access · Intzestraße 5 · D-52072 Aachen · Germany

Dr. Georg J. Schmitz
+49 241 80-98014
G.J.Schmitz@micress.de

Aachen, 9. Dezember 2014

TO OUR CUSTOMERS

New release of your MICRESS® software package.

Dear MICRESS user,

Enclosed please find the most recent release of your MICRESS® software package. The present release 6.2 of MICRESS® comprises a number of improvements and new functionalities. Of course we also attempted to fix all bugs being reported by our user community.

MICRESS® 6.2 has been carefully tested and now is available in different variants for different operating systems:

For the current standard installation of MICRESS® Release Version 6.2 (with coupling to TQ interface version 8) following platforms are supported:

- Windows 7 / 8
- SUSE Linux Enterprise 11 (SLES 11), resp. OpenSUSE 12.2
- CentOS 6.6
- Ubuntu 14.04.1 (LTS)

The usage of the older TQ version S with MICRESS® is still possible but only supported for the following operating systems

- Windows XP / 7
- SUSE Linux Enterprise 10,11 , resp. OpenSUSE 11.4
- CentOS 5.10

For each operating system 64 bit variants with or without coupling to thermodynamic databases are available. 32 bit variants can be made available upon request. Future MICRESS® releases will not further support 32bit. Creation of .ges5 files for MICRESS® 6.2 requires Thermo-Calc at least in version 3.0 (corresponding to TQ8).

Older .ges5 files being created using the TCC-S version are still supported in version 6.2. The next version of MICRESS® will however not further support .ges5 files being created with Thermo-Calc versions older than 3.0.

MICRESS® 6.2 is also supplied as a partly parallelized version. Diffusion, stress, flow and temperature solvers can be executed multithreaded based on OpenMP (www.openmp.org).

In addition, the following free tools are provided along with MICRESS either on the release DVD or as download from the MICRESS® website (www.micress.de) for both Windows and Linux operating systems:

The fully re-written DP_MICRESS (version 7.1) is now included into the present distribution of MICRESS® 6.2. This powerful new postprocessor contains all functionalities of the previous DP_MICRESS and additionally provides a variety of new functionalities. Operation of DP_MICRESS has become much more intuitive and the GUI has been significantly improved. Scripts allow customizing the appearance of the screen and pre-configured tools allow numerous operations on the result files.

MICpad (Version 1.0) has been developed as a new tool for editing driving files. Bookmarks, colored comments and input strings largely facilitate navigating and editing especially large driving files. MICpad further acts as a control center allowing starting and monitoring the simulations as well as monitoring and organizing the results. Some graphics have been implemented into MICpad to visualize e.g. the linearized phase-diagrams in case of noTQ coupled MICRESS® simulations.

An additional flow solver module complementing the MICRESS® elastic and MICRESS® TQ modules can now be procured and be used along with the new MICRESS® release 6.2.:

MICRESS® flow module

The MICRESS® flow solver is an additional module to be used along with MICRESS®. It simulates laminar fluid dynamics for an incompressible, isotropic, Newtonian liquid, and is applied to the liquid phase (phase 0). All other phases are considered as immobile obstacles which may be affected by phase field calculations but are not transported with the liquid. Advection is included in species transport for concentration coupled simulations. Concentration dependent density changes can be defined to drive convective currents. Some possible applications of the MICRESS® flow module are: Diffusion controlled dendritic growth in fluid flow, concentration driven convection scenarios and the determination of permeability for specific structures.

Physical phenomena by now not being taken into account are (without claiming completeness): shrinkage flow, heat driven convection, forces or pressures due to fluid flow affecting solid phases or phase transformations. When simulating later stages of solidification, isolated pockets of liquid may cause the flow solver to diverge. More information on the flow module and its use is depicted in the manual (volumes 2 and 4).

new input/output options:

The release 6.2 of MICRESS® comprises a number of new I/O options being depicted in the following:

- A new option allows the generation of .in-files with deterministically listed grain positions when using a driving file based on the “random option” to place the grains. This option is activated by selecting “deterministic_infile“ after choosing “random” in the driving file.

- A new output for the average velocity of the „moving frame“ has been defined. This option is especially useful when exploiting whether a “steady state” has been reached.

- When reading microstructures from files the „phase to grain“ (option: p) now allows the identification of more than one phase by different discrete field values. Interfaces between different phases are generated automatically. The lowest field value in the microstructure input file is interpreted as “interface”.

- The ternary interaction parameters (diagonal and off-diagonal partition coefficients for multi-ternary extrapolation) are now additionally included into the .TabLin output.

- The input scheme for updating of thermodynamic data has been improved and extended: The time interval for relinearisation of thermodynamic data can now also be read from a file as time-dependent. This holds for both global relinearisation as well as for each individual phase interaction.

- The interval for updates of the diffusion coefficients from database now can also be defined as time-dependent from file.

- The order of the optional parameters for automatic time stepping (pre-factors, min. and max. values of the time step) can now be read time-dependent from file.

- User defined comments characterized by an exclamation mark following the hash in the driving file (#! “This is a user defined comment”) can now be used as permanent comments in the driving files. These comments will not be removed when generating the in-file and thus remain visible.

