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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 6.1 of MICRESS® comprises a number of improvements and new functionalities. Of course we also attempted to fix all bugs reported by the user community.

MICRESS® 6.1 has been carefully tested and now is available in following variants for different operating systems:

Windows

- Windows XP
- Windows 7

Linux

- SUSE Linux Enterprise or OpenSuse (for both: versions 10 and 11)
- CentOS 5.4
- Fedora 12
- RedHat 4

For each operating system there are 32 and 64 bit variants with or without coupling to thermodynamic databases. Note that coupling to old databases resp. ges5 files having been with Thermo-Calc Version R is not further supported any more. Creation of respective .ges5 files for MICRESS 6.1 requires Thermo-Calc version S.

MICRESS 6.1 is also supplied as a partly parallelized version. Diffusion, stress and temperature solvers can be executed multithreaded (OpenMP based: www.openmp.org).



In total the following executables are provided for MICRESS 6.1 for both Linux and Windows (“par” indicates partly parallelized versions):

MICRESS_tqs_x64 (the new standard)

MICRESS_par_tqs_x64

MICRESS_tqs_x32

MICRESS_par_tqs_x32

MICRESS_noTQ_x32 (no coupling to databases)

MICRESS_par_noTQ_x32 (no coupling to databases)

MICRESS_noTQ_x32 (no coupling to databases)

MICRESS_par_noTQ_x32 (no coupling to databases)

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

DP_MICRESS, the MICRESS post-processing and visualisation tool being distributed along with the current release, is still unchanged. A fully re-written DP_MICRESS is however close to maturity and scheduled along with the next release of MICRESS. Beta-Versions will already be available for download from the website probably around early August 2013.

MICpad has been developed as a new tool to edit driving files. Bookmarks, colored comments and inputs strings largely facilitate navigating and editing especially large driving files. A pre-release version of MICpad will be available on the MICRESS website in early August as well. Any feedback for its further evolution and improvement is highly welcome

new Input/Output

Following the demands of some customers and different specifications in the literature, the input for the pinning force for the *grain boundary mobility* can now be specified either as a curvature (as before) or as a pressure (J/cm³ resp. MPa). Respective options (curvature + value resp. pressure + value) have to be selected and old driving files have to be adapted for this purpose.

There is a *new output for grain orientations* (results_TabO.txt) comprising quaternion descriptions and also further the orientation format, specified in the driving file like e.g. Euler angles or other orientation definitions.

Element extensions have been added to the nomenclature of result files comprising concentrations of alloy elements (e.g. results_conc1.mcr can now be stored including the chemical name of the element, e.g.



results_concFE.mcr if element Fe was assigned to element #1 in the driving file). For this purpose a respective switch has to be set in the “output definitions” in the driving file e.g.: out_conc element_extensions.

Reading *diffusion data from file* now is possible also for multicomponent diffusion data. The structure of a respective data file is described in the manual.

For the new features in the *recrystallisation model* (see below) local dislocation densities can now be read from a VTK file. The same values can also be saved in the vtk format. Orientations in this context can now also be specified by quaternions. For details of reading these files and their format please refer to the manual.

There is now an additional output for the TQ start concentrations in phases from a database, which is both stored in the log file and displayed on screen. This output is particularly interesting for identifying different composition sets of phases described in the database (e.g. if FCC_A1#1 is austenite and FCC_A1#2 is a MC-carbide).

A new input feature for generating a hollow sphere called „round invers“ has been implemented. This feature is particularly useful to define e.g. a spherical simulation domain.

The new “end_at_temperature” option allows finishing a simulation once a pre-specified temperature is reached. It complements the present simulation time options. The simulation will finish depending on which condition is reached first, i.e. either when the defined temperature or when the maximum simulation time is reached.

The keyword “first” allows requesting an additional output after the first time-step

improved performance

Finite difference correction „FD-correction“

All details of the FD correction being first introduced in Version 6.0 have meanwhile been comprehensively published in J. Eiken “Numerical solution of the phase-field equation with minimized discretization error” *Materials Science and Engineering* 33 (2012) 012105”. The implementation of this scheme has been further optimized in Version 6.1.

