

Applications Example:

## Titanium Alloy Design for Additive Manufacturing

Database(s):	<b>TCTI4 or newer</b>	Module(s):	
Version required:	<b>Thermo-Calc 2022b or newer</b>	Calculator(s):	<b>Property Model Calculator (Equilibrium, Liquidus, and Solidus)</b>
Material/Application:	<b>Titanium Alloys/Additive Manufacturing</b>		
Calculation name:	<b>PM_G_13_Ti_Alloy_Design_for_AM</b>		

### INTRODUCTION

Additive manufacturing provides new opportunities to fabricate complex parts. However, traditional alloys may not be readily printable using techniques such as laser powder bed fusion. As such, the development of new alloys may be necessary to fully realize the benefits of additive manufacturing technologies.

In this example, inspired by the work of Ackers et al. [1], batch calculations within the Property Model Calculator are used to identify candidate titanium alloy chemistries for biomedical implant applications using the thermodynamic TCS Ti/TiAl-based Alloys Database (TCTI). To optimize printability and material weight, the liquidus temperature, solidus temperature, and density of 2000 randomized titanium alloy chemistries from the Ti-Nb-Zr-Sn-Ta-Fe-Mo system are calculated. An estimate of alloy cost is also made for each alloy. Taken together, this methodology can be used to identify compositions of interest and accelerate material development activities.

### How to Run the Calculation

To run this example, open Thermo-Calc and navigate to the Help Menu → Example Files ... → Property Models → General. This example includes one calculation file:

- **PM\_G\_13\_Ti\_Alloy\_Design\_for\_AM:** requires a license for Thermo-Calc 2022b or newer and the Titanium and TiAl-based Alloys Databases TCTI4 or newer.

Other software and database versions may work, but results may vary.

**Note:** *The calculation example only includes 200 randomized titanium alloy chemistries to reduce the calculation time and the result will therefore look slightly different from what is presented in this document.*



Read additional in-depth [Application Examples available](#)

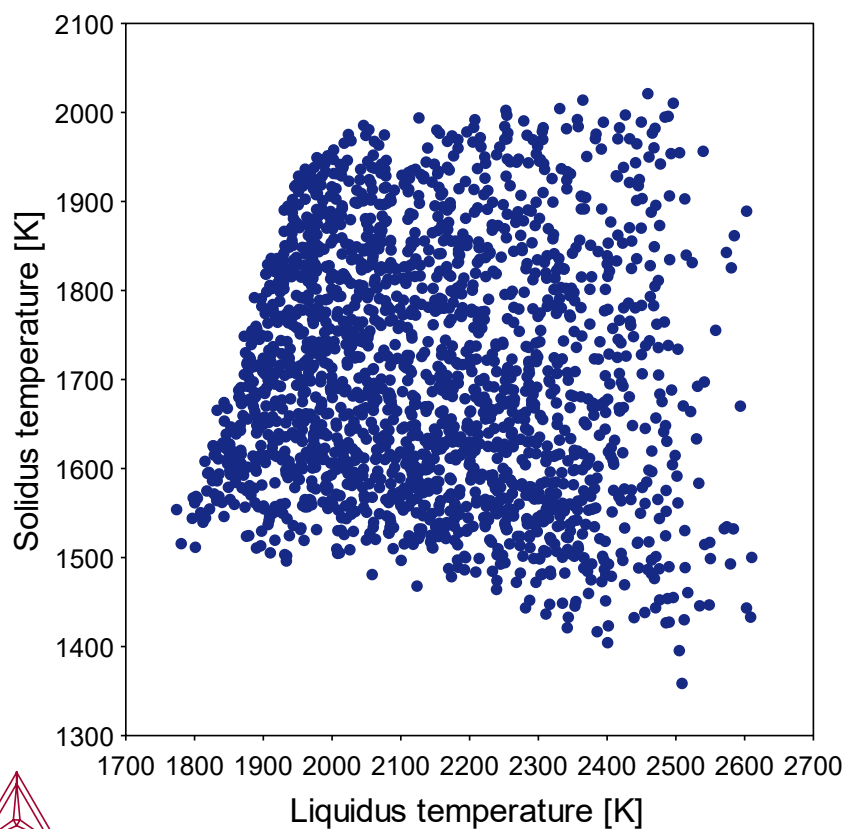
## EXAMPLE CALCULATIONS AND EXPLANATIONS

### Chemistry Variation

To explore the chemistry space, 2000 alloy chemistries are randomly generated with a uniform distribution. Each of the solute elements, Nb, Zr, Sn, Ta, Fe, and Mo are allowed to vary between 0 and 10wt%. These chemistries are then used as input for the batch calculations demonstrated in this example.

