Modelling Phase Transformations and Material Properties Critical to Simulation of Heat Treatment Distortion in Steels

Zhanli Guo, Nigel Saunders and Jean-Philippe Schillé

Sente Software Ltd., Surrey Technology Centre, The Surrey Research Park, Guildford, Surrey GU2 7YG, U.K.

Heat Treatments are widely used in various manufacturing processes to enhance the quality of a product. Distortion induced by heat treatment is a major industrial problem because it critically affects the dimensional accuracy of precision components , which may considerably increase the costs of operations and decrease the quality of core parts. Prediction of distortion induced by heat treatment is difficult because such prediction requires detailed knowledge of material properties that are normally lacking and difficult to evaluate, especially at high temperatures.

This paper describes the development of a computer model for the calculation of phase transformation and material properties required for prediction of distortion during heat treatment of steels. The success of the model is based on a model of all of the major phase transformations taking place, as well as the calculation of properties of different phases formed during the heat treatment process. In the past, predictive phase transformation models have mainly concerned carbon and low alloy steels. The current model has the advantage that it can be applied to many types of steel, including medium to high alloy types. A wide range of physical, thermo-physical and mechanical properties can be calculated, all as a function of time/temperature/cooling rate, even for an arbitrary cooling profile. Time-Temperature Transformation (TTT) curves and material data are readily exported to FE/FD based packages for simulating quench distortion.

Keywords: *Steels, phase transformation, material properties, quench distortion, JMatPro*

1. Introduction

The unwanted distortion generated during heat treatment is a major industrial problem because it critically affects the dimensional accuracy of precision components. If distortion can be predicted and controlled, then corrections can be made during the earlier machining stage so that the components reach their final desired shape and dimension after heat treatment.

Prediction of distortion induced by heat treatment has generally been based on prior experience or by a trial and error approach. In recent years, with the significant improvement of computing power, finite-element (FE) simulation tools have been developed to tackle this problem. While being successful in some cases, almost all of the FE packages suffer from one common problem: the lack of accurate material property data. This is because distortion prediction requires detailed knowledge of the material properties of each phase formed during heat treatment, all of which are a function of alloy composition, heat treatment procedures (microstructure) and temperature.

In summary, the following information on materials properties has to be known for distortion prediction:

- Phase transformation kinetics, i.e. TTT and CCT diagrams.
- Temperature dependent thermophysical properties of each phase formed, such as density, Young's modulus, thermal expansion coefficient, and thermal conductivity.
- Temperature dependent mechanical properties of each phase formed.

In the present paper, the development of a computer program, JMatPro, is reported which can calculate the above material properties for general steels. The success of the program is based on a sound description of all the major phase transformations taking place during heat treatment, as well as calculation of the properties of different phases formed in steels. This paper extends on previous work [1)] and focuses on the application aspects of JMatPro, generating material data that otherwise has to be measured through experiments, such as dilatometry, Jominy hardenability tests, and Gleeble® testing. To make JMatPro's material data more easily used by process modelers, the data can be organized in a format such that it can be directly read by FE simulation packages. Such linking has been successfully developed between JMatPro and forging/deformation simulation packages.

2. Modeling of Material Data for Distortion Prediction

2.1 TTT and CCT Diagrams

Significant work has been carried out over recent decades to develop models that can calculate TTT/CCT diagrams for steels, see for example refs. [2,34)]. Although successful for low alloy steels, such models are limited when it comes to more highly alloyed types. This problem has been solved by the development of a model that is able to calculate TTT/CCT diagrams for steels of all types, including highly alloyed ones [5]. The kinetic model is based on the approach of Kirkaldy et al.[2)] but with extensive modification to critical model parameters.

Figure 1 show a comparison between calculated experimental TTT diagrams for two steels. While Figure 1 provides detail for specific calculations, it is instructive to look at overall accuracy of the calculations. To this end we have taken the experimentally observed start times at the nose temperature of the various transformations to ferrite, pearlite and bainite from (i) the Atlas of Isothermal Transformation Diagrams of BS En Steels [6)] and (ii) the ASM Atlas of Isothermal Transformation and Cooling Transformation Diagrams [7)] and compared these to those calculated using the new model (Figure 2).

