

Estimation of the martensite start temperatures of steels using thermodynamic models

T. Sourmail, www.neuromat.org

Overview

This program implements the thermodynamics models for martensite nucleation as described by Ghosh and Olson [1–4], to predict the martensite start temperature of steels (M_s) as a function of their composition.

It is written in FORTRAN 77 (apologies, this is so that it can be interfaced with the thermodynamics calculation software MT-DATA [5]).

The program has been divided in different sources, one part containing the sub-routines which need MT-DATA to function, the other those which could be used independently.

Copyright and disclaimer blurb:

Permission is granted for anyone to copy, use, modify, or distribute these programs and accompanying documents for any purpose, provided this copyright notice is retained and prominently displayed, along with a note saying that the original programs are available from Thomas Sourmail's web page, and note is made of any changes made to these programs. These programs and documents are distributed without any warranty, express or implied. As the programs were written for research purposes only, they have not been tested to the degree that would be advisable in any important application. All use of these programs is entirely at the user's own risk.

Contents

1 Overall functioning	2
2 Installation and test run	2
3 Files	3
4 The source directory	4
5 Using the script for batch calculations	5

1 Overall functioning

The purpose of this program is to search for the temperature at which the conditions for martensite nucleation are satisfied. The criterion is simply that the driving force $\Delta G^{\gamma \rightarrow \alpha}$ should be greater or equal to the critical driving force ΔG_c .

ΔG_c is a function of the composition and, in the case of the more recent model of Ghosh and Olson [3,4], a function of the temperature.

The program reads the composition of your alloy from an input file, then searches for the temperature at which the criterion for martensite nucleation is satisfied.

The output has been kept very simple so as to simplify the use of the program in scripts. In the following, I assume that you have MT-DATA installed so that it can run/compile third-party applications. If this is not the case, you should contact the National Physical Laboratory.

2 Installation and test run

Once the archive file downloaded and save it in a directory of your choice. You can then extract the files using:

```
tar -zxf ms_prediction.tar.gz
```

There is a precompiled program called *Ms* together with all the required files for a test run. Compilation was made on RedHat 9.0 and should work on most Red-Hat version above 7.3. I have experienced problems with older versions as the gcc libraries have changed. Nevertheless, the program can easily be re-compiled and function properly.

To test the software, simply type

```
./Ms
```

at the command prompt, once in the directory containing the program.

You should obtain the following output:

```
result;2250.88;-321.97; 258.54;2250.88;-303.08; 304.64  
result;2435.00;-333.58; 230.19;2386.85;-311.04; 285.22
```

The first line refers to the results obtained with the first model of Ghosh and Olson [1,2]. There are six consecutive numbers which are: the critical driving force (absolute value) ΔG_c for the given composition, the Gibbs energy for ordering, calculated according to [6,7], and the M_s temperature in Kelvin. For the first three numbers, the ordering contribution is ignored, it is only shown but not included in the comparison of $\Delta G^{\gamma \rightarrow \alpha}$ and ΔG_c . The second set of three numbers corresponds to the case where the ordering effect is taken into account in the comparison of $\Delta G^{\gamma \rightarrow \alpha}$ and ΔG_c . Note that the ordering contribution is not exactly equal because it affects the M_s temperature and therefore the temperature at which it is evaluated.

The second set of six numbers correspond to the same results as obtained with the more recent method of Ghosh and Olson [3,4], where ΔG_c depends on the temperature through the temperature dependency of the austenite modulus. Note that the program includes a subroutine to evaluate the shear modulus of austenite as a function of composition and temperature that can be used indepently.

If you are not concerned about the detailed description of the files, you can jump to the section on practical use, which describes how to use the accompanying script to make batch predictions, that is predictions on a file containing a large number of compositions.

3 Files

The main directory should contain the following files:

- Ms: the main program, which needs a valid MTDATA license to function properly.
- input.dat: this file contains two pieces of information for the main program to use: the name of the thermodynamic file (mpi file) to be used. If you are not familiar with what an mpi file is, I suggest you consult either the MTDATA manual, or my online help, particularly: www.msm.cam.ac.uk/phase-trans/mtdata/advanced_databases.html
The second input is a number which is the precision to be satisfied for $\Delta G^{\gamma \rightarrow \alpha} = \Delta G_c$ this can and should be left as it is.
- composition.dat: this file contains the composition of the alloy you are using, in the following format:

Fe,Mn,C
1
95
4.7
0.5

The first line is for comments, anything can be written in it, but the line must be present. In general, I recommend copying there the names of the elements in the same order as in the mpi file to facilitate input. **NOTE:** the list of elements present in this file **does not** influence the reading. The order of the elements is determined by the mpi file, and it is therefore very important that you enter the weight or mole fractions in the same order.

Following is a parameter which indicates whether your input is in weight or mole (1 or 2 resp.).

Then, the mass or number of moles of each component, **in the same order** as in the mpi file.

- Z_phi.csv: contains pre-calculated values for the functions z and ϕ as described in [6, 7]. The exact value is linearly interpolated between the two closest values. This gives much better results than the algorithm distributed on www.msm.cam.ac.uk/map, particularly at high T/Tc.
- SRC: a directory containing the source code.
- FeMnC.mpi: is a demo mpi file containing data for the system Fe-Mn-C, phases ferrite (BCC_A2) and austenite (FCC_A1). This file has been created with the SGTE SSOL database to which you should have access by default with your MTDATA package.

