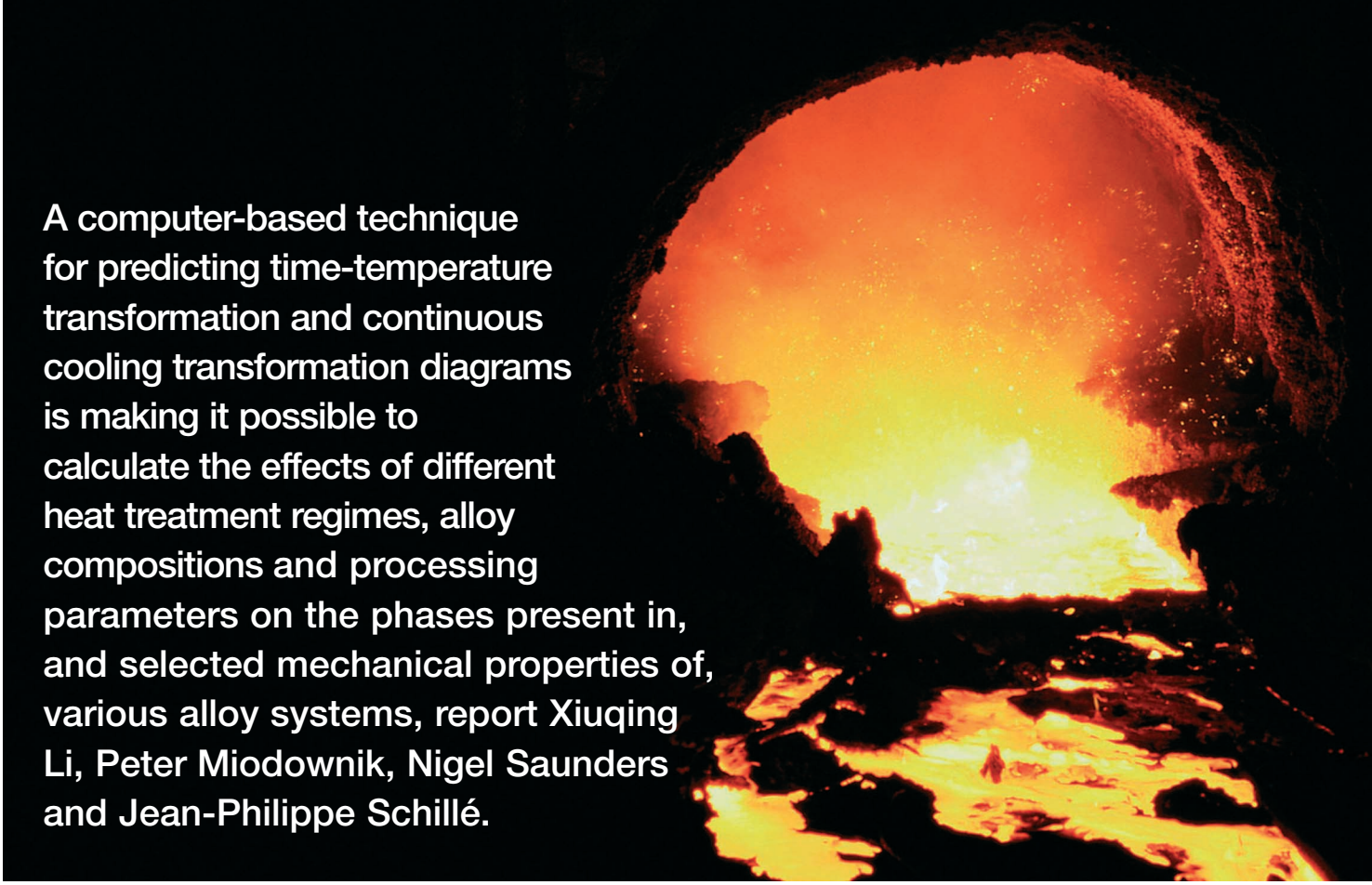

A computer-based technique for predicting time-temperature transformation and continuous cooling transformation diagrams is making it possible to calculate the effects of different heat treatment regimes, alloy compositions and processing parameters on the phases present in, and selected mechanical properties of, various alloy systems, report Xiuqing Li, Peter Miodownik, Nigel Saunders and Jean-Philippe Schillé.

