Modelling phase transformations and material properties critical to the prediction of distortion during the heat treatment of steels

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Abstract: This paper describes the recent development of models in JMatPro for the calculation of phase transformations and material properties that are critical to the prediction of distortion during the heat treatment of steels. The success of these models is based on the accurate description of all the major phase transformations taking place, including the formation of ferrite, pearlite, bainite and martensite, as well as the calculation of the properties of the different phases formed during the heat treatment process. One advantage of the current models is that they can be applied to many types of steels, including medium- to high-alloy types. A wide range of properties such as density, thermal expansion coefficient, thermal conductivity, strength and hardness can be calculated, all as a function of time, temperature and cooling rate, even for an arbitrary cooling profile. The material data calculated from JMatPro have been exported directly to Finite Element (FE)/Finite Difference(FD)-based packages for forging/deformation simulation.

Keywords: materials properties; modelling; distortion; TTT diagram; Jominy hardenability; heat treatment.

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Biographical notes: Dr. Zhanli Guo received his BEng and MEng from the Department of Materials Science and Engineering of Tsinghua University, China, in 1994 and 1997, respectively. His PhD was obtained from Queens University Belfast, UK, in 2000, where he continued working as a post-doctoral Researcher for about three years after graduation. He then joined Sente Software Ltd. in 2003, focused on developing and promoting JMatPro for the simulation of material properties in metallic systems. He has published more than 60 technical papers; over 30 are journal publications.

Dr. Nigel Saunders received a PhD from the University of Surrey, UK in 1984. He stayed on to become a Lecturer in the Department of Materials Science and Engineering. He left the university in 1990 to form Thermotech Ltd., a company specialising in thermodynamic phase diagram calculations. Along with a major consortium of international companies, Thermotech provided the launch pad for the development of JMatPro, a new software programme dedicated to the calculation and provision of material property data for the materials industry. He has published more than 100 technical papers, including 30 invited papers, and two books.

Seminal work on the crucial role played by magnetic forces in steels led to Professor Miodownik's becoming a founding member of the CALPHAD community in 1972. Since then he has continued to apply thermodynamics to other areas such as the calculation of stacking fault and antiphase boundary energies. From 1981 to 1989 he was the Head of the Materials Science and Engineering Department of the University of Surrey, UK. Since his retirement in 1994, he has been concerned with the calculation of physical and mechanical properties of individual phases. He is currently combining these activities as Co-Director of predictive material properties programmes at Sente Software.

Dr. Jean-Philippe Schillé received his PhD degree from the University Louis Pasteur in Strasbourg, France. He worked on magnetic materials for the Universities of York and Oxford in the UK before getting involved in the computer-aided simulation of material properties and behaviour. He currently works as the Managing Director of Sente Software Ltd.

1 Introduction

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/Finite Difference (FE/FD) simulation tools have been developed to tackle this problem. While being successful in some cases, almost all of the FE/FD packages suffer from one common problem: the lack of accurate material property data. This is because the prediction of distortion 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. 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, including tensile strength, yield strength and hardness.

In the present paper, the development of a computer program, *J*ava-based *Mat*erials *Pro*perty (JMatPro) simulation software, is reported which can calculate the above material properties for general steels. The success of the program is based on an accurate description of all the major phase transformations taking place during heat treatment (Saunders *et al.*, 2004), as well as an accurate calculation of the properties of different phases formed in steels. This paper is a natural extension of our previous work (Guo *et al.*, 2005), where model development was explained in details and extensive validation had been carried out. Consequently the present paper will focus on a specific application of JMatPro, which generates material data that otherwise has to be measured through experiments such as: dilatometry, Jominy hardenability test, and Gleeble® testing.

2 Modelling 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 (Kirkaldy *et al.*, 1978; Kirkaldy and Venugopolan, 1984; Bhadeshia, 1981; 1982; Lee and Bhadeshia, 1993). Although successful for low alloy steels, these models are limited when it comes to more highly alloyed types. This problem has been solved in the most recent version of JMatPro, which is now able to calculate TTT/CCT diagrams for steels of all types, including the highly alloyed ones (Guo *et al.*, 2005; Saunders *et al.*, 2004).

