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An Integrated Approach To The Calculation Of Materials Properties For Ti-Alloys

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Abstract

For the past 3-4 years work has been undergoing on the development of a new computer programme (JMatPro) for calculating general material properties of multi-component alloys. These properties are wide ranging, including stable and metastable phase equilibria, thermo-physical and physical properties (from room temperature into the liquid state), TTT/CCT diagrams, martensite temperatures, proof and tensile stress, hardness, stress/strain diagrams, etc. A feature of the new programme is that the models are based on sound physical principles rather than purely statistical methods. Thus many of the shortcomings of methods such as regression analysis can be overcome. For example, sensitivity to microstructure can be included. Prediction of physical properties relevant to solidification can now also be made, which is of vital importance for process simulation but extremely difficult to measure or otherwise estimate. This paper provides a background to the scientific models used by JMatPro and numerous examples of calculated results for various properties in Ti-based alloys will be presented, with the emphasis being placed on validation of calculated results against experimental observation in multi-component commercial alloys.

1 Introduction

Thermodynamic modelling tools for exploring equilibrium phase relationships in complex materials are being increasingly used in industrial practice [1]. Such calculations benefit the end user, whether they work in industry or academia, but the applicability of phase equilibrium calculations often falls short from directly providing the information that is actually required. For example, thermodynamic modelling helps towards the understanding of changes in phase constitution of a material as a function of composition or temperature. However, a considerable jump is then needed to convert this information into the properties being targeted by the end user, e.g. TTT/CCT diagrams, mechanical properties, thermo-physical or physical properties.

To overcome these limitations a new computer programme has been developed, called JMatPro, an acronym for *J*ava-based *Mat*erials *Pro*perties software. The approach adopted in the development of the new programme has been to augment the thermodynamic calculation by incorporating various theoretical models and additional property databases that will allow a quantitative calculation for the requisite materials property within a larger software structure. This then enables a clear path to be created between the thermodynamic calculation and the final product that is required, i.e. the materials property itself.

The purpose of the present paper is to demonstrate how the translation from thermodynamic calculations to general materials properties has been achieved and to present examples of applications to multi-component commercial alloys, with particular emphasis on the validation of the calculated property against experimental values.

2 Results and Discussion

2.1 Thermodynamic calculations

The current software utilises core minimisation routines developed for the PMLFKT software programme by Lukas et al.[2] and recently extended by Kattner et al [3]. to multi-component alloys. These sub-routines have been converted from Fortran to C and, in addition, a comprehensive set of new sub-routines written in C/C++. These new subroutines (i) provide automatic start points, (ii) original algorithms to ensure that highly reliable results for multi-component, multi-phase equilibria can be routinely calculated, (iii) algorithms for stability checking that also continually monitor the composition of the various phases that may have miscibility gaps or the potential for ordering and (iv) highly robust routines for finding phase boundaries. Thermodynamic calculations have been applied directly to commercial Ti-alloys [4] and Fig. 1 shows a comparison between experimentally observed and calculated β-transus temperatures for a wide variety of multi-component Ti-alloys, while Fig. 2 shows the comparison between experimentally observed vol% α and calculated mole % α for Ti-6Al-4V alloys as a function of temperature.

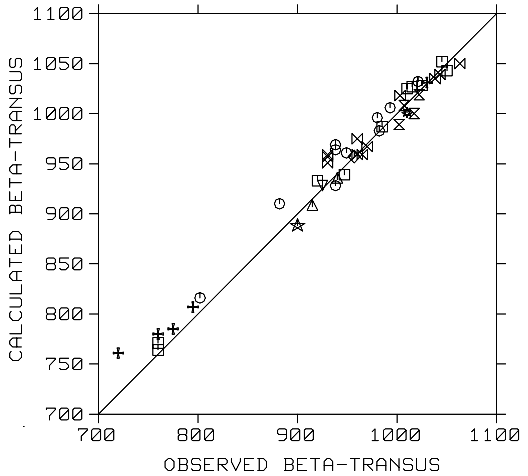

Figure 1. Comparison between experimentally observed and calculated β-transus temperatures for various multi-component Ti-alloys. (see Saunders [4] for references to experiment values).

