Chapter 10

Summary and future work

Following an extensive review of the work done on the topic, it can be said with certainty that precipitation phenomena in austenitic stainless steels are complex, and that controversies persists in many cases.

A part of this work was concerned with the microstructural evolution of a newly designed austenitic stainless steel named NF709, with a particular attention to phases which may be detrimental to long-term creep properties. In this regard, results obtained during this work indicate that the detrimental role of σ -phase is not systematic, as evidence is given that it has little effect on the ductility. It is also shown that significant differences in the precipitation sequences can appear from apparently similar compositions. Furthermore, by combining observations from the literature and the detection of Cr_3Ni_2SiN the role of nitrogen as a stabiliser for the η -structure can be clarified.

Of great interest is also the ability to predict the microstructural evolution of these steels. Based on previous work by Robson and Bhadeshia, and Fujita and Bhadeshia, a model has been created which makes full use of modern thermodynamic calculation tools. This model corrects approximations made necessary when using stand-alone programs, in particular, it is shown that using either the equilibrium tie-line, or the one corresponding to a zero gradient of carbon, is incorrect and does not lead to satisfactory predictions of the growth rate. The problem is only correctly solved when addressing it in terms of activities of the components rather than concentration. Also, the issue of capillarity in multicomponent systems has been examined, and earlier approaches have been corrected. A method has been designed which allows to tackle the problem through modification of the SGTE databases so that capillarity corrections can be calculated directly with MT-

DATA. With the program written so as to avoid too specific solutions, it is hoped that its scope of use will extend beyond austenitic stainless steels in future works.

However, for various reasons, this still has to be considered as a semi-quantitative approach. First, there is a serious lack in available thermodynamic data on phases that are commonly encountered in modern grades of heat-resistant austenitic stainless steels, which strongly limits the number of systems in which meaningful predictions can be made. Furthermore, the model still relies on the mean-field approximation. It is certainly a worthy challenge to overcome this so as to account for localised interactions, or grain-boundary and intragranular precipitation separately. Finally, fundamental reasons have been given which justify a re-examination of the way nucleation theory is used in multicomponent systems, so as to improve the prediction ability of the classical theory.

Given the difficulties in predicting quantitatively the precipitation reactions, it is yet too early to use these calculations as inputs in the further step which is to estimate the mechanical properties. It is clear that a meaningful model based on the precipitation state must include feature such as location, as, for example, grain boundary and intragranular precipitates are known to have different influences, and distribution, as a same phase finely dispersed or present as coarse particles also has different effects.

However, when using powerful empirical methods such as neural network modelling, these difficulties can be avoided; variables such as composition and test conditions can be used directly. With the use of creep data collected from a number of sources, such models have been built to estimate the creep strength and creep life of austenitic stainless steels. Predictions made with these models have been compared to known trends, and shown to grasp properly interactions between different input variables and to be superior to conventional extrapolation methods. It is also interesting to note that the use of physically relevant variables significantly improved the models; for example, the logarithm of time was used rather than time and a variable relevant for the estimation of the quantity of fine MX precipitates was added. This justifies the hope that future models, which may use predicted volume fractions and locations of precipitates as inputs, could help confirming or understanding the role held by the different precipitate phases in determining the creep strength of austenitic stainless steels.

APPENDIX ONE

MAP_STEEL_CREEP_LIFE_AUSTENITIC

This appendix presents the model described in chapter 9 and associated documentation following the MAP format, http://www.msm.cam.ac.uk/map/mapmain.html.

1 Provenance of Source Code

Thomas Sourmail

Phase Transformations and Complex Properties Group,

Department of Materials Science and Metallurgy,

University of Cambridge,

Cambridge, CB2 3QZ U.K.

The neural network program was produced by:

David MacKay,

Cavendish Laboratory,

University of Cambridge,

Madingley Road,

Cambridge, CB3 0HE, U.K.

Added to MAP: June 2001.

2 Purpose

A program for the estimation of the creep life of austenitic stainless steels as a function of elemental composition, test conditions and solution treatment.

3 Specification

Language: C

Product Form: Source Code

Operating System: tested on Solaris, SGI and Linux. Can be compiled on most UNIX

systems.