Two new features in the models deserve special attention. One is the determination of the austenite composition at the quenching temperature. When carbides or other second phases are present at this temperature, it would be inappropriate to use the overall alloy composition as the composition of the austenite to be decomposed. In the present treatment, the composition of the austenite present at the quenching is always calculated directly (Li *et al.*, 2002) and then used in the subsequent modelling. The other feature is that the formation of martensite and bainite is affected by the prior formation of ferrite. The carbon rejected by the formation of ferrite is then incorporated into the remaining austenite, which may have a significant impact on further transformations. For example, increased carbon in austenite reduces bainite and martensite start temperatures and increases the strength of the transformed phases.

2.2 Thermophysical and physical properties

Thermophysical and physical 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 (Sente Software Ltd., 2005; Guo *et al.*, 2005). The relevant properties that can be modelled include: 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 phase present when necessary.

2.3 Mechanical properties during heat treatment

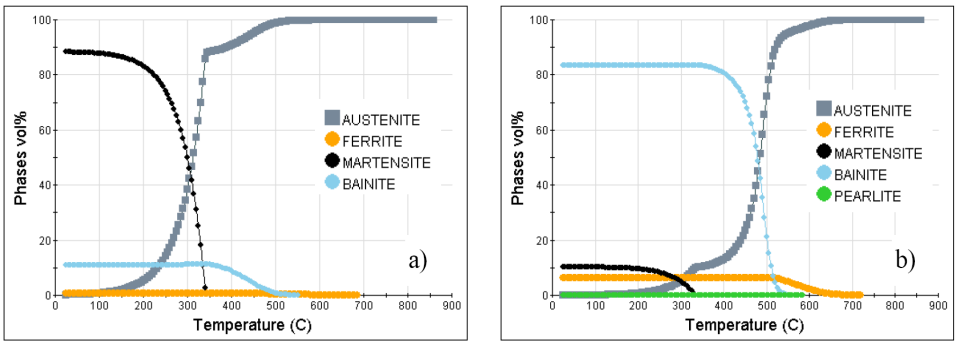
A heat treatment cycle typically includes heating, isothermal holding and cooling procedures. The mechanical properties, as well as physical and thermophysical properties, of steels during those procedures can now be calculated (Sente Software Ltd., 2005; Guo *et al.*, 2005). The microstructure is assumed to be 'frozen' when below the final heat treatment temperature, and reach equilibrium when above this temperature. The calculation of mechanical properties during isothermal holding or cooling has been demonstrated previously (Guo *et al.*, 2005).

3 Applications

3.1 Cooling rate on phase transformations and material properties

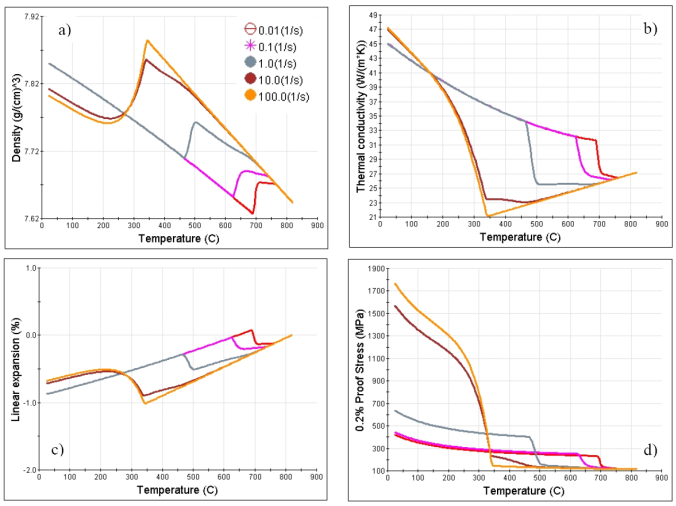
An example is given to demonstrate how cooling rate affects the phase transformations during quenching. The alloy is a 4140 steel, with composition (wt%): Fe-0.98Cr-0.77Mn -0.21Mo-0.04Ni-0.15Si-0.37C, and grain size ASTM 7 ~ 8. Figure 1 shows the evolution of various phases during cooling at 20°C/s and 5°C/s, respectively. A significant amount of martensite is formed during cooling at 20°C/s, but much less at 5°C/s. Cooling at 5°C/s results in about 4% and 6% ferrite formed before the start of bainite (Bs) and martensite (Ms) formation, respectively. The change of carbon concentration in the remaining austenite caused by the formation of such small amount of ferrite is enough to lower the Bs and Ms temperatures by 10°C.

