



MATERIALS STUDIO PHASEFIELD Datasheet



OVERVIEW

Simulation of microstructure evolution at the mesoscale is a powerful tool for understanding solidification, phase transformations, dendrite growth and coarsening and grain growth in solid-state materials. This is important because the resulting microstructures determine the overall thermomechanical properties of the material.

To make microstructural predictions BIOVIA Materials Studio PhaseField tools employ the OpenPhase_Core library [1], which is a highly validated implementation of the phase-field method [2,3]. Phase-field represents materials as distributions of grains at the mesoscale, where each grain is related to the composition and orientation of crystal phases. Processes of solidification are determined by equations that describe thermodynamic and kinetic character of the phases. These are embodied by a number of physical parameters that can be measured or simulated. BIOVIA Materials Studio PhaseField supports these calculations by providing convenient way to define the component phases, represent the nucleation of solid phases, manage the thermodynamic and kinetic input, and define the temperature and pressure conditions.

Phase-field is a scale bridging technology linking thermodynamics and kinetic parameters that are routed in atomistic interactions, to microstructure prediction, which can then be either homogenized to find representative average materials properties, or used to measure relative amounts of each phase that occur as a function of thermal history.



Figure 2: Example microstructure outputs from BIOVIA Materials Studio PhaseField simulation showing the boundaries between grains.

WHAT IS PHASEFIELD?

A phase field model is a mathematical model describing interfacial dynamics. The phase distribution is described by an order parameter (phase field) which changes smoothly as you move across an interface. The system can then be solved as a set of partial differential equations avoiding explicit treatment of the boundary conditions at the interface. Effects such as latent heat, heat diffusion and mechanical strain can also be included in the simulations. The time evolution of the problem is solved by integrating the set of partial differential equations on a regular grid starting from a defined starting condition and including appropriate boundary conditions. As part of the starting conditions of the simulation you can specify grains or provide a set of nucleation seeds during the cooling of the system. You can perform calculations using a 2D or 3D grid and to speed up the calculations the code is parallelized. The primary applications of the phase field method are for microstructure formation during solidification and grain growth scenarios in metal alloys [4].

KEY USES OF PHASEFIELD

Optimizing Alloy Manufacturing

Understanding how the microstructure of hard materials such as super-alloys change as a function of the thermal and mechanical history is extremely important for determining the performance of a manufactured part. Internal stresses will be frozen in during manufacturing and can lead to deformation of materials during machining or in use. These stresses occur on the length scales of the individual metal grains and can result in part failures. For example, through detailed understanding of the grain composition and evolution during processing, metallurgists and materials scientists work to optimize the material composition and processing conditions, to contain the highest proportion of the strongest phases within the constraints of the manufacturing process. Traditionally huge numbers of physical tests and material characterization experiments are required to achieve a thorough understanding of the material and eventual certification, but predictions of the response of the material microstructure to changes in composition or solidification conditions through simulation can significantly accelerate these investigations.

Phase-field simulation of microstructure evolution at the mesoscale [2,3] is a long established method focused on understanding solidification, phase transformations, dendrite growth, coarsening and grain growth in solid-state materials. To make microstructural predictions BIOVIA Materials Studio PhaseField employs the OpenPhase_Core solver [1], which is a mature and highly validated implementation of the phase-field method. Phase-field represents materials as distributions of grains at the mesoscale, where each grain is related to the composition and orientation of crystal phases. The evolution of the phases is determined by equations that describe the thermodynamic and kinetic character of the phases. These characteristics are embodied by a number of physical parameters that can be measured or simulated.

Pipeline Pilot Materials Studio Collection protocols provide access to the phase-field method and are available through the Pipeline Pilot Connector in Materials Studio. Tutorials are also provided in the Materials Studio Online Help to provide guidance in using these protocols.

BIOVIA Materials Studio PhaseField provides a convenient way to define the component phases, grain set up, thermodynamic and kinetic input, and temperature and pressure conditions, through an easy-to-use interface in the Pipeline Pilot Connector within Materials Studio.



Figure 2: Output from a BIOVIA Materials Studio PhaseField simulation showing nucleation and growth of aluminium-magnesium alloy during cooling.