In view of the good experiences we and our customers made when using this correction scheme, from version 6.1 we recommend to always activate this option by adding the key-word 'fd_correction' to the choice of the phase-field potential. In view of compatibility issues with old driving files we did not opt to make this selection “default”. However, a respective “recommendation message” will be given in case the option is not selected.

A new option to stabilize the interface profile in case of high driving forces has been included. This option draws on an additional numerical interface stabilization energy being added to the physical interfacial energy. It should be only used in conjunction with the FD correction scheme. It is very helpful in case an increased grid resolution is not possible in view of excessive memory usage.



The averaging algorithms for the *Anti-trapping currents* (ATC) have been substantially improved with respect to both speed and accuracy.

new functionalities

Recrystallization models

A number of new functionalities have been introduced especially in the *recrystallization model*:

In addition to specifying an average energy per grain (as being implemented up to version 6.0) also an *average dislocation density per grain* can now be specified alternatively. This provides the basis for future extensions and coupling to crystal plasticity finite element methods and also yields new outputs like e.g. the average mean stress being calculated on the basis of analytical formula without explicit coupling to the stress solver. A new result file <name>.rhoD is created, if the model is defined via dislocation densities per grain. A residual energy or dislocation density per nucleus is now introduced as well as a threshold to distinguish new from old grains.

Further a *local recrystallisation model* based on the local dislocation densities has been implemented. The local dislocation densities can e.g. be read from a vtk file. An empirical model to describe recovery has been implemented as well in this model. For more details about using the new functionalities please refer to the manual.

Description of anisotropic phases

A significant amount of new functionalities refer to a largely broadened and generalized description of anisotropy. The crystallographic symmetry of solid phases can now be defined by selecting one of the following options: none cubic hexagonal tetragonal orthorhombic.

The standard MICRESS' anisotropy model is based on predefined anisotropy functions determined by the crystal symmetry defined for the phase of the anisotropic grain. A new model, which can be selected by the optional keyword 'harmonic_expansion', is especially helpful to incorporate quantitative interfacial data from experiments or Molecular Dynamics simulation. Here, the anisotropy functions are formulated by linear combination spherical harmonics selected in accordance with the crystal symmetry.

Along with the improved description of anisotropy new models for faceted growth in cubic and hexagonal systems have been introduced. These new functionalities have already successfully been applied to study e.g. the refinement of eutectic silicon in aluminum alloys in 2 and 3 dimensions. For more details about using the new functionalities please refer to the manual.



The Read-Shockley model describing the decrease of interfacial energies as function of misorientation for low-angle grain boundaries has been included. The Humphreys model describing the decrease of interfacial mobility as a function of misorientation has been implemented as well.

Nucleation models

Additional parameters like a “nucleation distance” and an additional “nucleation radius” have been introduced to allow for better control of nucleation rates in simultaneous nucleation events. Please refer to the manual for further details. The parent-relation algorithm for determining orientation of nuclei on substrates has been revised and improved.

enhanced thermodynamics in MICRESS

A description of ternary interactions (interactions in systems with three and more elements) has been introduced as an alternative to the present multi-binary extrapolation scheme. The benefits of this option are especially in simulations in high alloyed materials where the multi-binary scheme reaches its limits

A new feature allows setting pressure values different from atmospheric pressure for the calculation of thermodynamic equilibria. This feature is particularly interesting for the definition of partial pressures in the gas phase at solid/liquid - gas interfaces.

The expert option „start_value_1/2“ allows selecting the phase from which start concentrations are taken for iterative calculation of quasi-equilibrium.

various

The new „infinite_limit“ option extends the previous “infinite” option and allows switching diffusion coefficients to “infinite” diffusion in case a pre-selected threshold value resp. limit is exceeded. It can be applied for each component independently and amongst others provides benefits in simulation time.

Noise can now be added to the driving force allowing for more realistic simulations based on fluctuations in the driving force

Several example files have been up-dated and re-worked.

Several changes in internal data formats and algorithms lead to improved performance.

A warning is now issued in case of incompatible architectures (32/64 bit) of MICRESS executable and .ges file.



documentation

The distribution of MICRESS 6.1 comprises the following 5 volumes of the manual, which have been up-dated 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
Support MICRESS®