- All Tab Output can now also be written in .csv format (comma separated values) facilitating import e.g. into Excel sheets.

improved performance:

- The ternary extrapolation scheme has been strongly improved. A new improved criterion for ternary demixing has been implemented.

- The ”local” extrapolation of diffusion coefficients (i.e. extrapolation of their composition dependence) has been completely reworked. A user-defined limit of the extrapolation range helps avoiding problems such as entering into spinodals.

new functionalities/new features:

A number of new functionalities relates to the simulation of diffusion:

The input keywords for diffusion data have been chosen more systematic, based on the two mayor keywords “diagonal” and “multi” for Fick and Fick-Onsager Definition (only diagonal elements vs. full diffusion matrix), and commonly used single characters (“n”, “d”, “g”, “l”, “f”, “z”, “i”, “I”). The old notation is still accepted.

Diffusion coefficients from databases can now be corrected by the user via a pre-factor. These pre-factors can be specified individually for each diffusion term (i.e. for each alloy element or line of the diffusion matrix).

A new segmentation scheme is added which allows for the calculation of diffusion data for a user-defined number of equidistant layers in z-direction. This allows for a better matching when diffusion data strongly vary along a wide temperature gradient, or in case of the simulation of diffusion couples.

further important new features:

The new feature "add_to_grain" allows repeated nucleation of already existing grains, e.g. for nucleation of the liquid-phase as grain 0 with multiple occurrences, but also for changing the phase-ID, the grain orientation or the reX-energy during simulation runtime. A detailed description of this feature is found in the manual and also in the MICRESS® forum (see "new features"). This feature has already turned out as very powerful and useful for removing resistant rest liquids in solidification, in the context of modeling melting e.g. during welding processes, or when simply “switching” a martensite (being modeled as a supersaturated ferrite) to austenite is required when crossing a preselected process condition.

The feature **"restart structure_only"** allows reading initial structures from restart files of preceding simulations. These structures can be combined with structures from other simulations, with input structures being defined in the driving file or with microstructures being specified in .txt or .vtk files. This feature turns out to be most valuable when combining different materials in a single simulation domain as e.g. required for welding processes, or when “filling” a larger simulation domain with a representative microstructure or for the simulation of process chains in ICME type settings (Integrated Computational Materials Engineering), where microstructures are handed over from one process to the next.

The new feature **“globalF”** represents an extension of the “global” relinearisation scheme in the sense that only interconnected interface regions are approximated by a common set of linearization parameters. This is not only useful in connection with categorization, but also when interfaces split up into independent regions which cannot be satisfactorily described by the traditional “global” option.

For simulations of recrystallization a minimal mobility has been implemented in the Humphreys model (describing the reduction of the mobility as a function of misorientation in small-angle grain boundaries). This minimum mobility is set to zero by default and then reduces to the previous Humphreys model with tiny mobility for misorientations <3°.This model extension is of particular interest for the description of the orientation dependence of phase boundary mobilities like e.g. the gamma / alpha phase boundary.

A minimal value for the interface mobility of each interface can now be specified. This value will be exceeded neither by anisotropy or by minimum time step definitions, nor by direct specification. Use of this feature is however recommended for MICRESS experts only.

The new feature init_fraction assists in the TQ-initialization of phase interactions. This initialization can sometimes be difficult, e.g. when the structure_only option of restart is used to combine different materials at the beginning of a simulation.

New functionalities have further been implemented in the area of nucleation:

A shield group number can be specified as a second optional parameter together with the shield time. It specifies the phase number or shield group number for which shielding shall take effect.

Another new feature is region_restrictive allowing regions for nucleation to be specified in combination with the "restrictive" feature. This means that nucleation is only allowed inside the specified region and e.g. only in the bulk and not at interfaces, and not at triple junctions.

new examples:

Several example files have been added, up-dated or re-worked:

Especially the Gamma_Alpha- examples (Gamma_Alpha_dri, Gamma_Alpha_TQ_dri, Gamma_Alpha_PARA_dri and Gamma_Alpha_PARATQ_dri) have been fully re-worked.

A new example for a 10-component superalloy (CMSX_4) has been added.

A number of further new examples refer to the flow solver and to the recrystallization functionality.

various

- Several changes in internal data formats and algorithms lead to improved performance.
- The license manager (FlexNetPublisher Version 11.11.1 (FlexLM)) supports also IPv6 type domain specifications
- Installation of MICRESS® now proceeds via an executable installer

documentation

The distribution of MICRESS® 6.2 comprises the following 5 volumes of the manual, which have been updated to include descriptions for all new features and options:

MICRESS® manual Vol.0: MICRESS® - phenomenological background
MICRESS® manual Vol.1: MICRESS® installation
MICRESS® manual Vol.2: running MICRESS®
MICRESS® manual Vol.3: MICRESS® post processing
MICRESS® manual Vol.4: MICRESS® examples

We do hope that these improvements will assist you in solving your problems and will continue to make MICRESS® a valuable tool for your research. For more details, please don't hesitate to ask us, preferentially via the MICRESS®-Forum (www.micress.de/forum)

Yours sincerely
ACCESS e.V.

Dr. Georg J. Schmitz
Global Marketing, Sales & Support MICRESS®