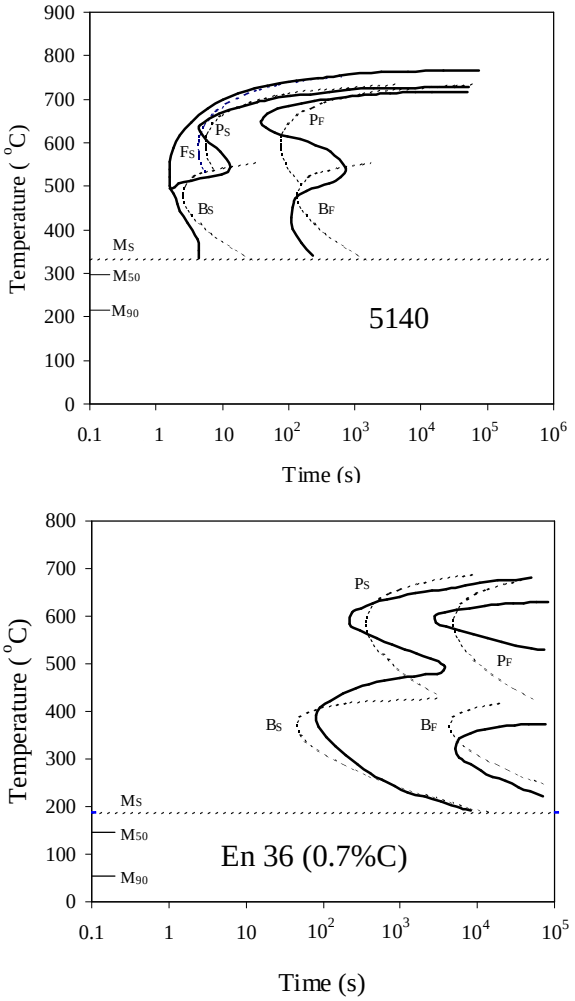

Figure 1. Comparison between experimental (bold lines) and calculated TTT diagram (dashed lines) for (a) a 5140 steel and (b) a En36 NiCr carburised steel

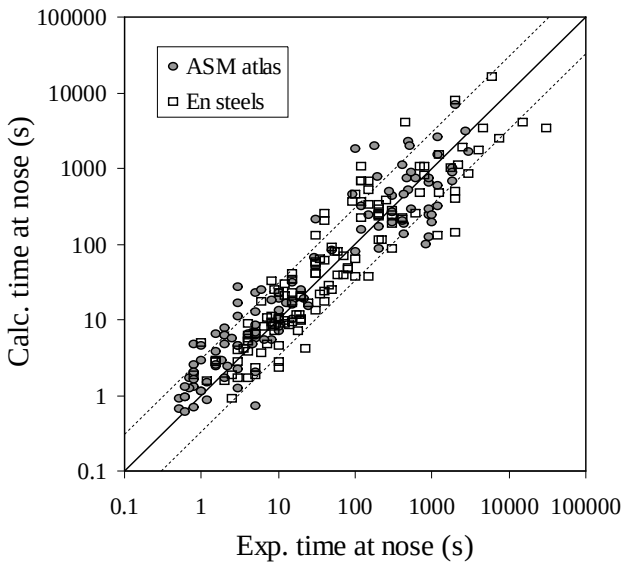

Figure 2. Comparison between experimental [6,7] and calculated start times at the nose temperature of the C-curves for various steels

2.2 Material Properties

Thermophysical, physical properties and mechanical properties are critical parameters for the prediction of distortion induced by heat treatments or processing. JMatPro's ability to model these properties has been well documented in previous published work for various metallic systems [1,8,9,10]. In summary, the properties that can be modelled include yield strength, stress/strain curves, density, molar volume, thermal expansion coefficient, Young's, bulk and shear moduli, Poisson's ratio, thermal conductivity and diffusivity, electrical conductivity and resistivity. All are provided for each available phase when necessary.

2.3 Combining Phase Transformation and Material Property Modeling During the Quench Process

To model the quench process we calculate phase transformation from austenite at small isothermal steps and utilize standard additivity models to calculate the total amount of transformation. The partitioning of C to austenite during the austenite→ferrite transformation is considered. Either a constant cooling rate or an arbitrary cooling profile can be used.

An example demonstrating how cooling rate affects the phase transformations during quenching is give for a 4140 steel with a prior austenite grain size of ASTM 7.5. Figure 3 shows the evolution of various phases during cooling at 20°C/s and 1°C/s, respectively.