Transformed –

Software simplifies alloy heat treatment, production and design

The steel industry is a severely competitive place to do business. So any technique for rapidly evaluating alternative alloy compositions, estimating the properties of off-specification melts and highlighting potential ways of reducing costs could offer companies considerable advantages. A versatile new software-based approach is now available that should prove useful to producers and end-users alike who are looking to improve their materials, heat treatment regimes and other processing operations. The software enables users to predict key transformation diagrams for the materials they are making and processing.

Time-temperature transformation (TTT) and continuous cooling transformation (CCT) diagrams are acknowledged as the best reference points for steel heat treatment, alloy production and alloy design. However, a large number of practical experiments are required to generate sufficient diagrams to cover the multitude of alloy compositions and heat treatments found in industry. The measurements themselves are time-consuming, and their interpretation is not always straightforward.

As a result of these factors, TTT and CCT diagrams are often not available for the specific compositions required, nor do they always cover the full range of cooling rates, temperatures and grain sizes that may be of interest for a specific application.

Many years ago, this problem was partially solved by the introduction of the Jominy Hardenability test, which pro-

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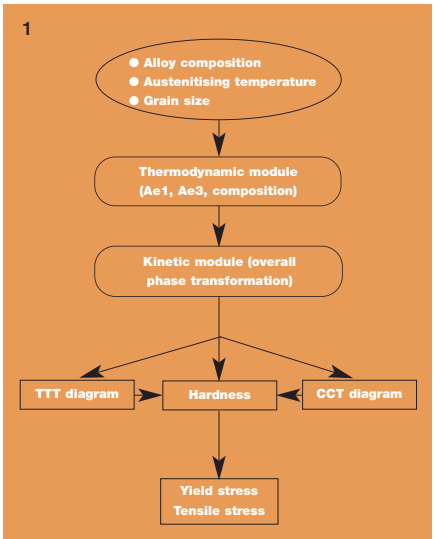
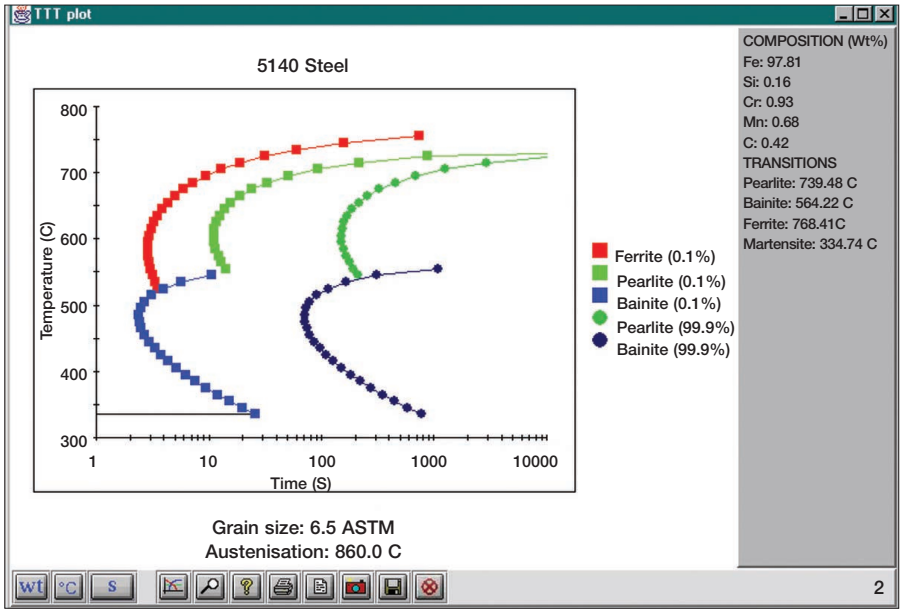
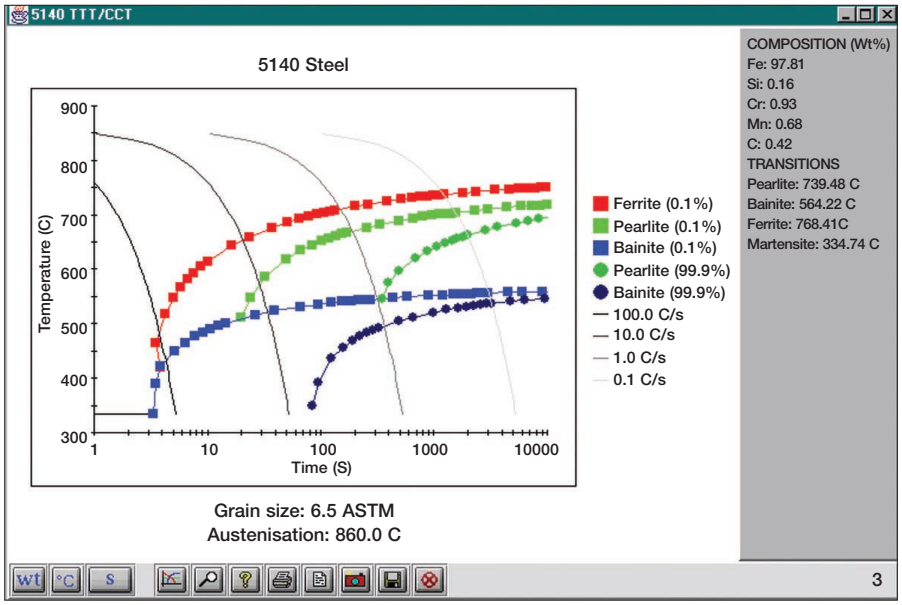