### Liquidus and Solidus Temperature

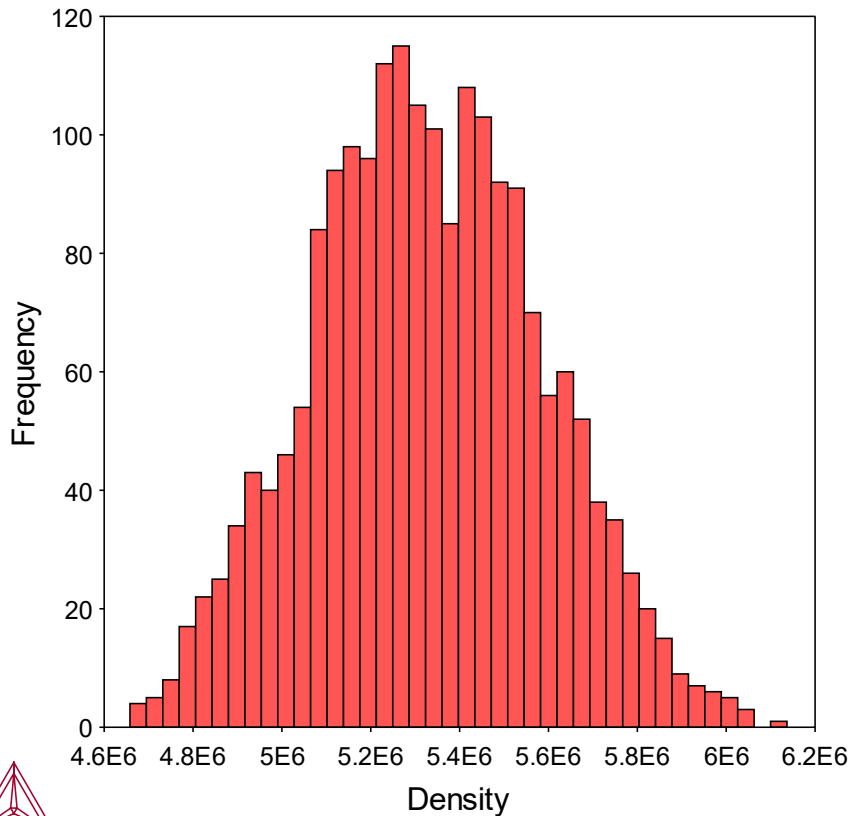
A narrow solidification temperature interval is favorable to minimize the risk of defect formation during printing. In this case, the liquidus and solidus temperatures can be used to calculate the equilibrium solidification temperature interval for each of the randomized titanium alloy chemistries. Using the Batch calculation type and the Liquidus and Solidus Temperature Property Models, the liquidus and solidus temperature data for each of the titanium alloy chemistries are calculated. The results are presented in Figure 1. Although the equilibrium solidification temperature interval differs from what would be expected during additive manufacturing thermal cycles, it can serve as a useful calculation for rapidly screening candidate alloy chemistries.



*Figure 1: Calculated liquidus and solidus temperature data for 2000 randomized chemistries from the Ti-Nb-Zr-Sn-Ta-Fe-Mo system.*