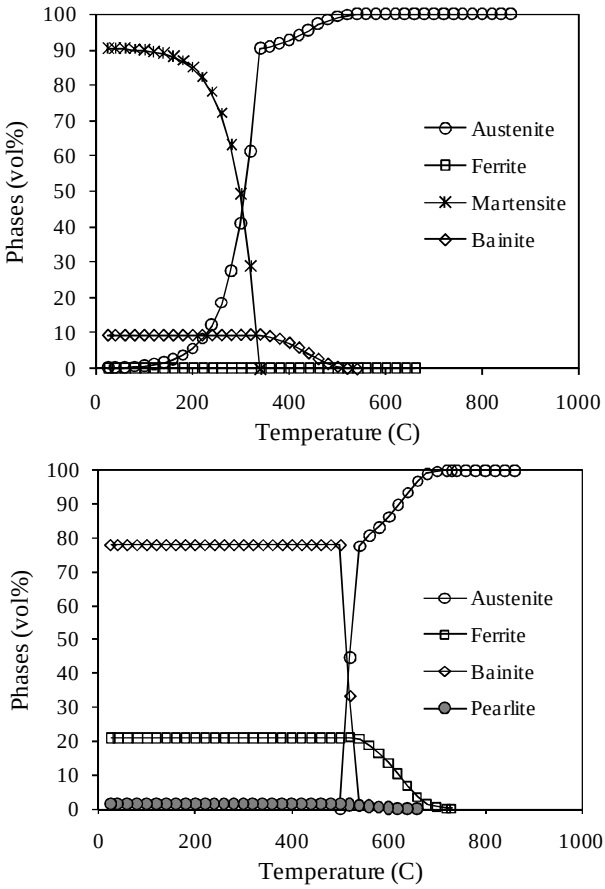

Figure 3. Phase evolution in a 4140 steel, composition Fe-0.98Cr-0.77Mn-0.21Mo-0.15Si-0.37C (wt%), during cooling at (a) 20°C/s and (b) 1°C/s

The cooling rate effect on physical and mechanical properties is shown in Figure 4, again using steel 4140 as an example. Five cooling rates are used: 100, 10, 1, 0.1, and 0.01 °C/s respectively. Typical material properties relevant to the prediction of distortion such as linear expansion coefficient, thermal conductivity and yield stress at different cooling rates are plotted.

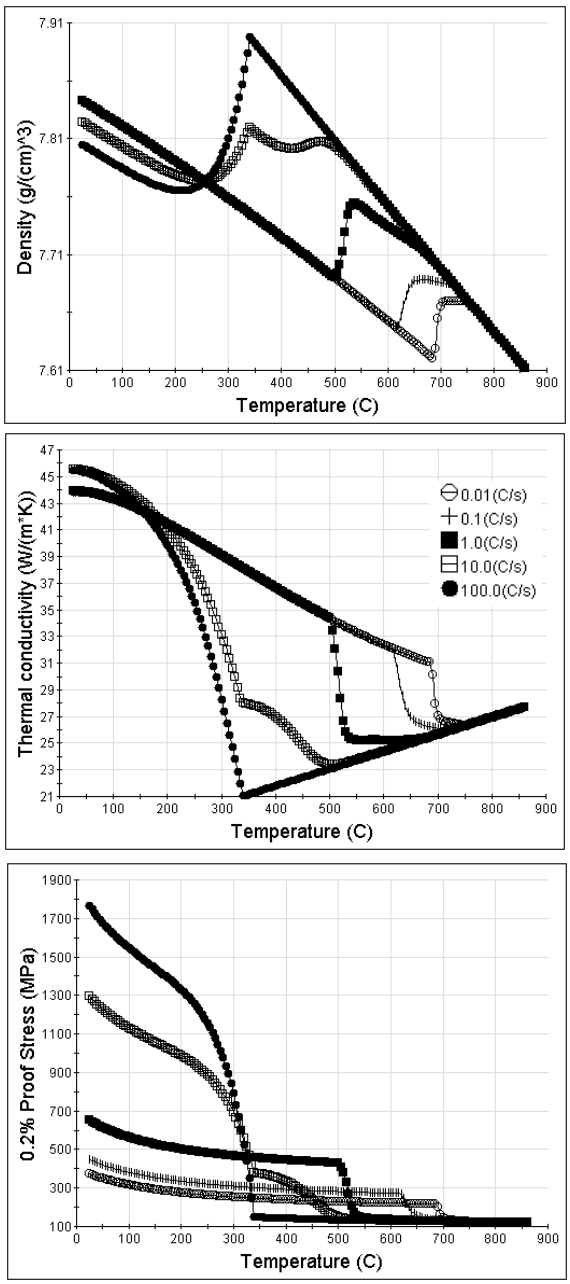

Figure 4. Various properties calculated for a 4140 steel at various cooling rates ranging from 0.01 to 100 °C/s.