Flow diagram of the prediction system



Calculated TTT diagram for a 5140 steel



Calculated CCT diagram for a 5140 steel

vides indirect information about critical cooling rates and related mechanical properties via the measurement of hardness values. However, this test does not provide any basic structural information.

A more comprehensive computerised approach was developed by Kirkaldy in response to the oil crisis of the 1970s. But this approach could only function through the use of many empirical correlations, largely because the complex interaction between alloying elements could not be formulated explicitly at that time.

Since then, techniques for the calculation of multi-component phase diagrams such as CALPHAD have become well established. These new techniques can handle more than a dozen components in the case of steels, and can more accurately account for various interactions between components than the earlier methods.

This means it is possible to derive more accurate driving forces for the precipitation of individual phases or of two-phase products such as pearlite. When combined with theories of nucleation and growth, it is possible to make quantitative predictions of TTT and CCT curves, derive the related Jominy Hardenability and extend the calculations to other mechanical properties.

The new software tool JMatPro, which is an acronym for Java-based Materials Properties software, is a suite of computer programs that has been developed by Thermotech and Sente Software for the prediction of a broad range of materials properties. Figure 1 shows the procedure adopted for the prediction of TTT, CCT and Hardenability diagrams. The user simply inputs their choice of alloy composition, austenite grain size and austenitising temperature, together with a choice of how the answers should be displayed.

The thermodynamic module then calculates all the necessary critical equilibrium temperatures, such as the Ae_3 for ferrite and the Ae_1 for pearlite, together with the equilibrium compositions and amounts of all the phases concerned. This is particularly important for cases in which there are undissolved carbides at the austenitising temperature. Other critical temperatures, such as the formation temperatures for bainite and martensite, are calculated from empirical formulae, which are related as far as possible to thermodynamic information.

The relevant information is passed to a kinetic module that applies the appropriate kinetic equation, depending on the transformation process being modelled. Finally, the software calculates the time taken for a set amount of transformation at the desired temperature(s).

Figure 2 shows a TTT diagram calculated using JMatPro for a 5140 alloy. Thermodynamic calculation indicates that, at the austenitising temperature of 860°C, the alloy is fully austenitic and the equilibrium transformation temperatures for ferrite and pearlite are 768°C and 739°C respectively. The diagram shows five well defined curves – ferrite start, pearlite start and finish, and bainite start and finish. 'Start' is taken as 0.1% transformed and 'finish' as 99.9% transformed. Once the martensite start temperature is reached, transformation of the other phases is suppressed.

The key question for the software is whether critical values can be calculated quantitatively, with respect to both temperature and time, for a large range of

compositions, without making arbitrary changes to the thermodynamic input. This has been successfully achieved and defines the methodology as a true predictive tool rather than a mere simulation exercise based on empirical correlation coefficients.

