FIRST DRAFT

Modelling Properties of Titanium Alloys: during Solidification or at Elevated Temperatures

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Abstract: This paper describes the development of a computer software, JMatPro, for calculating the properties and behaviour of commercial alloys. These properties are wide ranging, including but not limited to: thermodynamic properties, physical and thermophysical properties, mechanical properties, and TTT/CCT diagrams of multi-component alloys. The aim of this paper is to demonstrate some of its features on simulating the properties and behaviour of titanium alloys, concentrating on two areas:

- Physical and thermophysical properties during solidification (from room temperature to the liquid state).
- High temperature mechanical properties, including creep properties and high temperature strength.

Key words: Modelling, Material properties, High temperature strength, Solidification, Titanium alloys

1 Introduction

The physical, thermophysical and mechanical properties of materials are vital inputs for process design/modelling. However, while such properties are relatively easy to measure at room temperature, they become increasingly difficult or even impossible to determine experimentally at high temperatures. To overcome these difficulties and provide reliable and cost effective data for process modelling, sound physical models are required so that such properties can be readily calculated. The present paper demonstrates the capabilities of a well-established computer software JMatPro that is able to provide many of the properties required.[1,2]

In earlier papers, capabilities of JMatPro on titanium alloys have been introduced in details.[3,4] Phase diagram modelling has reached a stage where light elements C, O and N can be accurately accounted for in titanium alloys. Not only are critical features such as the β-transus predicted successfully but further information such as the amount of α and β as a function of temperature, elemental partitioning, and activity of all elements are all readily obtained.[3] JMatPro can also provide a wide range of information regarding TTT/CCT diagrams, mechanical properties, physical and thermophysical properties for titanium alloys.[4] The calculations utilise well-established material models and have taken into account the effect of microstructure. It is the aim of this paper to demonstrate some new features of the JMatPro software on calculation the properties and behaviour of titanium alloys, concentrating on the following two areas:

- Physical and thermophysical properties are critical to cast/solidification simulation. These properties are calculated for the whole temperature range including in the liquid phase. Where relevant, properties are given for each phase.
- High temperature mechanical properties, including creep properties and high temperature strength. The proof/tensile strength and hardness are calculated at any temperature up to the melting point.

The calculated results have been extensively validated against experiment for a wide range of commercial titanium alloys.

2 Use in solidification modelling

Casting process simulation is now widely accepted as an important tool in product design and process development to improve yield and casting quality. However simulation packages ultimately rely on high quality inputs concerning physical, thermophysical and mechanical properties of the relevant alloys. Although they usually have a built-in property database where experimental property data of known alloys are stored, the number of alloys for which information is available is generally limited. Also, the information for a given alloy may be incomplete in that not all properties have

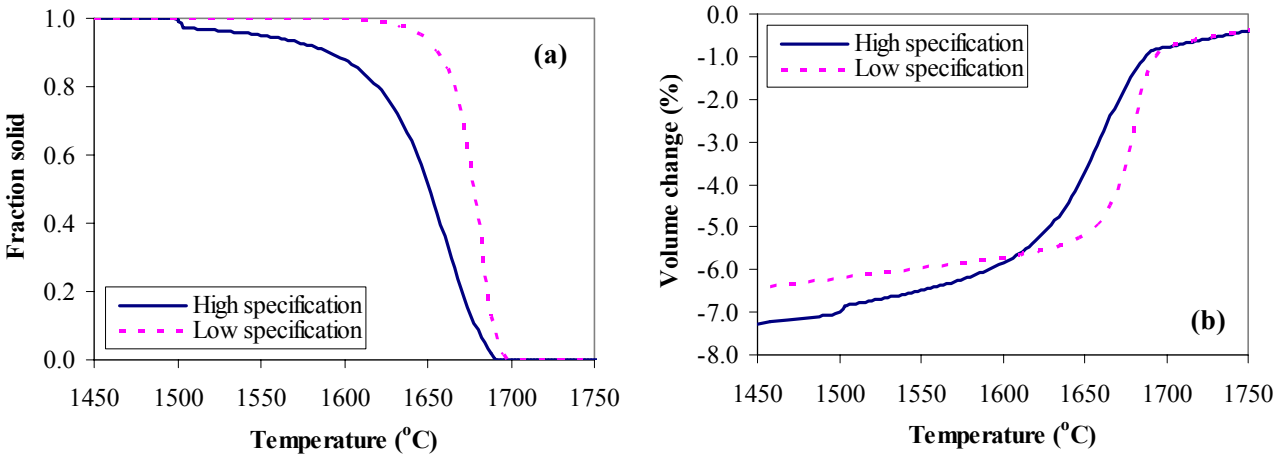

Figure 1. Calculated properties as a function of temperature plots for IMI 834 alloy of hign/low specification, (a) fraction solid, and (b) volume change.

been measured. Furthermore, information from a variety of sources is sometimes used to build up the database for one specific alloy. This can lead to inconsistent results as the composition of the alloys used for database creation may not be identical. It is known that various important properties are sensitive to small changes in composition. To overcome the lack of data, it is highly desirable to develop computer models for calculation of the physical and thermophysical properties of specific multi-component alloys during solidification. JMatPro, an acronym for ***J***ava-based ***Mat***erials ***Pro***perties software, provides such a capability [5].