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4 Description

MAP_STEEL_CREEP_LIFE_AUSTENITIC contains the programs which enable the user to estimate the creep life of austenitic stainless steels as a function of chemical composition, solution-treatment temperature, and stress and temperature of the creep test. It makes use of a neural network program called generate44, which was developed by David MacKay and is part of the bigback5 program. The network was trained using a large database of experimental results [1]. 4 different models are provided, which differ from each other by the number of hidden units and by the value of the seed used when training the network. It was found that a more accurate result could be obtained by averaging the results from all models [1]. The programs calculate the results of each model and then combines them, by averaging, to produce a committee result and error estimate, as described by MacKay [2].

The source code is accompanied by a program to install the program, which should run on most versions of UNIX. Once uncompressed, and once the 'install' program run, the directory contains:

README

A text file containing step-by-step instructions for running the program, including a list of input variables.

MINMAX

A text file containing the minimum and maximum limits of each input and output variable. This file is used to normalise and unnormalise the input and output data.

test.dat

An input file containing the input variables used for predictions.

model.gen

This is a UNIX shell file containing the commands required to run the model. It can be executed by typing 'sh model.gen' at the command prompt. This shell file normalises the input data, executes the neural network program, unnormalises the results and combine them to produce the final *committee* result.

.normalise

Hidden executable file, to normalise the input data.

.generate44

Hidden executable file, for the neural network program. It reads the normalised input file

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and also uses a configuration file spec.t generated by $.generate_spec$ and the weight files, located in the subdirectory c.

.generate_spec

Hidden executable file, generates the configuration file read by .generate44.

.gencom

Hidden executable file, combines the output of the different models in a committee result.

.treatout

Unnormalise the results.

SUBDIRECTORY c

$_{\mathbf{w}}$ *f

The weight files of the different models.

*.lu

Files containing information for calculating the size of the error bars for the different models.

_c*

Files containing information about the perceived significance value [1] for each model.

\mathbb{R}^*

Files containing information about the noise, test error and log predictive error [1] for each model.

SUBDIRECTORY d

outran.x A normalised output file which was created during the building of the model. It is accessed by .generate44.

SUBDIRECTORY outprdt

out1, out2, etc.

The normalised output files for each model.

com.dat

The normalised output file containing the committee results. It is generated by .gencom.

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5 References

1. Thomas Sourmail, H. K. D. H. Bhadeshia and D. J. C. MacKay, A neural network model for the creep strength of austenitic stainless steels., Materials Science and Technology, in press.

2. D. J. C. MacKay, *Mathematical modelling of weld phenomena 3*, eds. H. Cerjak and H. K. D. H. Bhadeshia, Institute of Materials, London (1997) 359, 3. D. J. C. MacKay's website at http://wol.ra.phy.cam.ac.uk/mackay/README.html

6 Input parameters

The input variables are listed in the README file in the corresponding directory. The maximum and minimum values for each variable are given in the file MINMAX.

7 Output parameters

These give the creep life in log h. The output is written in the file result.txt.

Accuracy

A full calculation of the error bar is presented in reference 1.

Program data

See sample file test.dat

Program results

See sample file result.txt

Keywords

Neural networks, creep life, austenitic stainless steels.

APPENDIX TWO

MAP_STEEL_CREEP_STRENGTH_AUSTENITIC

This appendix presents the model described in chapter 9 and associated documentation following the MAP format, http://www.msm.cam.ac.uk/map/mapmain.html.

1 Provenance of Source Code

Thomas Sourmail

Phase Transformations and Complex Properties Group,

Department of Materials Science and Metallurgy,

University of Cambridge,

Cambridge, CB2 3QZ U.K.

The neural network program was produced by:

David MacKay,

Cavendish Laboratory,

University of Cambridge,

Madingley Road,

Cambridge, CB3 0HE, U.K.

Added to MAP: June 2001.

2 Purpose

A program for the estimation of the creep strength of austenitic stainless steels as a function of elemental composition, temperature of creep test and required life.

3 Specification

Language: C

Product Form: Source Code

Operating System: tested on Solaris, SGI and Linux. Can be compiled on most UNIX

systems.