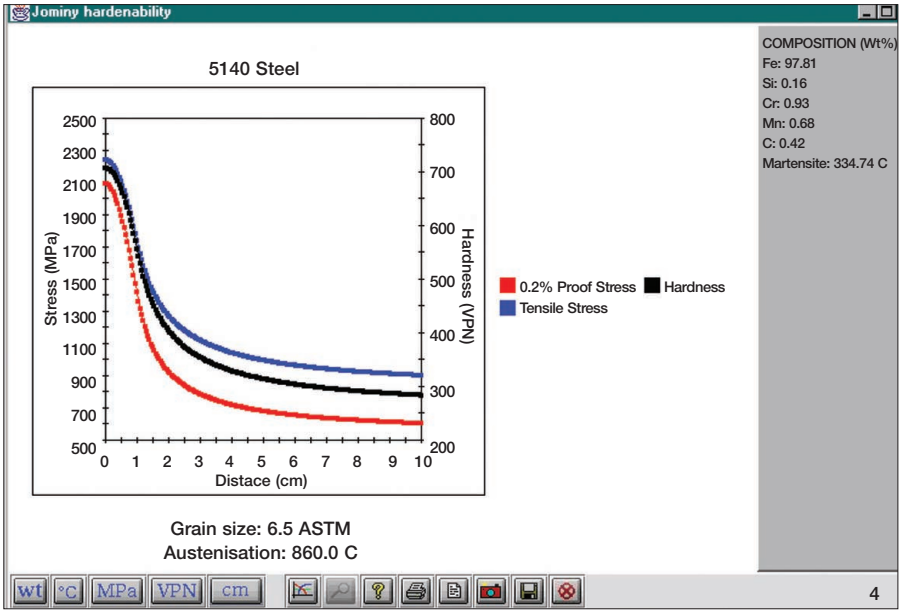
From the TTT diagram it is relatively easy to calculate the equivalent CCT diagram, figure 3, and Jominy hardness curve, figure 4, following mathematical treatments established by Kirkaldy – but using reassessed hardness values for ferrite, martensite and pearlite. JMatPro also takes this one step further by not only calculating the hardness at a given cooling rate, but also by deriving the associated yield and ultimate tensile strength using a long-established theoretical route. In many previous treatments, such properties have been related to hardness values only through regression analysis.

Among the many benefits of a system such as JMatPro are the following:

- TTT and CCT diagrams, Jominy Hardenability curves and mechanical properties can be generated for specific compositions, instead of relying on general diagrams available in the literature
- It is possible to show the effect of minor variations in individual alloying additions within a given specification, or to investigate the optimum combination of elements that would yield more reproducible properties
- Decisions can be made regarding the permissible level of local segregation that will still lead to the material having the required performance criteria
- Entering a change in the austenitising temperature not only generates the corresponding change in the kinetics and properties, but also gives information on the phases present at that temperature – this has an important corollary in that JMatPro can be readily used for dual phase steels
- It is possible to investigate the consequences of inhibiting the formation of a particular phase
- It is possible to investigate the effects of changes in grain-size during different processes such as controlled rolling and welding.

An important attribute is the range of alloy compositions that can be handled. A number of alternative methods have been developed to calculate TTT diagrams in the past decade, but their applicability and accuracy vary with the carbon content and the level of alloying additions in the alloys used during validation. This is inevitable when some of the key operational parameters have been derived by regression analysis, and there is insufficient information about multi-component interactions. The latter factor has an important consequence – the quotation of higher permissible composition ranges for individual elements does not necessarily mean that these are valid for all possible combinations of these elements.

In this context, software such as JMatPro combines accuracy with a broad range of applicability because it has a sound thermodynamic basis as well as a reduced number of arbitrary input parameters. Additionally, JMatPro also offers a number of other property modules, notably for physical properties such as elastic modulus and thermal conductivity.



Calculated Jominy hardness, yield stress and tensile stress for a 5140 steel

Therefore, it is possible to extract additional information about the alloy as a whole, or the properties of individual phases. The examples given here are drawn from HSLA steel, but JMatPro has been successfully applied to the generation of TTT diagrams for other materials such as stainless steels, Ti- alloys and Ni-base superalloys.

Future developments will include the calculation of a broader range of associated properties and will encompass the effects of more complex heat-treatments for a broader range of materials.

Authors' details

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Further reading

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