Application Example

Titanium Alloy Design for Additive Manufacturing

Identify candidate alloy chemistries for additive manufacturing applications.

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.

Learn How Thermo-Calc Can Help You:

- **Rapidly screen candidate alloy chemistries for additive manufacturing**
- **Identify candidate chemistries for use in specific applications**
- **Improve your final product by selecting for optimized properties**
- **Reduce the risk of defect formation during manufacturing**
- **Obtain a cost estimate of candidate alloys based on raw materials**

Products Used

Thermo-Calc

Databases:
Titanium and TiAl-based Alloys Database (TCTI)

Add-On Modules:
None used

SDKs:
None used

Materials & Applications

- Titanium Alloys
- Alloy Design
- Additive Manufacturing

Thermo-Calc Software

ABOUT THE EXAMPLE

This example shows how Thermo-Calc can be used to accelerate the design of titanium alloys for additive manufacturing to be used in biomedical applications.

In this example, inspired by the work of Ackers et al.[1], the Property Model Calculator in Thermo-Calc is used to run batch calculations that are used to identify candidate titanium alloy chemistries for biomedical implant applications. The example uses the thermodynamic and properties database TCTI, which is our Ti/TiAl-based Alloys Database.

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.

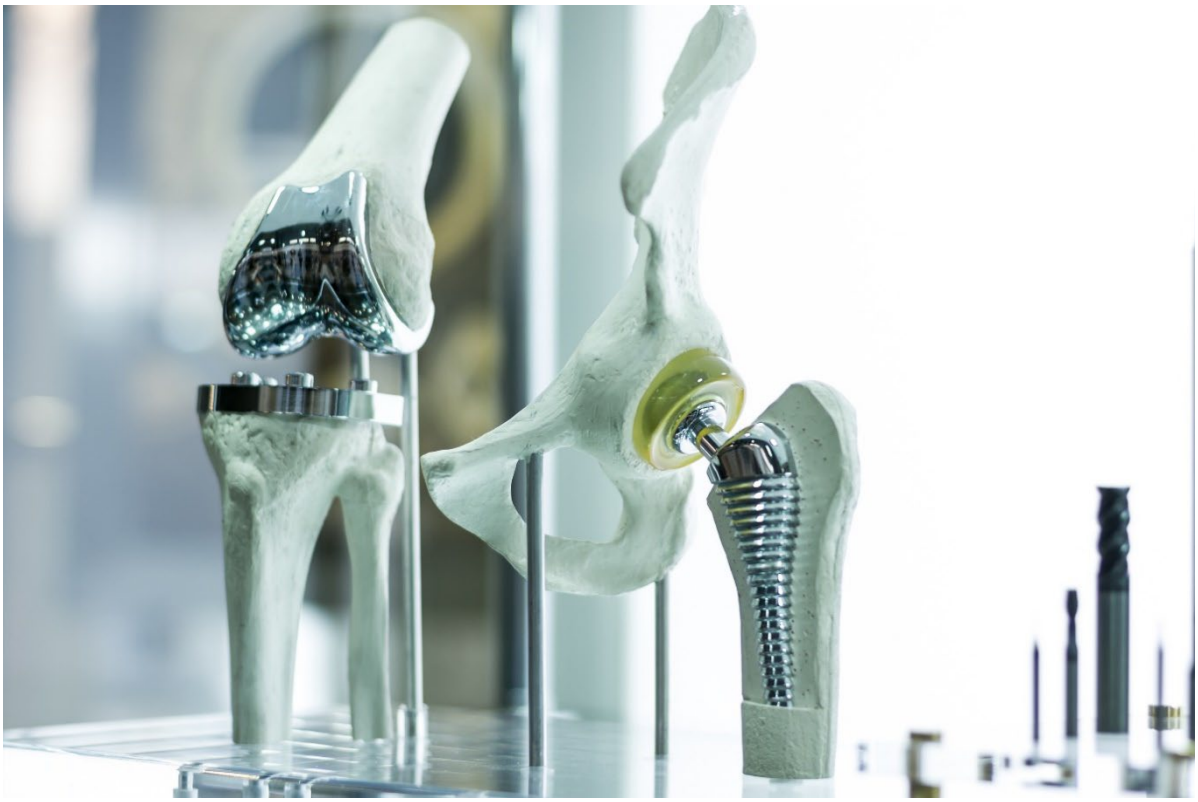

Figure 1: A display of biomedical implants. Thermo-Calc can be used to accelerate the development of alloys used in such applications.

[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).

EXAMPLE CALCULATIONS AND EXPLANATIONS

Chemistry Variation

To explore the chemistry space, 2000 alloy chemistries are randomly generated in the software 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.