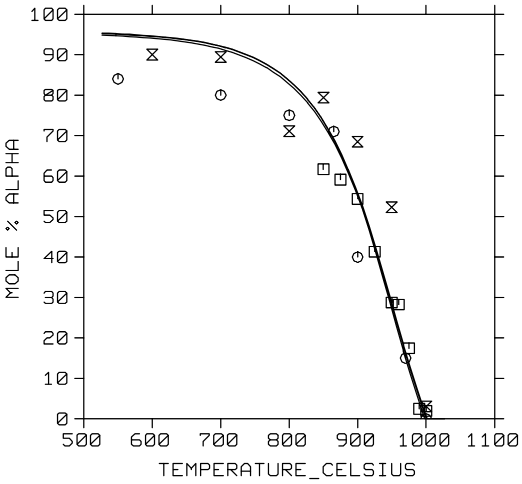

Figure 2. Comparison between experimentally observed vol% α and calculated mole % α for Ti-6Al-4V alloys. (see Saunders [4] for references to experiment values).

2.2 TTT/CCT calculations

The evolution of volume fraction during solid-state transformation can be described using the well known Johnson-Mehl-Avrami (JMA) equation, which, for spherical particles and isothermal conditions, can be expressed as [5]:

$$x = \frac{V}{V_{eq}(T)} = 1 - \exp\left(-\frac{\pi}{3} N_r G_r^3 t^4 \right) \tag{1}$$

where T is the temperature, V is the volume fraction transformed at time t, V_{eq} is the equilibrium amount of precipitate, N_r is the nucleation rate and G_r is the growth rate. A more general equation is usually used in practice, taking the form

$$x = 1 - \exp(-\mathrm{k}\, t^{\mathrm{n}}) \tag{2}$$

where *k* is a constant and usually empirically evaluated for each temperature. *n* is often called the Avrami exponent which usually has to be evaluated empirically and takes values between 1-4. The various values of *n* are usually linked to factors such as the shape of the precipitate, whether the nucleation or growth rate is constant, or varying with time, or whether nucleant site saturation has been achieved.

Recently an approach has been developed [6] with the aim of including a more explicit representation of nucleation and growth rates as shown in eq.1 while maintaining the flexibility of approach more inherent in the generalised form shown in eq.2. This has been achieved by incorporation of the effect of shape in the basic equations after Martin et al. [7]. Excellent results have been obtained for various alloy types using this approach [8]. A significant factor in its success has been the capacity to use explicit values for transformation temperatures, equilibrium amounts and compositions for the precipitating phase, and allied thermodynamic factors such as driving forces obtained from thermodynamic calculation.

A further advantage of the current modelling method is that it reduces the number of input parameters that otherwise need to be evaluated. In consideration of nucleant density and precipitate shape, specific values are defined for the various types of precipitates, consistent with the dimensionality of the precipitate and potential nucleant site. We have considered the case of Widmenstatten growth, where the morphology of α is considered as having dimensional characteristics associated with a complex mixture of plates and needles rather than spheres. Two types of α precipitate are considered, those at the prior β grain boundary (GB) and those in the prior β grain interior (bulk) that have an increased barrier to nucleation. Nucleant densities consistent with formation at GBs and dislocation sites [9] are utilised.

Fig. 3 shows the subsequently calculated isothermal Time-Temperature-Transformation (TTT) diagram for Ti-1023 (α transformed=5%) compared with experimental observation [10,11]. It is possible to convert this diagram to a Continuous-Cooling-Transformation (CCT) diagram using well known additivity rules [12] and the subsequently calculated CCT diagram is shown in Fig. 4. It is recognised that phase transformations in Ti-alloys can be complex and the approach used here considers a fairly simple scenario. However, kinetics are dominated by the temperature of the β-transus because transformation rates increase rapidly at higher temperatures. This is shown in Fig. 5 for (i) Ti-6242Si, (ii) SP700 and Ti-1023 whose respective β-transus temperatures are typically 1000°, 900° and 800°C. Note that as the β-transus temperature increases, the critical cooling rate is increasingly controlled by the formation of bulk α rather than GB α. This is due to the preferential increase in kinetics of bulk α transformation in comparison to GB α as the temperature increases.