## Density

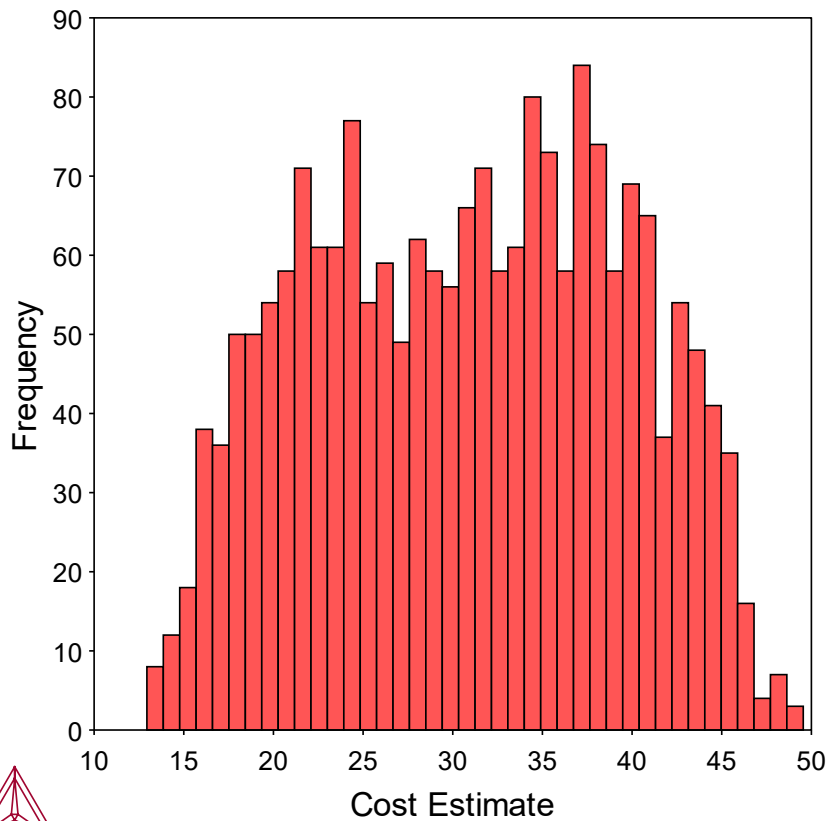
Alloys with low density are favorable for biomedical implant applications to minimize weight and improve patient comfort. The density of each randomized titanium alloy chemistry is calculated at 350 °K, using the Equilibrium Property Model and the Batch calculation type. The distribution of calculated densities is presented in Figure 2.



*Figure 2: Calculated density of 2000 randomized chemistries from the Ti-Nb-Zr-Sn-Ta-Fe-Mo system*

## User-defined Functions

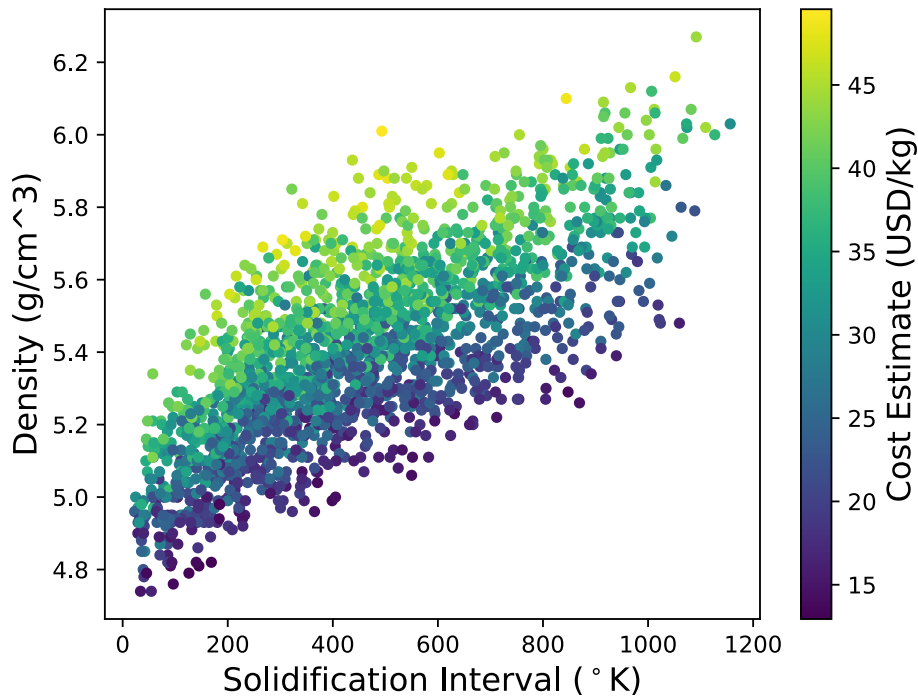
Custom user-defined functions can be used in the Property Model Calculator. In this example, alloy cost is estimated based on a user-defined function that accounts for raw material costs and the concentration of each element in each randomized titanium alloy chemistry. A histogram of the cost estimate for each randomized alloy chemistry is presented in Figure 3.