Row	Ti	Nb	Zr	Sn	Ta	Fe	Mo	Composition unit
2	62.3587	9.3369	9.6195	0.9041	7.6729	1.2911	8.8167	mass_pct
3	78.8754	0.7386	2.2268	0.0910	7.6715	3.4857	6.9111	mass_pct
4	68.8677	1.6185	9.8662	3.6442	5.6279	3.4887	6.8868	mass_pct
5	67.9341	9.7190	2.6998	9.5054	2.1664	3.7831	4.1921	mass_pct
6	68.4690	8.5234	1.5777	1.1610	3.8797	8.9117	7.4776	mass_pct
7	61.0659	8.8489	9.9402	9.9985	0.6289	3.2166	6.3010	mass_pct
8	79.1175	4.8786	2.4185	0.5925	8.9232	2.6322	1.4374	mass_pct
9	55.0382	8.6810	2.3114	8.7500	9.1645	8.5843	7.4705	mass_pct
10	71.7643	9.6840	0.4953	1.4800	0.8186	6.7158	9.0418	mass_pct
11	82.7582	1.4871	4.3851	0.4264	2.3989	1.3257	7.2186	mass_pct
12	77.5186	4.3771	1.2897	4.9145	6.5420	2.4371	2.9209	mass_pct
13	59.5487	6.6860	9.4573	9.2022	5.6950	6.7131	2.6977	mass_pct
14	63.9840	7.2456	6.3935	5.7221	2.7397	6.4077	7.5075	mass_pct
15	79.9129	1.5096	0.8807	4.9083	2.1926	9.7852	0.8107	mass_pct
16	69.0185	9.4997	1.2520	5.3210	1.7614	9.3769	3.7705	mass_pct
17	71.3783	5.2489	2.4214	7.9737	7.0815	2.0980	3.7982	mass_pct
18	73.5836	0.1734	3.6913	8.4834	6.7711	6.6507	0.6466	mass_pct
19	72.2557	4.3117	3.9514	5.3429	2.7111	2.7514	8.6759	mass_pct
20	61.5221	8.5778	3.4971	2.5214	6.5553	9.6018	7.7246	mass_pct
21	72.8899	1.4153	0.7985	9.2022	4.6391	4.9649	6.0900	mass_pct
22	71.7877	1.1679	4.7851	6.8302	0.4809	5.2596	9.6885	mass_pct
23	69.1699	8.4940	3.0962	5.5482	1.8971	3.4442	8.3505	mass_pct
24	57.9056	3.0363	8.8786	9.9721	8.6502	2.6491	8.9081	mass_pct
25	69.1788	8.4272	5.8203	4.0018	3.4381	0.5675	8.5663	mass_pct
26	72.1222	6.5906	5.9411	4.6207	0.1849	5.5116	5.0288	mass_pct
27	67.4834	1.8842	4.9695	1.0659	5.2487	9.8929	9.4554	mass_pct
28	65.1552	1.9061	7.7995	7.2938	7.6326	4.4187	5.7942	mass_pct
29	59.0726	5.5256	5.0888	4.7176	9.1839	6.7739	9.6376	mass_pct
30	81.2528	1.8499	1.3792	0.3294	3.9906	9.4744	1.7237	mass_pct
31	58.9996	6.3094	9.5181	6.6043	9.8360	0.8103	7.9223	mass_pct
32	73.0018	5.5267	7.8706	2.0157	4.1689	6.3873	1.0291	mass_pct
33	59.1130	8.7706	9.7123	0.8968	9.3997	7.8082	4.2993	mass_pct
34	77.5449	5.6347	0.9450	6.9149	4.5393	0.4862	3.9350	mass_pct
35	60.6973	6.4159	9.3904	2.3318	8.2238	9.2143	3.7266	mass_pct
36	66.7385	5.5399	8.3456	4.8116	2.8268	1.8821	9.8556	mass_pct
37	65.1947	1.7369	9.1878	7.8322	8.4691	7.3469	0.2325	mass_pct
38	63.9936	6.2596	6.5683	6.2586	9.9062	5.9898	1.0239	mass_pct
39	66.2970	8.0817	2.8942	9.6753	4.6502	2.3008	6.1007	mass_pct

Figure 2: A sampling of the 2000 alloy chemistries that were randomly generated in Thermo-Calc.

Liquidus and Solidus Temperature to Rapidly Screen Alloy Chemistries

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 3. 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. If required, users can get a more accurate estimate of the solidification interval using the Scheil calculator in Thermo-Calc.