The physical and thermophysical properties of the liquid and solid phases critical to casting/solidification modelling include the fraction solid transformed, heat release, thermal expansion and conductivity, volume, density and viscosity, all as a function of temperature. Within the framework of the development of JMatPro, extensive work has been carried out on the creation of sound, physically based models for these properties. As well as providing comprehensive data for all critical properties, it is possible to examine (1) how changes in the composition of an alloy within its specification range can affect properties during solidification, and (2) how properties of the liquid can vary in the mushy zone, rendering simple extrapolation of high temperature experimental data inadequate for estimating properties in the mushy zone.

Titanium alloy IMI 834 has been used as an example to demonstrate the composition sensitivity of physical and thermophysical properties. This alloy has a wide specification range: Al: 5.5~6.1, Sn: 3.0~5.0, Zr: 3.0~5.0, Nb: 0.5~1.0, Mo: 0.25~0.75, Si: 0.2~0.6, O: 0.075~0.15 (wt%). In later context, HS (high specification) means that each alloying element takes its maximum amount, whereas LS (low specification), the minimum amount. Figure 1(a) shows the calculated fraction solid as a function of temperature for IMI 834 of HS and LS. The solidification of the alloy follows the Scheil-Gulliver condition in the calculations, which assumes that solute diffusion in the solid phase is small enough to be considered negligible and that diffusion in the liquid is extremely fast, fast enough to assume that diffusion is complete. As can be seen that the solidification curve of HS and LS differs significantly. The solidus/liquidus temperatures for HS and LS are 1500/1691°C and 1600/1698°C, respectively. As a result of this difference in the solidification curve, the change of volume, density, thermal expansion coefficient and thermal conductivity of the alloy of HS and LS during solidification all differ. The difference in the volume change is shown in Figure 1(b) as an example. Other properties that JMatPro can provide include Young's/bulk/shear moduli, Poisson's ratio, electrical conductivity/resistivity, liquid viscosity, enthalpy, specific heat and latent heat.

Another advantage of JMatPro is that the properties of each phase during solidification can be calculated[4]. Such information can be critical for predicting casting defects but is difficult or impossible to obtain experimentally, e.g. the behaviour of the liquid phase in the mushy zone. Figure 2 shows the density of different phases in IMI 834 of LS during solidification.

3 High temperature mechanical properties

A key element in process modelling of metallic alloys is the high temperature mechanical behaviour, particularly

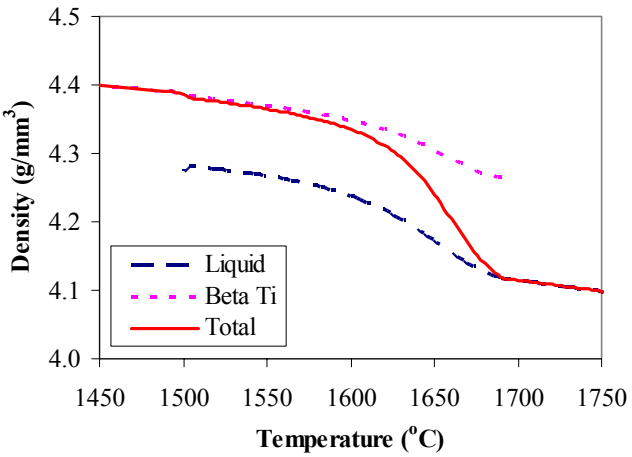

Figure 2. Calculated density of IMI834 of low specification during solidification.

with respect to flow stress as a function of temperature and strain rate. It is therefore of substantial interest to develop physically based models that can both account for known experimental data and be extrapolated into new and very different regimes with great confidence.

3.1 Creep properties

Creep of metals and alloys is generally analysed in terms of three components: here we will consider steady-state or secondary creep rate. The creep rate of beta titanium alloys is described by the following expression:[6,7]

$$\dot{\varepsilon}_s = AD(Gb/RT)(\sigma/E)^n \qquad (1)$$

where $\dot{\varepsilon}_s$ is the secondary creep rate, A a material dependent parameter, D the diffusion coefficient, b the Burgers vector, σ the applied stress, G and E the shear and Young's modulus of the matrix at the creep temperature, respectively. The creep rate is independent of grain size in the practical range for temperature and stress for beta alloys.[8] The value of n is related to the mechanism of the creep and can take on a range of values.[Error! Bookmark not defined.] The effect of grain size on the creep properties of alpha and alpha+beta alloys can be quite complicated.