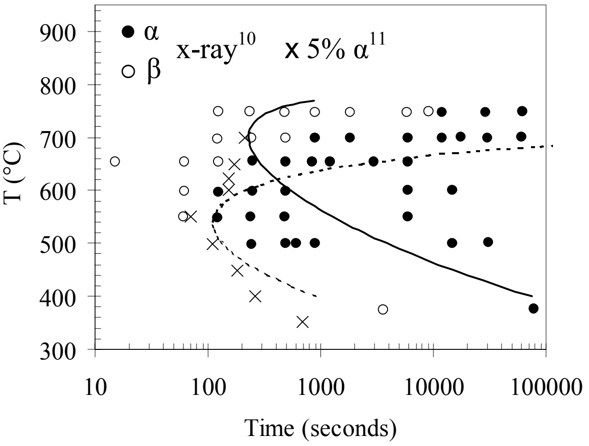

Figure 3. Experimentally observed[10,11] and calculated TTT diagram for Ti-1023. Full lines indicate α(GB), dashed lines denote α(bulk).

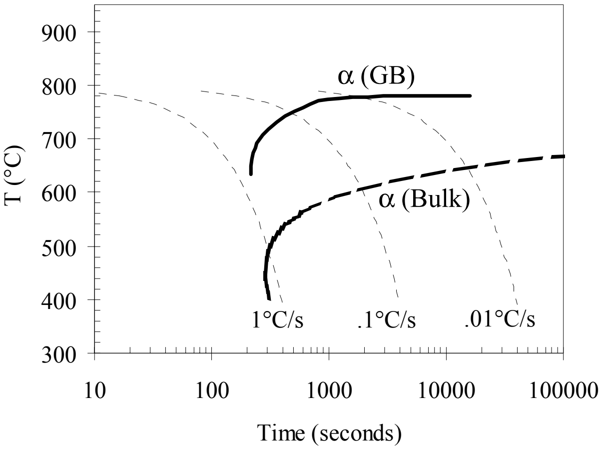

Figure 4. Calculated CCT diagram for Ti-1023

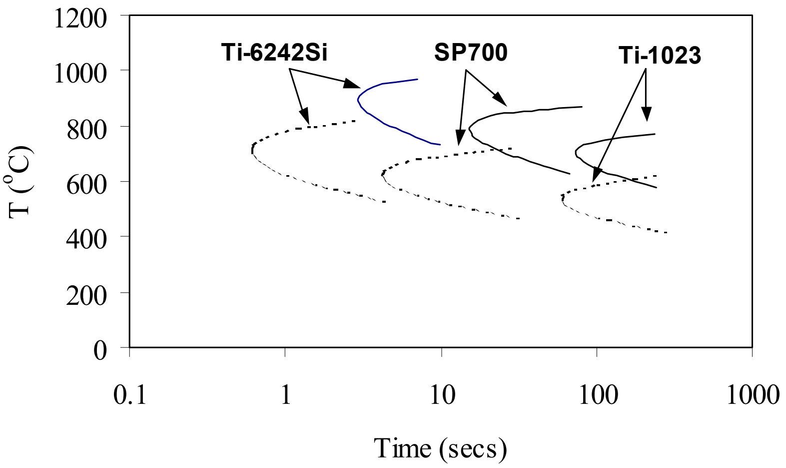

Figure 5. Calculated TTT diagrams (α transformed=1%) for Ti-6242Si, SP700 and Ti-1023. Full lines indicate α(GB) and dashed lines denote α(bulk).

2.3 Mechanical Properties

Many Ti-alloys are predominantly solid solution strengthened and, as such, the proof stress of the α and β phases can be calculated using the standard Hall-Petch equation [13], $\sigma_y=\sigma_o+k^{-1/2}$, where σ_y is the yield or proof stress, σ_o is the intrinsic flow stress, k is the Hall-Petch coefficient and d is the grain size. So that mechanical properties can be calculated for Ti-alloys, two types of databases have been created; one for flow stress and the other for Hall-Petch coefficients. These databases are similar in format to the thermodynamic ones in that they comprise input coefficients for the pure metals and solid solution strengthening coefficients as a function of pair-wise mixing of the various elements. All that is then required to calculate σ_y is the composition of the α and/or β phase and the grain size.