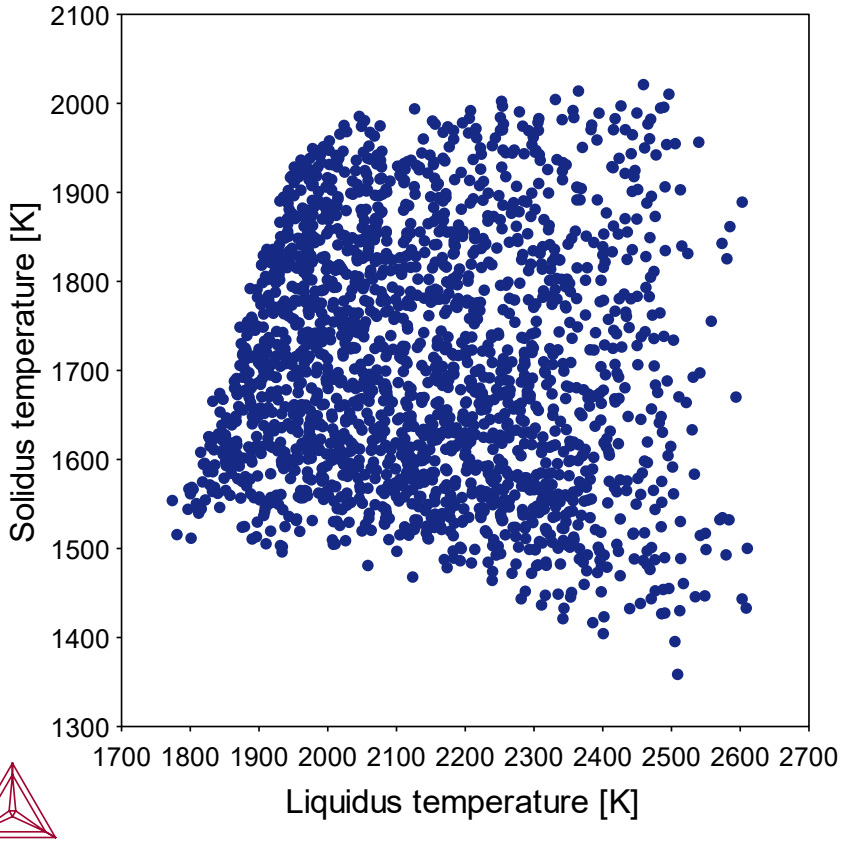

Figure 3: Calculated liquidus and solidus temperature data for 2000 randomized chemistries from the Ti-Nb-Zr-Sn-Ta-Fe-Mo system.

Low Density for Improved Patient Comfort

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 4.

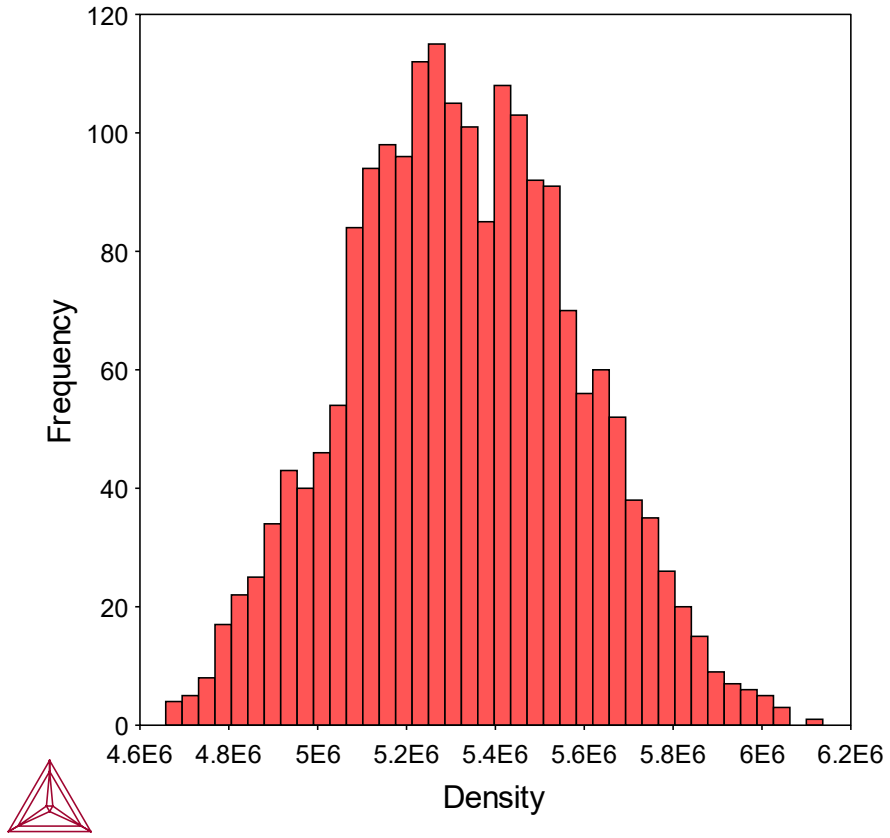

Figure 4: Calculated density of 2000 randomized chemistries from the Ti-Nb-Zr-Sn-Ta-Fe-Mo system. Low density is favorable for biomedical applications.