4 The source directory

There are 5 source files in this directory, and a small script to compile the program.

- Calculate_Ms.f: is the main program, it initialises MT-DATA, reads the data, produces the output. It also contains a number of subroutines which you may

want to re-use in MTDATA interfaced programs: FIND_DG to estimate driving forces (details in source code), FIND_MS which is responsible for calling the different bits and pieces (evaluation of ΔG_c , of $\Delta G^{\gamma \rightarrow \alpha}$, of order) and evaluate the M_s temperature. TO_MOLS resize the system to 1 mole, so that all values are molar. All these subroutines call MTDATA and therefore cannot be used without the appropriate license.

- MS_temperature.f: contains all the subroutines to evaluate ΔG_c (CALCULATE_DGMS_I and _II for 1994 method and 2002 method resp.), the shear modulus of austenite (SHEAR_MODULUS_AUSTENITE), the free energy for ordering (CALCULATE_DG_ORDERING). All these subroutines do not require MTDATA, they need a list of element names and amounts.
- data_ghosh_olson_acta_mat_1994.f and data_ghosh_olson_athermal_2001.f contain the data for the models of Ghosh and Olson. These could have been included in the subroutines for estimation of ΔG_c and shear modulus, but have been separated for readability and ease of access.
- compile is a small script to compile the program. You should edit the line

```
export MTOBJ=/opt/mtdata/objects
```

to match your environment. To compile the program, simply type, in the SRC directory:

```
./compile ../Ms
```

in this case we indicate we want the binary file to be written to 'Ms' in the directory above. You must provide an output file name to compile the program.

5 Using the script for batch calculations

A script is provided to perform batch calculation on large number of compositions. It is written in Tcl. The Tcl interpreter is installed on most linux distribution by default. If it is not installed on your machine, you need to install first.

To perform a batch calculation, you need a database of compositions saved in the following format (for example, when working with Fe-Mn-C):

```
Mn C
4.8 0.2
4.7 0.3
...
4.0 1.0
```

NOTE: in this case, the composition is **always assumed to be given by wt%**, and the amount of Fe is set to the balance (100%). Changing the script to alter this behaviour should however be trivial. Lines to modify are indicated in the script.

It is important that the file *input.dat* is present and pointing to the correct mpi file. The mpi file and *Z_phi.csv* must also be present as described in section 1. There is no need however to worry about *composition.dat*.

To start the calculation, type:

```
./calculate_batch.tcl test_FeMnC.csv
```

where test_FeMnC.csv is the database as described above.

The program writes the result to the standard output (*i.e.* most likely your terminal), but also generates a number of files containing the results:

- results_Gc contains the ΔG_c as evaluated at the M_s temperature for the different compositions you entered. There are four numbers in a line, corresponding to Ghosh and Olson 1994 method with and without ordering (first and second values, always identical as the ordering is not added to ΔG_c and ΔG_c does not depend on the temperature), then Ghosh and Olson 2001/2 with and without ordering (third and last value, which can be different as ΔG_c depends on the temperature).
- results_Zener: the contribution of the ordering in the same conditions (four values).
- results_Ms: the M_s temperature in Kelvin, also four numbers as above.

If the SGTE database are used, I have found that the best agreement is obtained using the original method of Ghosh and Olson and accounting for ordering, that is, the second value in all cases.

An example file is provided, called *test_FeMnC.csv*, it should return the following results for *results_Ms*:

```
561.47 561.47 594.07 594.07
522.58 522.58 548.56 548.56
...
298.29 331.76 278.07 318.1
258.54 304.64 230.19 285.22
```

NOTES ON THE DATABASE FORMAT: it is very important that your file columns are separated by **ONLY ONE SPACE**. Do not use tab, comma or anything else to separate columns. Most good spreadsheet softwares such as Open Office (www.openoffice.org) allow you to export files as column separated values, and to select the separator.

6 Troubleshooting

The program writes considerably more information to a file called debug. The first few lines should contain the results of the calculation used to resize the system to one mole:

```
Moles and components mole fractions
```

```
-----
FCC_A1      Fe      Mn      C
.100000E+01 0.9159642 0.0392050 0.0448307
-----
```

```
1
```

```
Weight and components weight fractions
```

```
-----
FCC_A1      Fe      Mn      C
.538462E-01 0.9500000 0.0400000 0.0100000
-----
```

If this is not the case, MTDATA hasn't done the job properly. A good guess is that `input.dat` does not point to the right `mpi` file, or that the latter is absent or corrupted. A second possibility is that the file `composition.dat` is not correctly formatted.

If you have other problems, please feel free to contact me.

References

- [1] G. Ghosh and G. B. Olson. *Acta Mat.*, 42:3361–3370, 1994.
- [2] G. Ghosh and G. B. Olson. *Acta Mat.*, 42:3371–3379, 1994.
- [3] G. Ghosh and G. B. Olson. *J. Phase Eq.*, 22(3):199–207, 2001.
- [4] G. Ghosh and G. B. Olson. *Acta Mat.*, 50:2655–2675, 2002.
- [5] MT-DATA. National Physical Laboratory, Teddington, Middlesex, U.K., 1989.
- [6] C. Zener. *Trans. AIME*, 167:513, 1946.
- [7] J. C. Fisher. *Metals Trans.*, 185:688–690, 1949.