Most Ti-alloys are two-phase where the properties of the two phases are reasonably similar, in which case the total yield/proof stress can be obtained through the classical linear law of mixtures, which is a special case of a more generalised approach [14], and has worked extremely well for duplex stainless steels [6]. However, it is recognised that the approach will fail if morphologies become too complex, such as in certain aged β-alloys where omega is formed or when α_2 or martensite is present. Once the proof stress has been calculated, the ultimate tensile stress (UTS) and hardness can be derived from the inter-relationship between the proof stress, hardness and UTS described previously [15].

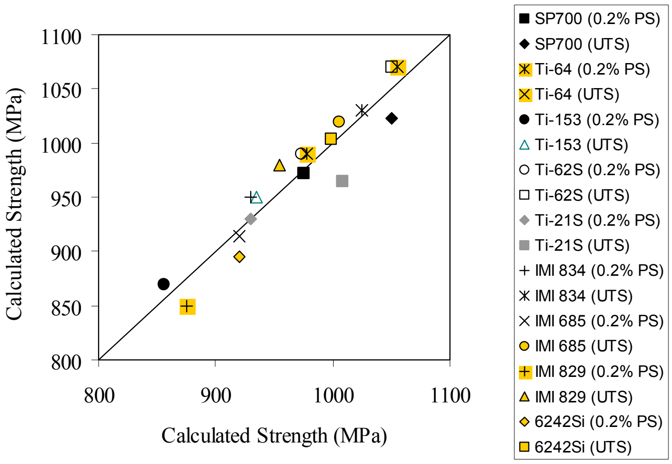

Figure 6. Comparison between calculated and experimentally observed 0.2% proof stress of various commercial Ti-alloys

Fig. 6 shows the agreement between calculated and experimentally observed 0.2% proof stress and UTS of a range of alloys comprising α, α/β and β types. The experimental results are taken from various manufacturers data sheets [16,17,18,19] and where information concerning grain size can be straightforwardly extracted. For the case of Ti-153 and Ti-62S, grain sizes after Niwa et al. [20] and Fanning [21] respectively, were used. For the case of the β alloys, these are considered in the solution treated condition rather than the aged condition where omega may form providing additional strength. Such strengthening can be taken into account but has not, as yet, been implemented. Where microstructures are predominantly Widmenstatten, eg. in α types, the lathe width is used as input for *d*. For the α/β types such as Ti-64 and SP700 an average grain size has been used. Fig. 7 shows a more detailed calculation for Ti-6Al-4V, where proof stress, UTS and hardness are shown as a function of grain size, while Fig. 8 shows stress strain curves calculated for average grain sizes of 1, 10 and 100μm.

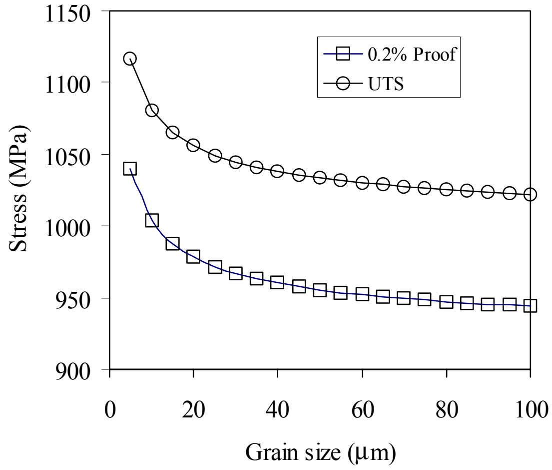

Figure 7. Calculated 0.2% proof and UTS for Ti-64 as a function of grain size.

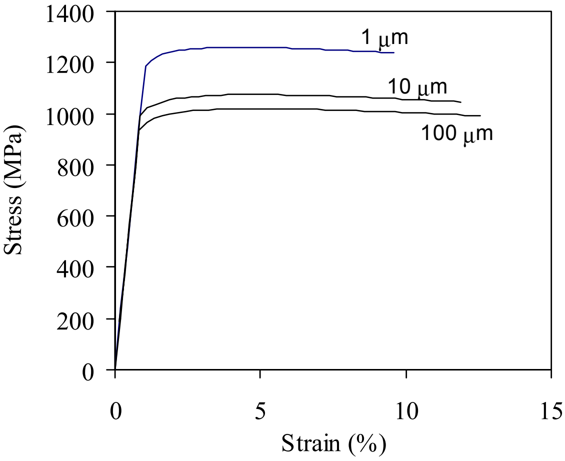

Figure 8. Calculated stress/strain curves for Ti-64 as a function of grain size.