User-defined Functions for Cost Estimates of Raw Materials

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 5.

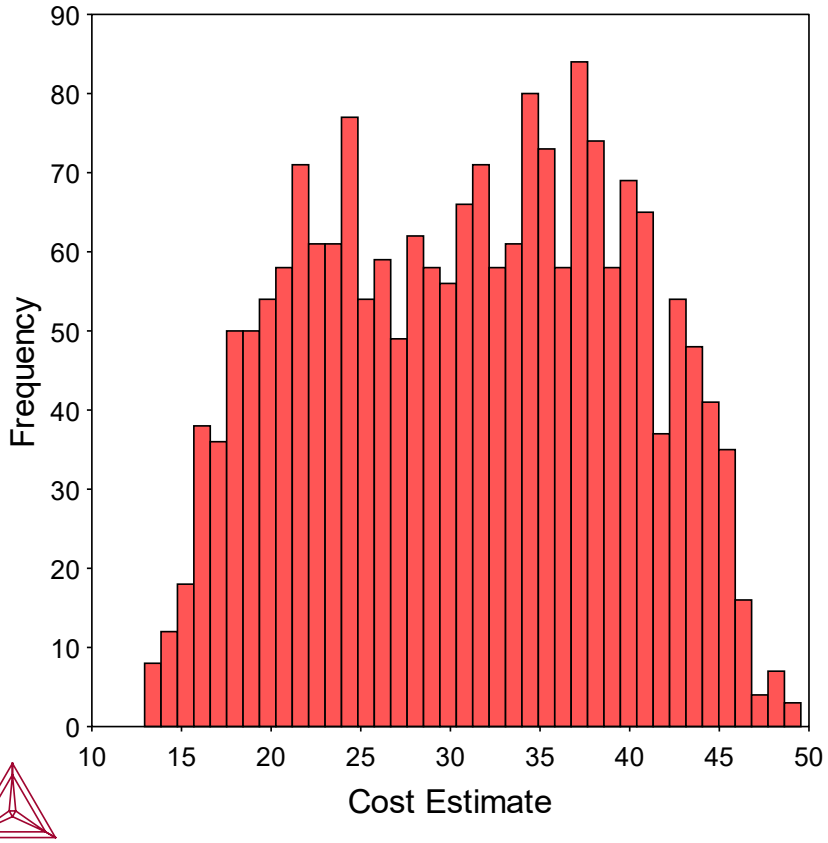

Figure 5: Cost estimate histogram for 2000 randomized chemistries from the Ti-Nb-Zr-Sn-Ta-Fe-Mo system. The cost estimate was calculated using a user-defined function in the Property Model Calculator.

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 6. 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 6.