Almost all of the input parameters for Eq.(1) can be obtained through JMatPro. G and E are calculated through the physical property calculations, and D is calculated from the diffusion database. This leaves A as the only adjustable parameter, fitted with experimental results. Figure 3 shows a comparison between calculated and measured secondary creep rates for beta titanium alloys, where the value of n is taken as 4.[7] The work presented here on the creep properties of beta titanium alloys is part of an ongoing project, where research on alpha and alpha+beta alloys is in progress. As rupture strength is an alternative design criterion in practice, the calculation procedure has been extended to include this property by employing Monkman-Grant relationship.[9]

$$t_r = \alpha \dot{\varepsilon}_s^{\beta} \qquad (2)$$

where t_r is the time to rupture while α and β are evaluated empirically, Figure 4. The values of α and β derived from the present work is in very good agreement with those from Monkman and Grant. It should be noted that this relationship applies to all titanium alloys regardless of alloy type and microstructure.

3.2 High temperature strength

JMatPro utilises well-established strength equations for yielding and utilises the classic Hall-Petch equation to calculate strength as a function of grain size.[4] The

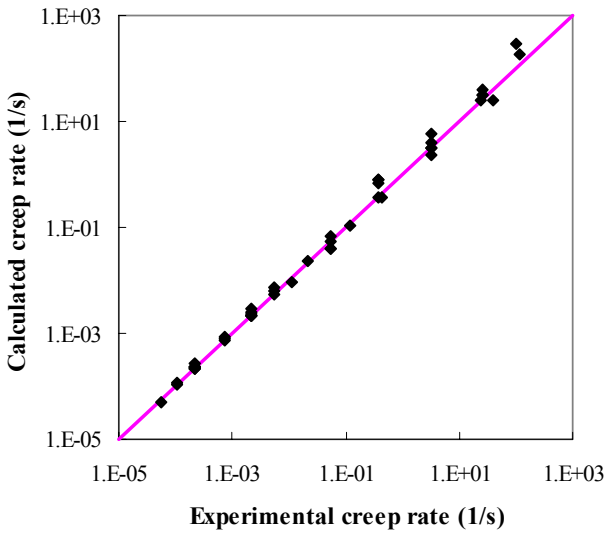

Figure 3. Comparison between experimental and calculated secondary creep rate for titanium alloys

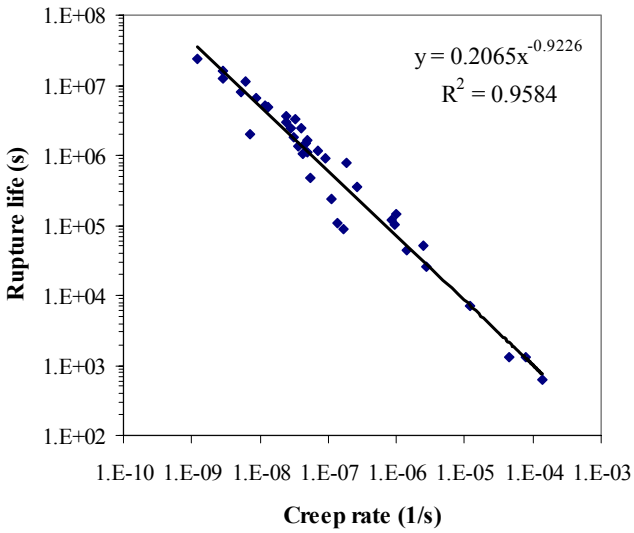

Figure 4. Monkman-Grant relationship for titanium alloys

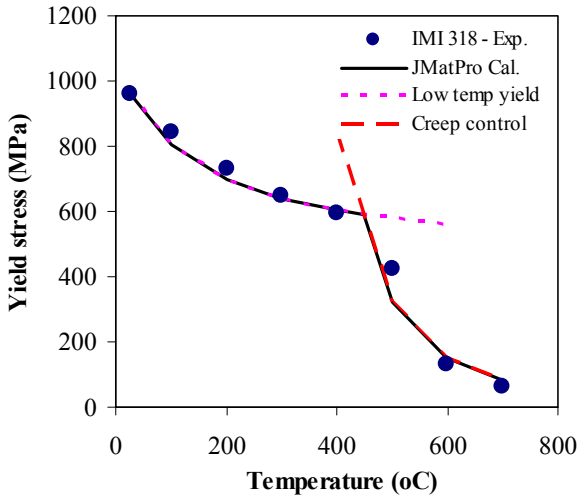

Figure 5. Comparison between experimental and calculated yield stress for IMI 318 (Ti-6Al-4V).