*Figure 3: Cost estimate histogram for 2000 randomized chemistries from the Ti-Nb-Zr-Sn-Ta-Fe-Mo system. The cost estimate was calculated using a user-defined function in the Property Model Calculator.*

## Identification of Candidate Alloys

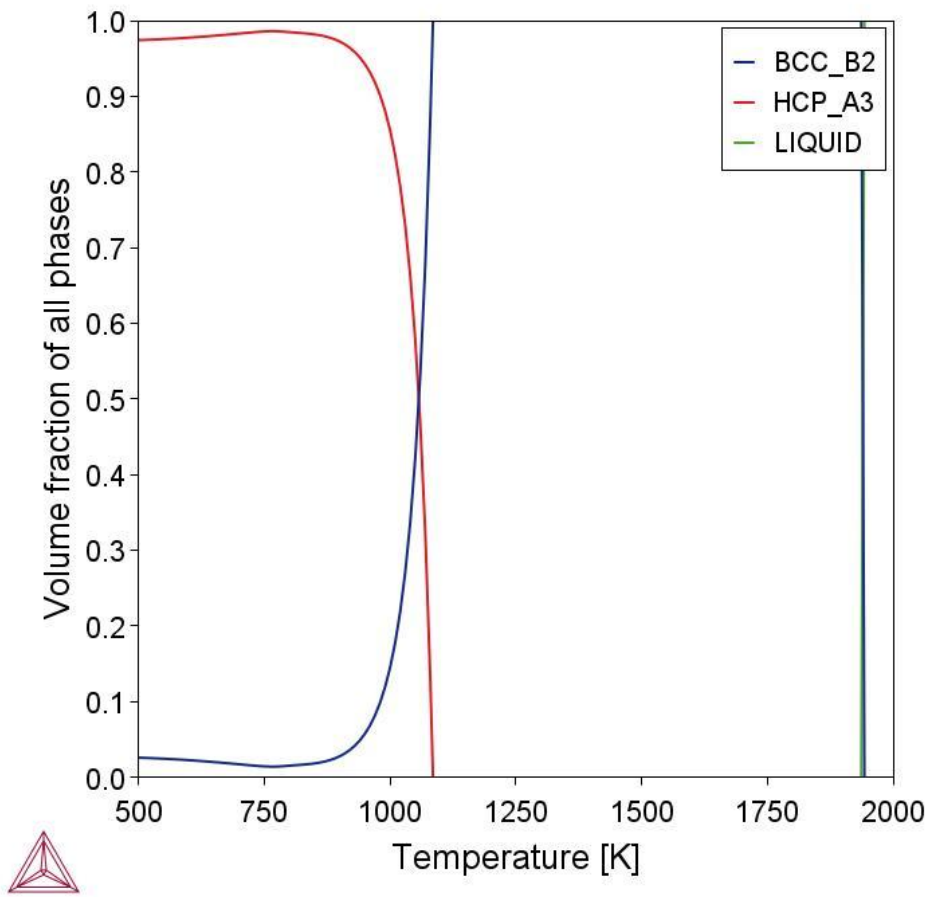
The results from the equilibrium solidification temperature interval, density, and cost estimate calculations for the randomized titanium alloy chemistries are exported and plotted in Python and presented in Figure 4. This plot gives an overview of the different properties and facilitates the alloy selection. Chemistries with a low solidification temperature interval, low density, and low-cost estimate are desirable for additively manufactured biomedical implants. The alloys satisfying these conditions lie in the lower left corner of Figure 4.



*Figure 4: Solidification interval, density, and cost estimate of 2000 randomized chemistries from the Ti-Nb-Zr-Sn-Ta-Fe-Mo system.*

### Phase Diagram of Candidate Alloy

Ackers et al. [1] performed calculations such as those shown in this example and supplemented the data with additional alloy design calculations. Through an alloy optimization procedure, four target titanium alloy chemistries are identified for further investigation in their study. The calculated phase balance as a function of temperature for one of the identified chemistries is presented in Figure 5. This shows the alloy has a narrow solidification temperature range, a beta transus of 1085 K, and that no deleterious phases are predicted to form.



*Figure 5: Phase fractions of a Ti-5Nb-3Zr-1.5Sn [wt.%] alloy as a function of temperature.*

## Reference

[1] M. A. Ackers, O. M. D. M. Messé, U. Hecht, Novel approach of alloy design and selection for additive manufacturing towards targeted applications. *J. Alloys Compd.* 866, 158965 (2021).