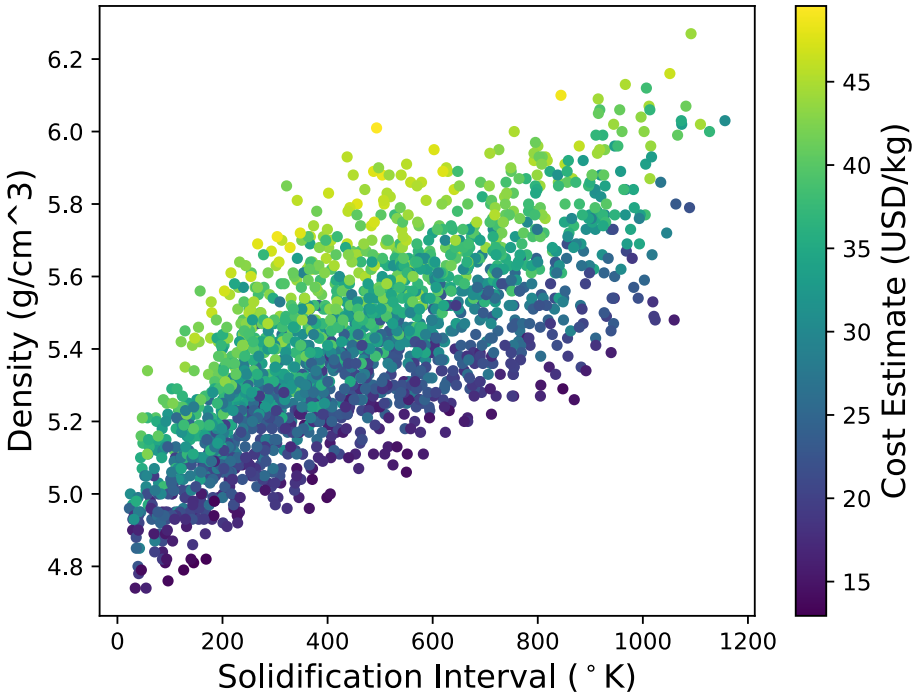

Figure 6: Solidification interval, density, and cost estimate of 2000 randomized chemistries from the Ti-Nb-Zr-Sn-Ta-Fe-Mo system. The alloys in the lower left corner are most suitable for biomedical applications.

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 7. 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.

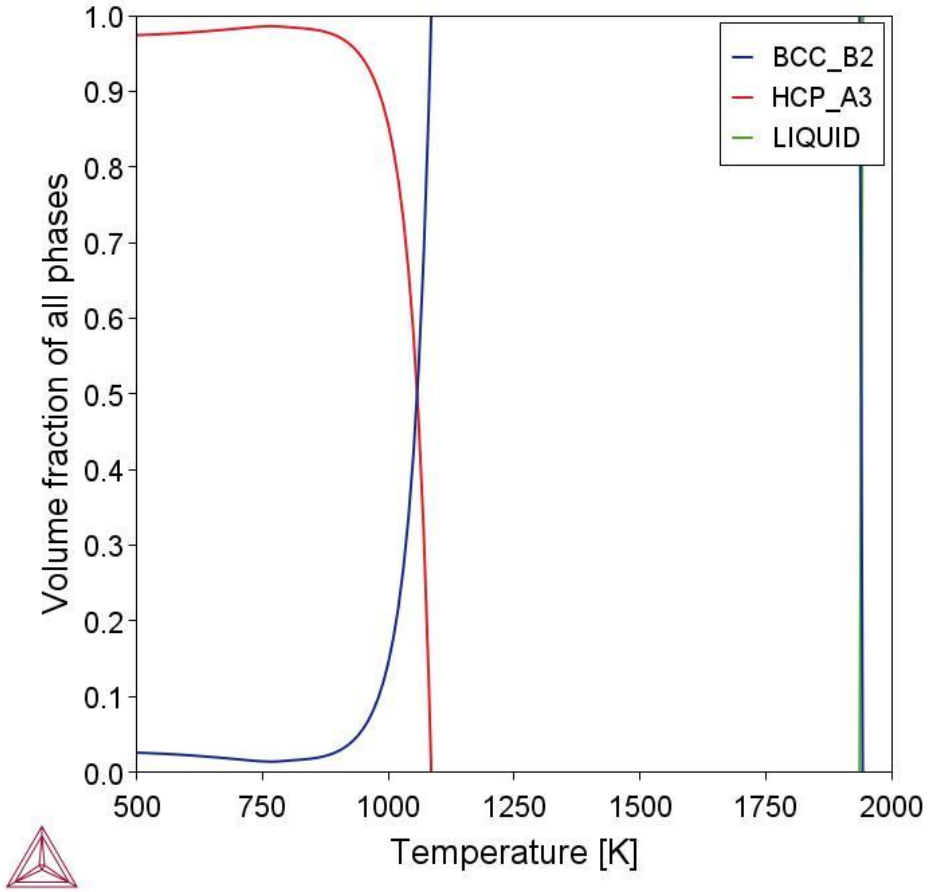

Figure 7: Phase fractions of a Ti-5Nb-3Zr-1.5Sn [wt.%] alloy as a function of temperature.

RUN THE CALCULATION

If you have a license for Thermo-Calc 2022b or newer and database TCTI4 or newer, you can run the calculations this example was based on. Results may vary as the source calculations may differ slightly from the calculations presented here.

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.*

ADDITIVE MANUFACTURING TOOLS IN THERMO-CALC

Thermo-Calc Software offers a range of calculators and tools that can be used for applications to additive manufacturing. For example, once users have identified candidate AM alloy chemistries using the methods described in this example, you can move on to modeling the powder bed fusion process using the Additive Manufacturing Module, an Add-On Module in Thermo-Calc. The Module has a unified treatment of process parameters and alloy dependent thermophysical properties, making it unique amongst AM simulation software. You can learn more about the Additive Manufacturing Module by watching our webinar, which you can access by clicking the image below.