Figure 1 Microstructure evolution in a 4140 steel during cooling at (a) 20°C/s and (b) 5°C/s (see online version for colours)



The cooling rate effect on physical and mechanical properties has been shown here, again using steel 4140 as an example. Five cooling rates are used: 100°C/s, 10°C/s, 1°C/s, 0.1°C/s, and 0.01°C/s respectively. Typical material properties relevant to the prediction of distortion such as density, linear expansion coefficient, thermal conductivity and yield stress at different cooling rates are plotted in Figure 2. The properties at 100°C/s and 10°C/s are very close, since the amount of martensite is over 90% in both cases.

Figure 2 Properties calculated for a 4140 steel at cooling rates from 0.01°C/s to 100°C/s (see online version for colours)



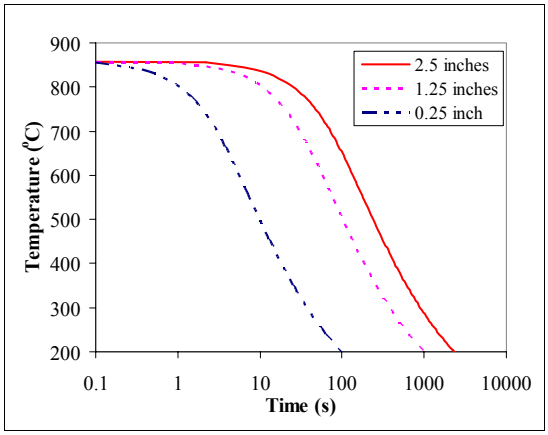
Notes: (a) density, (b) thermal conductivity, (c) linear expansion, and (d) proof stress.

3.2 Complicated cooling profile: Jominy hardenability test

The major steps for predicting Jominy hardness using this model are explained below. One has to calculate the microstructure evolution (final microstructure) and hardness for each position along the Jominy bar.

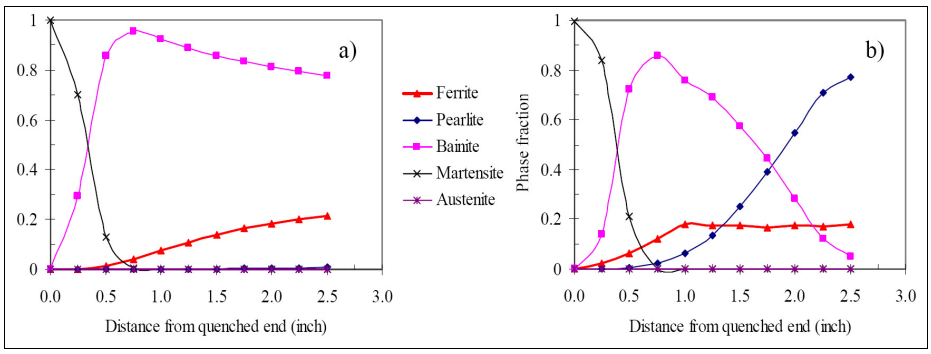
Each position along the Jominy bar is associated with a complex cooling pattern. Kirkaldy *et al.* (1978) established a formula to calculate the cooling curve for each position (Kirkaldy and Venugopolan, 1984). The calculated curve is in fairly good agreement with curves calculated from other analytic or finite-element methods (Li *et al.*, 1998). Figure 3 shows the cooling curves for three positions along the Jominy bar, *i.e.*, 0.25, 1.25 and 2.5 in from the quenching end.

