Element Interaction in Titanium

Interaction of Alloying Elements in Titanium Alloys

***M. Bäker**, Institut für Werkstoffe, Technische Universität Braunschweig*

In Short

- How do alloying elements interact with a titanium matrix?
- How do alloying elements in titanium interact with each other?
- Is it possible to quantitatively describe the interaction in different configurations?
- Is it possible to find a way to simulate pure titanium in the unstable β phase?

Due to their excellent strength, low density and high bio-compatibilty, titanium alloys are widely used in different applications. Titanium can exist in two different crystal structures, a low-temperature α-phase (crystal structure hexagonally closed-packed) and a high-temperature β-phase (crystal structure body-centered cubic). This allows to design titanium alloys with widely varying microstructures. For example, the standard titanium alloy Ti6Al4V that has been used in aerospace engineering since the middle of the 20th century contains both α and β phase. In recent years, the interest in other alloys, especially those that have a β structure, has increased due to their high biocompatibility and low Young's modulus. Futhermore, designing alloys for additive manufacturing is of growing importance.

When designing new alloys, understanding the influence of alloying elements is crucial to predict the properties of the alloys and to chose the optimal composition. The interaction of alloying elements plays an important role here: It can be energetically favourable or unfavourable for elements to be positioned in nearest- or next-nearest neighbouring positions. These interactions can lead to the formation of ordered structures in the alloy (intermetallic phases), but also to local ordering effects (short-range order) that are known to influence the mechanical properties. Understanding these effects is therefore important.

To achieve this understanding, simulations using density functional theory (DFT) are a versatile tool. Current DFT methods are able to calculate the energy of diferent structures with a sufficiently high precision to study interaction effects, phase transitions and other phenomena. In the current project, the software package VASP wil be used.

In a previous research project [1,2], interaction effects have been studied for nickel alloys. In one part of the project, the interactions between transition metals of the 6th period (Y–Cd in the periodic table) were studied in detail. The behaviour of these elements is dominated by the electrons in the so-called $4d$-electron shell that is gradually filled when going from Y to Cd. It was shown that the interaction of such alloying elements, when placed in a nearest-neighbour position, is strongly repulsive when both elements have less than 5 d electrons on average. This can be explained from the interaction of the elements with each other and with nickel, with has an almost full d shell so that bonds between nickel and and element with few d electrons are attractive. It was possible to show that all interaction energies in the 55 possible combinations between the elements Y–Cd can be mapped to a "master curve".

When placing elements on next-nearest neighbour positions, the pictures reverses. In this case, the interaction is strongly atractive when both elements have less than 5 d electrons. Although the interaction energies can be explained qualitatively, a simple quantitative description of the energy has not been found in the project.

The main objective of the current project is to perform similar calculations for titanium. Titanium is an ideal choice because it is technologically highly relevant as explained above and has a d electron shell that is only slightly filled and thus can be considered as a complement to nickel.

The alloying elements to be investigated are the elements with gradually filled $4d$-shells, Y–Cd, and the technologically important elements Al, V and Ta.

In the first part of the project, single elements will placed into the titanium α-phase. These calculations serve as reference for the interaction calculations, but also allow to study the properties of the elements in titanium, like bond strength or charge transfer between the alloying element and the surrounding atoms. In addition, it is known that for some elements, spontaneous symmetry breaking occurs, with the element moving closer to some of its neighbours than to others. This effect will also be studied here.

Next, two alloying elements will be placed on different neighbouring positions as nearest or next-nearest neighbours etc. Due to the large number of possible element combinations and the large number of crystallographically different lattice positions, this part of the project requires a large amount of CPU time.

For nearest neighbours, the main goal is to investigate whether the situation is comparable to that in nickel and whether a similar quantitative understanding can be achieved. If the same variables are involved in determining the interactions energies, a more unified picture of alloying element interactions would emerge which would also be interesting for other applications like the so-called medium or high entropy alloys.

For next-nearest neighbour interactions in nickel, it was not possible to achieve a quantitative understanding in the case of a nickel matrix. The comparison with the situation in titanium hopefully allows to better understand the effects occuring when elements are placed in this configuration which is of crucial importance in understanding intermetallic phases. Configurations with the elements in greater distances will be used as reference and to better understand the effects alloying elements have on titanium atoms that are bonded to two other elements.

All calculations described so far will be performed for the α-phase. The β-phase is unstable in pure titanium both experimentally and in density functional theory simulations. Therefore, studying interaction effects in this phase is difficult. In the third part of the project, it wil be attempted to find a way that allows for the simulation of these effects by adding stabilizing terms to the calculation that hinder the transformation to another lattice structure. If this can be done successfully, interactions in the β phase will be investigated in future phases of the project.

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More Information

[1] M. Bäker, *Understanding Element Solution Energies In Nickelbase Alloys Using Machine Learning*, Materials Research Express, 2023, doi:10.1088/2053-1591/acbe28

[2] M. Bäker, J. Rösler, *Influence of transition group elements on the stability of the γ''-phase in nickelbase alloys* , Modelling and Simulation in Materials Science and Engineering, **29** 2021, 055006, doi:: 10.1088/1361-651X/abd043

DFG Subject Area

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