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4 Description

MAP_STEEL_CREEP_STRENGTH_AUSTENITIC contains the programs which enable the user to estimate the creep strength of austenitic stainless steels as a function of chemical composition, temperature of the creep test and required life. It makes use of a neural network program called generate44, which was developed by David MacKay and is part of the bigback5 program. The network was trained using a large database of experimental results [1]. 14 different models are provided, which differ from each other by the number of hidden units and by the value of the seed used when training the network. It was found that a more accurate result could be obtained by averaging the results from all models [1]. The programs calculate the results of each model and then combines them, by averaging, to produce a committee result and error estimate, as described by MacKay [2].

The source code is accompanied by a program to install the program, which should run on most versions of UNIX. Once uncompressed, and once the 'install' program run, the directory contains:

README

A text file containing step-by-step instructions for running the program, including a list of input variables.

MINMAX

A text file containing the minimum and maximum limits of each input and output variable. This file is used to normalise and unnormalise the input and output data.

test.dat

An input file containing the input variables used for predictions.

model.gen

This is a UNIX shell file containing the commands required to run the model. It can be executed by typing 'sh model.gen' at the command prompt. This shell file normalises the input data, executes the neural network program, unnormalises the results and combine them to produce the final *committee* result.

.normalise

Hidden executable file, to normalise the input data.

.generate44

Hidden executable file, for the neural network program. It reads the normalised input file

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and also uses a configuration file spec.t generated by $.generate_spec$ and the weight files, located in the subdirectory c.

.generate_spec

Hidden executable file, generates the configuration file read by .generate44.

.gencom

Hidden executable file, combines the output of the different models in a committee result.

.treatout

Unnormalise the results.

SUBDIRECTORY c

$_{\mathbf{w}}$ *f

The weight files of the different models.

*.lu

Files containing information for calculating the size of the error bars for the different models.

_c*

Files containing information about the perceived significance value [1] for each model.

\mathbb{R}^*

Files containing information about the noise, test error and log predictive error [1] for each model.

SUBDIRECTORY d

outran.x A normalised output file which was created during the building of the model. It is accessed by .generate44.

SUBDIRECTORY outprdt

out1, out2, etc.

The normalised output files for each model.

com.dat

The normalised output file containing the committee results. It is generated by .gencom.

Appendix Two

5 References

1. Thomas Sourmail, H. K. D. H. Bhadeshia and D. J. C. MacKay, A neural network model for the creep strength of austenitic stainless steels., Materials Science and Technology, in press.

2. D. J. C. MacKay, *Mathematical modelling of weld phenomena 3*, eds. H. Cerjak and H. K. D. H. Bhadeshia, Institute of Materials, London (1997) 359, 3. D. J. C. MacKay's website at http://wol.ra.phy.cam.ac.uk/mackay/README.html

6 Input parameters

The input variables are listed in the README file in the corresponding directory. The maximum and minimum values for each variable are given in the file MINMAX.

7 Output parameters

These give the creep life in log h. The output is written in the file result.txt.

Accuracy

A full calculation of the error bar is presented in reference 1.

Program data

See sample file test.dat

Program results

See sample file result.txt

Keywords

Neural networks, creep strength, austenitic stainless steels.

APPENDIX THREE

MAP_DATA_MTDATA_CAPILLARITY

This appendix presents the databases created to include capillarity effects in MT-DATA calculations, as decribed in chapter 5 and associated documentation following the MAP format, http://www.msm.cam.ac.uk/map/mapmain.html.

1 Provenance of Source Code

Thomas Sourmail

Phase Transformations and Complex Properties Group,

Department of Materials Science and Metallurgy,

University of Cambridge,

Cambridge, CB2 3QZ U.K.

The original data were from the SGTE (Scientific Group Thermodata Europe) databases included with MT-DATA,

National Physical Laboratory,

Teddington,

Middlesex,

TW11 0LW, U.K.

Added to MAP: December 2001.

2 Purpose

To allow calculation of capillarity corrected equilibrium with thermodynamic calculation softwares such as MT-DATA.