It is possible to compare calculated results with experiment using Jominy hardenability curves and information on phases formed as a function of cooling rate. Figure 5 shows a comparison between calculated and experimental [7] Jominy hardenability for the 4140 alloy, while Figure 6 shows the comparison between calculation and experiment [11] for phase formation and hardness at various cooling rates for a 20MnCr5 steel.

In this case the cooling rate is calculated from the lamda value which is equal to the time taken to cool between 800 and 500°C, divided by 100.

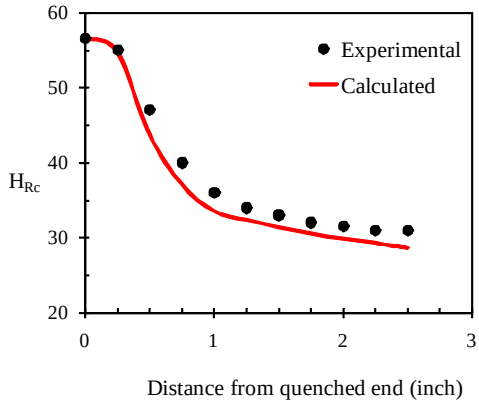

Figure 5. Comparison between calculated and experimental [7] Jominy hardenability for a 4140 steel

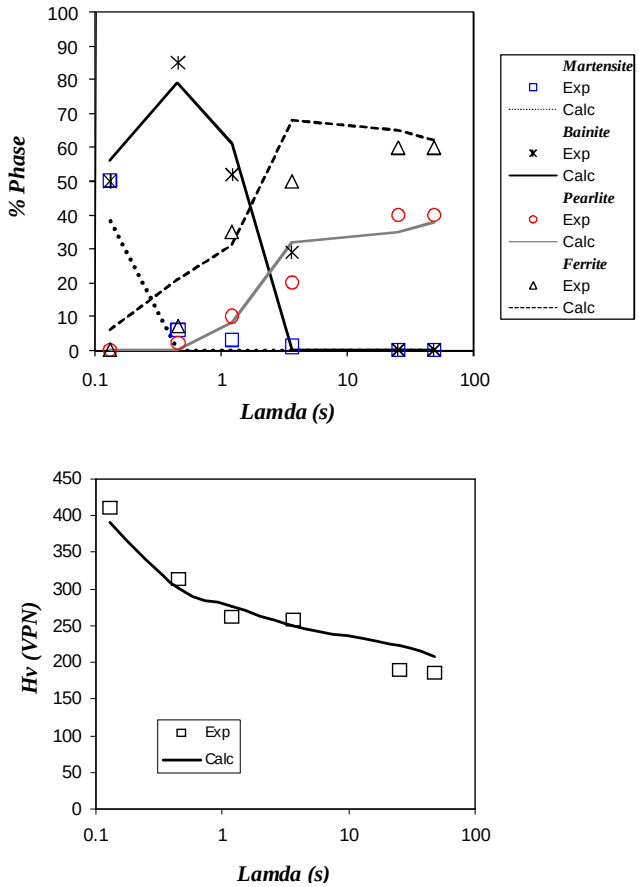

Figure 6. Comparison between calculated and experimental [11] phase formation and hardness as a function of cooling rate for a 20MnCr5 steel

2.4 Linking with FE-based Deformation Simulation Packages

Material data calculated by JMatPro have been used by users of many FE/FD-based process simulation packages, from MAGMASOFT and PROCAST for casting, DEFORM and FORGE-3D for forging and rolling, to ANSYS as a general simulation tool. To make JMatPro's data more easily used by process modelers, new

subroutines have been created within JMatPro so that the property data will be written as files that can be directly used by the simulation packages.

Simulation packages for quench distortion utilize kinetic models to calculate the amount of phase transformed as a function of temperature and time during the quench process. Such models are invariably not predictive and require experimental information so that model parameters can be empirically fitted to fit the in-built equations. It is straightforward to export TTT curves directly so that such a fitting process can be undertaken and Figure 7 shows TTT curves of the various phases, ferrite, pearlite and bainite using the steel 4140 as an example. For this case, two transformation curves corresponding to 5% and 50% were requested by the user

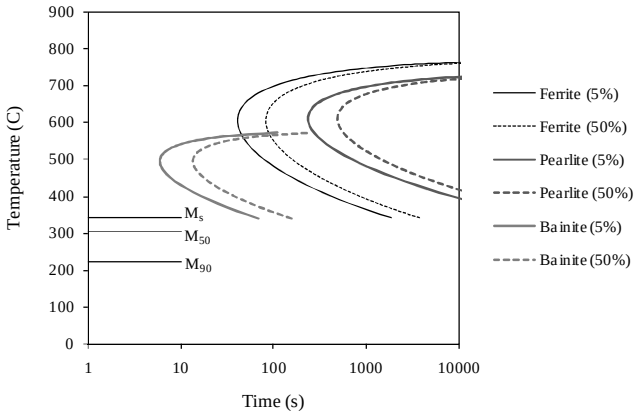

Figure 7. TTT curves for a 4140 steel corresponding to 5 and 50% transformation

The material properties that are usually required for distortion and deformation simulation are for each phase formed and Figure 8&9 show properties for all relevant phases during cooling of steel 4140, using yield stress and density as examples. Flow stress curves as a function of temperature and strain rate can be calculated as well.