Figure 3 Cooling curves for three positions from quenching end on a Jominy bar (see online version for colours)



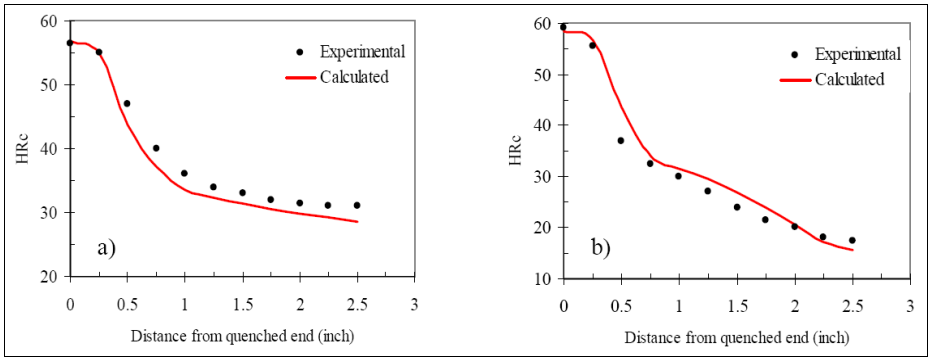
The model applied in JMatPro allows one to input user-defined cooling profiles, for instance those shown in Figure 3. The basic idea is to treat such cooling curves as a series of isothermal steps, each with different holding time. The microstructure evolution during cooling at each position can then be calculated, and the final microstructure is used to calculate the Jominy hardness. Two alloys were used as examples here, one is the 4140 steel (same as in 3.1), and the other is a 5140 steel (Fe-0.42C-0.93Cr-0.68Mn -0.16Si, grain size ASTM 6.5). The microstructure change along the Jominy bar for the two alloys is shown in Figure 4.

Figure 4 Microstructure change along the Jominy quench bar for (a) 4140, and (b) 5140 alloys (see online version for colours)



The hardness can be readily calculated when the microstructure at room temperature is known. The Jominy hardenability curve was calculated and compared with the experimental curve (ASM, 1977) for the two alloys in Figure 5. Good agreement was achieved for both alloys. It should be noted that the Jominy curve of alloy 5140, Figure 5(b), exhibits two zones: a fast hardness drop from the quenching end to 0.75 in depth, and a slow hardness drop between 0.75 and 2.5 in. This behaviour can be readily explained by the microstructure change along the Jominy quench bar shown in Figure 4(b). The initial fast drop in hardness is mainly due to the formation of bainite at the expense of martensite. At positions over 0.75 in in depth, pearlite starts to form at the expense of bainite (the stronger of the two phases), which leads to the second slow drop in hardness.

Figure 5 Jominy hardenability comparison between experimental and calculated curves for (a) 4140, and (b) 5140 alloys (see online version for colours)



3.3 Linking JMatPro with FE/FD-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 which is a general simulation tool. To make JMatPro's data more easily used by process modellers, new subroutines have been created within JMatPro so that the property data is written as files that can be directly used by the simulation packages. Such linking has been successfully developed between JMatPro and the simulation packages mentioned above and is being extended to heat treatment and welding simulation packages. Some examples relevant to deformation/distortion simulation are given below.

Figure 6 shows TTT curves of the various phases, ferrite, pearlite and bainite using the steel 4140 as an example. For this case, two curves were shown for each transformation, corresponding to 10% and 90%, respectively. Amongst the properties required as input in formulae for determining distortion and deformation are the yield stress and density (inverse of molar volume) of each phase as a function of temperature. Figure 7 shows these properties for each phase during cooling of steel 4140. Similar calculations of flow stress curves as a function of temperature and strain rate are also available.

Figure 6 TTT curves of steel 4140, corresponding to 10% and 90% of the transformation (see online version for colours)