2.4 Thermophysical and physical properties

Thermo-physical and physical properties are an important part of materials science, particularly for process modelling software, where properties such as thermal conductivity, various moduli, density, etc., are required as input before a simulation can proceed. Such properties can be readily measured at room temperature but, increasingly, these properties are required from room temperature well into the liquid state. A major achievement of the JMatPro programme is that such data can now be readily calculated for many types of different alloys [8,15,22,23,24]. The methodology is similar to that for solid solution strengthening but, instead, databases incorporating pure element data and pair interaction coefficients are required for physical properties rather than mechanical properties [8,15,22]. Firstly, the requisite properties for the α and β phases are calculated and then combined using a model accounting for the effect of microstructure on the final property [14]. Although such models have been implemented in JMatPro, they only have an important effect when the properties of the phases in the alloy differ significantly.

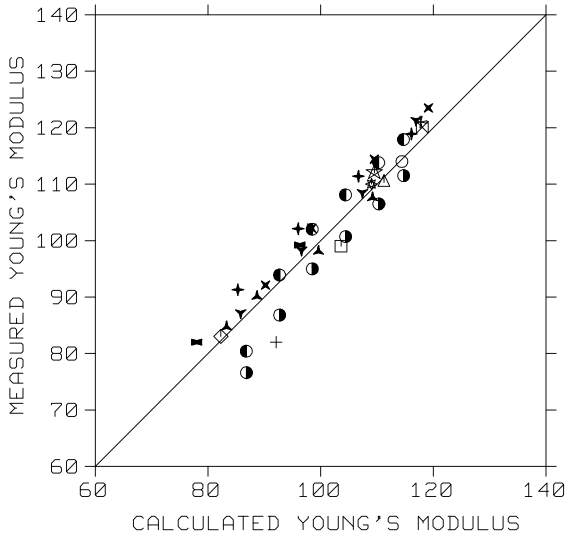

Figure 9. Comparison between experimentally observed [16,17,18,19] and calculated Young's moduli (GPa) for various Ti-alloys.

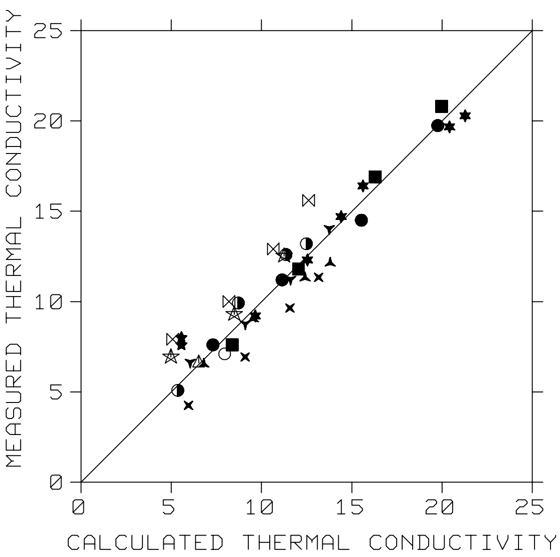

Figure 10. Comparison between experimentally observed [16,17,18,19] and calculated Thermal Conductivities (W m^{-1} K^{-1}) for various Ti-alloys.

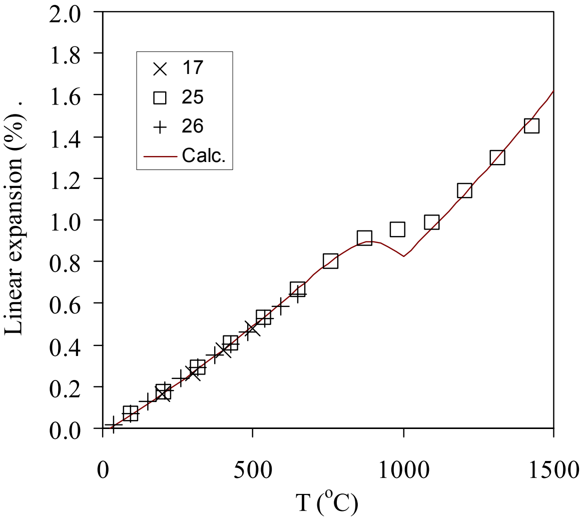

Figure 11. Comparison between experimentally observed [17,25,26] and calculated linear expansion for Ti-64.