3. Summary

Properties critical to the prediction of distortion induced by heat treatment have been calculated using the software program JMatPro. These properties include

• Phase transformation kinetics, i.e. TTT and CCT diagrams.
• Temperature dependent thermophysical properties of each phase formed, such as density, Young's modulus, thermal expansion coefficient, and thermal conductivity.
• Temperature dependent mechanical properties of each phase formed.

The success of the model is based on a sound description of all the major phase transformations taking place, as well as calculation of the properties of different phases formed during heat treatment process.

Links between JMatPro and many FE-based process simulation packages have been established and JMatPro's property data can be organized in such a format that can be directly read by those packages

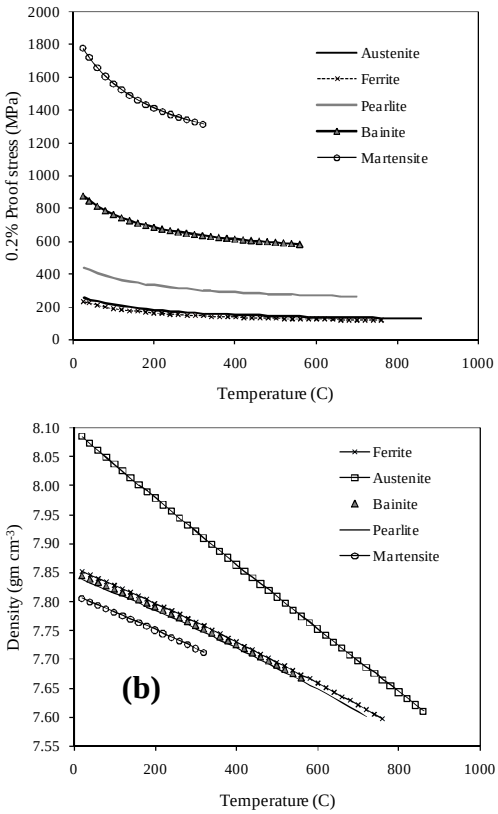

Figure 8. (a) 0.2% Proof stress and (b) density of the various phases formed during quenching of a 4140 steel

References

1) Z. Guo, N. Saunders, A.P. Miodownik and J.-P. Schillé, presented at *2nd Int. Con. Heat Treatment and Surface Engineering in Automotive Applications*, 20-22 June, 2005, Riva del Garda, Italy
2) J.S. Kirkaldy and D.Venugopolan, *Phase Transformations in Ferrous Alloys*, eds. A.R. Marder and J.I. Goldstein, AIME, (Warrendale, PA: AIME, 1984), 125.
3) H.K.D.H. Bhadeshia, Met. Sci., **16** (1982), 159.
4) J.L. Lee and H.K.D.H. Bhadeshia Mater. Sci. Eng. A, **171**, (1993), 223.
5) N. Saunders, Z. Guo, A.P. Miodownik, J.-P Schillé, *The Calculation of TTT and CCT Diagrams for General Steels*, Internal report of Sente Software Ltd., 2004, www.sentesoftware.co.uk/resources/TTT_CCT_Steels.pdf
6) *Atlas of Isothermal Transformation Diagrams of BS En Steels*, Special report 56 (Iron & Steel Institute, 1956)
7) *Atlas of Isothermal Transformation and Cooling Transformation Diagrams*, (ASM, 1977).
8) N. Saunders, Z. Guo, X. Li, A.P. Miodownik and J-Ph. Schillé, *Superalloys 2004*, eds. K. A. Green et al (TMS, 2004), 849.
9) N. Saunders, X. Li. A.P. Miodownik and J.-Ph. Schille, in *Ti-2003 Science and Technology*, ed. G. Luetering, (Wiley-VCH, Weinheim, Germany, 2004), 1397.
10) Z. Guo, N. Saunders, A.P. Miodownik, J.P. Schillé, *Material properties for process simulation*, Materials Science and Engineering A, in press, 2008
11) *Material Specification Sheet*, Saarstahl AG