti2AlNb is formed by the Ti 3d-orbital and Al 2p-orbital. Our investigation suggests that the stability and bonding character of O-Phase Ti2AlX can be significantly influenced by alloying with X. Hence, ordering nature, stability, and directionality of bonding combined effects the structure properties of O-Phase Ti2AlX intermetallics.

### Future work

- Bader charge analysis of two or more X= Nb, V, Ta, W, Mo Atoms on Ti2AlX.
- Characterization of the charge transfer between particular types of elements in the O-Phase.
- Calculate effects of alloying elements on the elastic properties.
- Extend stability calculations to higher temperatures.

## References

[1] Lobna Saeed, et al. "Ab-initio DFT investigation of phase stability and transformation paths of Ti-Al-Nb", Master Thesis, Dept. of Micromechanical and Macroscopic Modelling Interdisciplinary Centre for Advanced Materials Simulation Ruhr-Universität Bochum, 2018.
[2] Lee, June Gunn. Computational Materials Science: An Introduction. Second edition, CRC Press, Taylor & Francis Group, CRC Press is an imprint or the Taylor & Francis Group, an informa business, 2017.
[3] Y. Wang et al, Computer Coupling of Phase Diagrams and Thermochemistry 28,79–90, 2004.