3 Description

Two types of binary files are provided: .dbs and .inx files for direct use with MT-DATA. These data are replicated from the original databases, but a pressure dependency term has been added so that the MT-DATA user can increase the Gibbs energy of any of the precipitates by a given amounts.

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The user should be aware that this pressure dependency terms are in no way real volumetric data. There only purpose is to allow the addition of 10^{-6} J mol⁻¹ per Pascal. When using these database, a conventional calculation can be performed by setting the pressure to 1 Pa. If the Gibbs energy of, say, M23C6 is to be raised by 1000 J mol⁻¹, the pressure should be set to 10^9 Pa.

Once the file map_data_mtdata_capillarity uncompressed, the directory databases contains the following files:

README

Contains detailed instructions on how to install the databases and set up MT-DATA to use them.

cementite.dbs and cementite.inx

Binary files (database and index) providing thermodynamic data for cementite.

m23c6.dbs and m23c6.inx

Binary files (database and index) providing thermodynamic data for M23C6.

hcpa3.dbs and hcpa3.inx

Binary files (database and index) providing thermodynamic data for HCP_A3

sub_p.dbs and sub_p.inx

Binary files (database and index) providing thermodynamic data for the following substances: NTi, CTi, NNb, CNb, C0.479Nb, C0.877Nb, C0.98Nb.

SUBDIRECTORY loa_files

Contains the plain text load files corresponding to the above binary files.

Keywords

capillarity, coarsening, MT-DATA

APPENDIX FOUR

MAP_MT-DATA_KINETICS

This appendix presents the model described in chapter 6 and associated documentation following the MAP format, http://www.msm.cam.ac.uk/map/mapmain.html.

1 Provenance of Source Code

Thomas Sourmail and H. K. D. H. Bhadeshia Phase Transformations and Complex Properties Group, Department of Materials Science and Metallurgy, University of Cambridge, Cambridge, CB2 3QZ U.K.

This program is interfaced with MT-DATA, National Physical Laboratory, Teddington, Middlesex, TW11 0LW, U.K.

Added to MAP: December 2001.

2 Purpose

A program to estimate the kinetics of diffusion-controlled, multiple precipitation reactions in austenitic stainless steels. This program can also be used for the same purpose in different systems for which the SGTE databases provide thermodynamic data, but the user will be required to input the diffusion coefficients.

3 Specification

Language: FORTRAN

Product Form: Source Code

Operating System: tested on Solaris.

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4 Description

MAP_MT-DATA_KINETICS contains the program which enable the user to obtain an estimate of the volume fraction of various precipitates forming in austenitic stainless steels during ageing at elevated temperature, as a function of time.

All thermodynamic calculations are handled internally by MT-DATA, therefore suppressing the need for the user to input driving forces or equilibrium compositions.

The software uses MT-DATA .mpi files, from which the user selects required phases. This file has to be created in first place, using the ACCESS module of MT-DATA.

Once uncompressed, MAP_MT-DATA_KINETICS contains:

kinetics.f

The source code for the program.

compile

A unix shell script to compile the program and link it to MT-DATA object files. It needs to be edited to point to the directory where the latter are found.

precipitate_data

A file containing information about a number of precipitates, that is, lattice parameter, number of atoms per unit cell, and parameters for nucleation (nucleation site density and interfacial energy).

spheregrowth.out and planargrowth.out

Contains 500 precalculated points for the solution to the sphere growth and planar growth equations as described in [1].

README

Complete instructions for installation and use.

5 References

1. Thomas Sourmail, $PhD\ thesis$, $Chapter\ 6$, available on http://www.msm.cam.ac.uk/phasetrans/

6 Input parameters

The user is only required to select the phases allowed in the calculation and the elements which are expected to control their growth, for example Cr and C in the case of $M_{23}C_6$. For most other input parameters, such as composition, ageing temperature and solution-treatment temperature, the user has the possibility to create, with the software files which

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can be used for faster access in later calculations.

7 Output parameters

The default output is

Time /s — Vf of precipitate 1 — Vf of precipitate 2 — etc
where Vf is the volume fraction.

This can be easily modified by editing the subroutine SNAPSHOT.

Keywords

Simultaneous precipitation reaction kinetics, austenitic stainless steels.

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