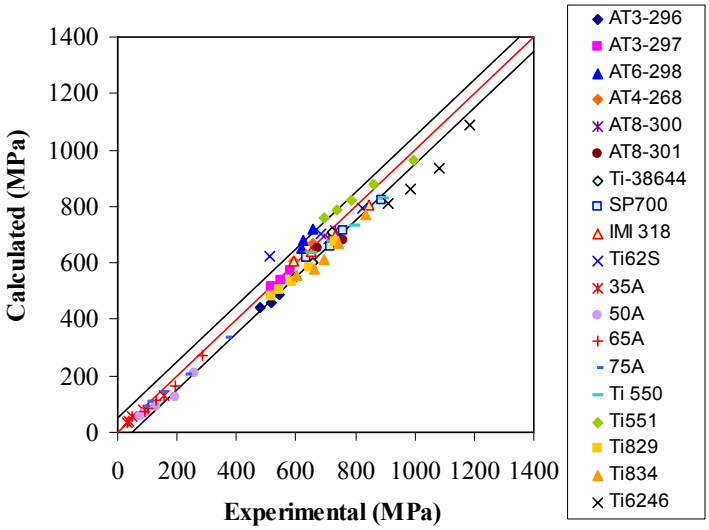

Figure 6. Comparison between experimental and calculated yield stress for various titanium alloys.

model utilises a generalised pair interaction approach for solid solution strengthening that has been validated for many types of alloys, including steels, Ti-alloys and Ni-based alloys. Generally speaking, room temperature strength decays monotonically with increasing temperature. Examination of the yield stress as a function of temperature, $\sigma(T)$, for many steels, nickel superalloys and titanium alloys shows a clear correlation between the rate of decrease in $\sigma(T)$ with increasing temperature and the room temperature yield stress (σ_{RT}). The decay is well matched using an exponential form of the following type:[1]

$$\sigma(T) = a + \beta \exp(-Q/RT) \qquad (3)$$

where α and β are constants directly related to σ_{RT} and the value of Q, which is determined empirically through regression analysis based on the data for a wide range of titanium alloys.

As the temperature is raised to high levels the alloy will yield via creep when the strain rate of the mechanical test is equal to or slower than the creep rate at the testing temperature. In this region, the critical stress is calculated by employing Eq.(1) in reverse and assuming the creep rate $\dot{\varepsilon}$ equals the strain rate. Figure 5 shows the good agreement between experimental and calculated yield stress vs. temperature for an IMI 318 alloy (equivalent to Ti-6Al-4V). The sharp fall in strength at around 450°C corresponds to the point where flow is being controlled via creep mode. The switch from low temperature yield to creep controlled yield is very obvious. High temperature strength calculations were carried out for a wide range of commercial titanium alloys and comparison against experimental values is shown in Figure 6. Flow stress as a function of strain rate can also be calculated.[10]

4 Summary

It has been demonstrated that the JMatPro software can provide a wide range of physical, thermophysical, and mechanical properties for Ti-alloys over a wide temperature range. The calculations are based on well-established physical models and the sensitivity to composition/microstructure has been considered. The calculated results have been extensively validated against experiment for a wide range of commercial titanium alloys. The good agreement gives confidence for calculations made for new combinations of alloying elements and heat treatments, which would otherwise require time consuming and expensive experimentation.

References

[1] N. Saunders et al., JOM, 2003, 55(12): 60-65
[2] Z. Guo et al., in "Modelling of Casting and Solidification Processes 2004", Kaohsiung, Taiwan, 2004: 563-570
[3] N. Saunders, in "Titanium '95: Science and Technology", Institute of Materials, London 1996: 2167
[4] N. Saunders et al., in "Ti-2003: Proc. of The 10th World Conference on Titanium", Hamburg, Germany, 2003: 1397
[5] http://www.sentesoftware.co.uk/biblio.html, Sente Software Ltd., 2005.
[6] J. Koike et al., Mater. Sci. Eng. A, 1996, A213: 98-102
[7] C. Schuh, D.C. Dunand, Scripta Mater., 2001, 45: 1415-21
[8] G. Malakondaiah, P.R. Rao, Scripta Metal., 1981, 15: 1107-1110
[9] F.C. Monkham, N.J. Grant, Proc. Amer. Soc. Test. Mater., 1956, 56: 593-620
[10] N. Saunders et al., in "22nd CAD-FEM Users' Meeting 2004", 10-12 Nov. 2004, Dresden, Germany, No.2.4.6