Extensive validation has been undertaken for solid-state properties and Figs. 9-10 show plots comparing experiment with calculations for Young's modulus and thermal conductivity for many commercial Ti-alloys. Note that Figs. 9 and 10 include results measured at various temperatures up to 500-600°C. Fig. 11 shows the linear expansion of Ti-6Al-4V up to 1500°C with experimental results [17,25,26] shown for comparison. The calculations were made assuming the α/β structure was "frozen in" below a final heat treatment of 700°C and the phases in equilibrium were then considered above this temperature. Agreement is very good, even in the region close to the β-transus where the amounts of α and β change rapidly with temperature. In this case the experiments were conducted on heating and differ slightly from the calculations, which consider that equilibrium is achieved.

It is instructive to briefly consider the use of JMatPro in solidification. Due to the difficulty in containing liquid Ti-alloys, there is almost no experimental data available for their thermo-physical and physical properties with which to compare the calculations against, except for *fe*

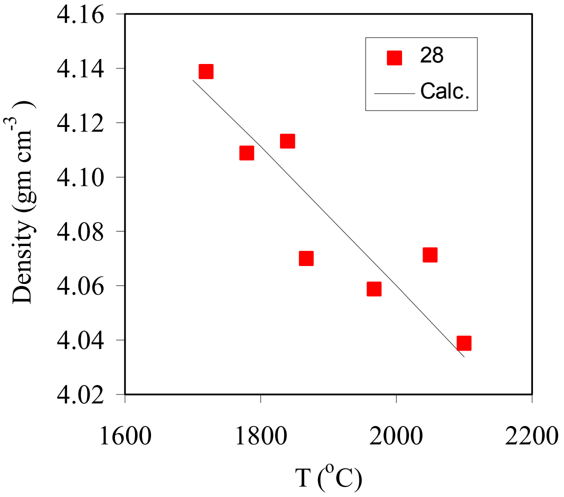

Figure 12. Comparison between experimentally observed [28] and calculated density of liquid Ti.

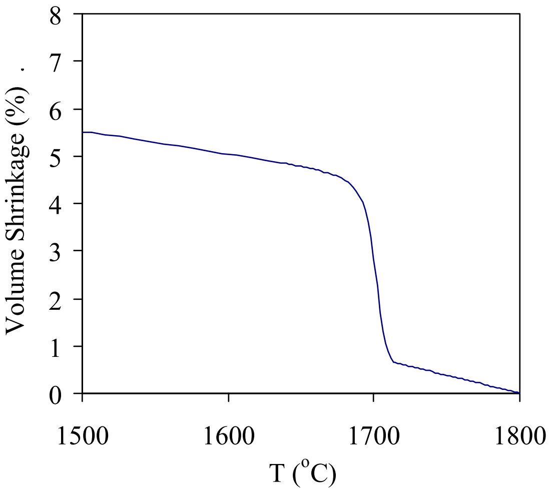

Figure 13. Calculated volume shrinkage during solidification of Ti-64.

the case of pure Ti where thermal conductivity [27] and density measurements [28] have been made. Fig. 12 shows the calculated density of liquid Ti in comparison to that measured by Saito et al. [28]. A strength of the current approach is that the models used are physically based and can be self-consistently applied for various alloy types where measurements have been made. It is therefore possible to demonstrate that the approach inherently provides excellent results for liquid alloys [29]. Using a Scheil-Gulliver model it possible to simulate non-equilibrium solidification for many types of multi-components alloys [29] and, using this model, the phases formed as a function of temperature were calculated. From this calculation, the volume change during solidification of Ti-6Al-4V was calculated and is shown in Fig. 13.

3 Summary and Conclusions

It has been demonstrated that an integrated approach to the modelling of materials properties can provide a wide range of information regarding phase equilibria, TTT/CCT diagrams, mechanical properties and physical properties for Ti-alloys. The calculations utilise well-established material models and consider the effect of microstructure. The calculated results obtained for a wide range of commercial Titanium alloys have been extensively validated against experiment.

The good agreement for known alloys gives confidence for calculations made for new combinations of alloying elements and heat-treatments, which would otherwise require time consuming and expensive experimentation.

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