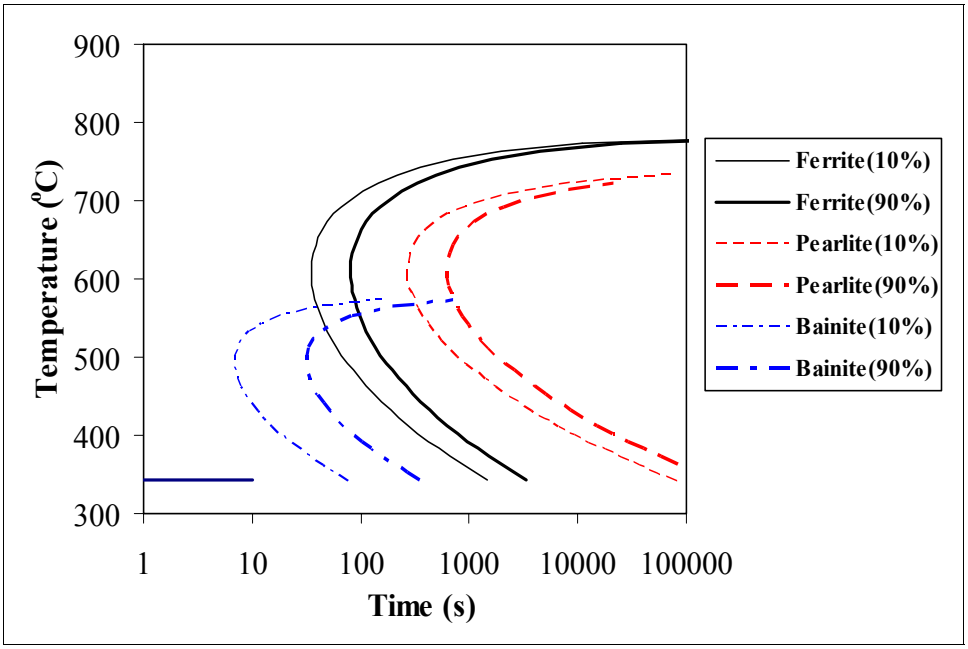
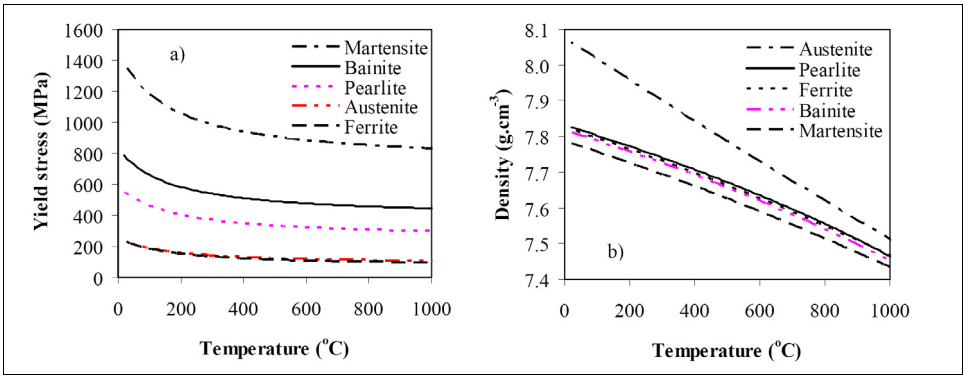


Figure 7 Properties for each phase during cooling of steel 4140 (see online version for colours)



Notes: (a) yield stress and (b) density.

4 Summary

Properties critical to the prediction of distortion induced by heat-treatment have been calculated using JMatPro, which embodies integrated software for the prediction of both the structure and properties of a wide range of alloys. TTT and CCT diagrams, as well as the density and yield stress of key microstructural constituents such as ferrite, pearlite, bainite and martensite for the two steels 4140 and 5140 have been calculated as examples of a larger range of physical, thermophysical and mechanical properties that can be handled in a similar way. Such calculations are available as a function of temperature, including elevated temperatures for which experimental results are often not readily available.

The way that arbitrary cooling profiles can be handled is demonstrated by the calculation of Jominy hardenability profiles which are the result of a complex interplay between thermal and microstructural properties. The variation of properties of different constituents for different cooling rates substantially increase the understanding of the hardness variation along the Jominy bar.

The success of the model is based on accurate description of all the major phase transformations taking place, as well as an accurate calculation of the properties of different phases formed during heat treatment process. The output from JMatPro has already been linked to other FE/FD-based process simulation packages such as MAGMASOFT and PROCAST for casting, DEFORM and FORGE-3D for forging and rolling, and ANSYS which is a general simulation tool. The desired properties could therefore also be linked to any packages that describe the development of the internal stress patterns originating from both elastic and plastic mechanisms.

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