Additive Manufacturing

One important application of phase-field method is in metal additive manufacturing. BIOVIA Materials Studio PhaseField can be used to understand dependence of microstructure on the print conditions during powder bed fusion additive manufacturing in which individual layers of metal alloy powder are melted by laser or electron beam and then cool down. Microstructural simulations provide an opportunity to design the material composition and manufacturing conditions together, in order to meet the required specifications of the printed part.

The microstructures predicted by BIOVIA Materials Studio PhaseField provide a direct view into the grain size and distribution of phases, but can also be used to provide homogenized materials properties for the representative volume element (RVE) it models. PhaseField produces SIMULIA Abaqus ready versions of the RVE to streamline this activity.

With BIOVIA Materials Studio material scientists and metallurgists can bridge to the macroscopic world of metal casting and additive manufacturing from the first principles prediction of metal alloy mixtures at atomistic scales. With end-to-end simulation of these materials now incorporating the impact of processing conditions on microstructure, the development and certification of metal alloys for part manufacture can be significantly accelerated.

Dendrite Growth

By controlling the degree of undercooling and thermal gradient the growth of dendrites can be manipulated to achieve a desired microstructure. Control over growth of dendrites provides control over material properties such as temperature resistance. Phase field modeling can predict dendritic growth both from solution and surface. E.g. in directional solidification of gas turbine engine blades.

HOW DOES MATERIALS STUDIO PHASEFIELD WORK

The PhaseField module is deployed using a set of pipeline pilot protocols supplied by the BIOVIA Materials Studio Collection.

- Solidification (PhaseField)
- Grain Growth (PhaseField)
- TTT Diagram (PhaseField)

General parameters such as grid size and temperature are defined through the protocol input parameters. Component and phase dependent properties such as interface mobility and composition are specified in a study table.

SETTING UP CALCULATIONS

PhaseField tasks are available through the Pipeline Pilot Connector dialog, which provides for specification of the simulation parameters and submission of the job to Pipeline Pilot from the Materials Studio Visualizer.

Thermodynamics Interface

CALPHAD thermodynamic databases are one convenient way to provide the thermodynamic input to PhaseField calculations. These can be developed from first principles simulation using tools already available in the Pipeline Pilot Materials Studio Collection Metal Alloys or by connecting to existing CALPHAD databases.

CALPHAD thermodynamic databases can be found at:

Thermodynamic DataBase DataBase

NIST Materials Data Repository

NIMS Materials Database (registration required)

Supported CALPHAD database APIs are:

- ThermoCalc
- OpenCALPHAD

Alternatively a simple linearized database model can be created by hand through the study table. You can define this by specifying the linear phase equilibrium slopes for each phase pair and the equilibrium composition of the phases at this temperature. You can also enter the entropy difference and the diffusion coefficient for each phase pair. A diffusion activation energy for Arrheniustype diffusion modelling, can also be defined.



Figure 3: Phase diagram for a low carbon steel, showing the linearized phase diagram boundaries used for thermodynamic input.

Composition & Tessellation

For the solidification protocol initial grain sites can specified while for the grain growth protocol the Nucleation Sites and Nucleation Phase parameters specifies the tessellation setup.

Optionally continuous nucleation can also be employed. Nucleation options specifies whether Phase1 is allowed to nucleate in Phase2 in the bulk, at the grain boundary or bottom of the cell.

Elastic Properties

You can take Elastic effects into account during the simulation stress or strain can be applied to the cell through the boundary conditions.

TTT Diagrams

By running a series of PhaseField calculations time-temperaturetransformation diagrams can be constructed which represent the degree of isothermal transformation from one phase to another as a function of time. Construction of these diagrams from experiments are very time consuming and expensive.

PHASEFIELD ANALYSIS IN MATERIALS STUDIO

A PhaseField simulation returns a number of results files. A 3D Atomistic Trajectory document containing the field data for properties such as:

- Phase field
- Composition
- Temperature
- Stress & Strain

Time evolution of scalar data properties are returned in a study table tracing properties such as:

- Temperature
- Interface Energy

- Grain volumes
- Phase fractions
- Latent heat
- Stress & Strain

The final microstructure is also returned in Abaqus format.



Figure 4: A voxel representation inside SIMULIA Abaqus software of as example grain microstructure generated by PhaseField. Textures like this can be homogenised to create FEA materials models in Abaqus

THE BIOVIA MATERIALS STUDIO ADVANTAGE

BIOVIA Materials Studio PhaseField is part of the comprehensive BIOVIA Materials Studio modelling and simulation suite. The integrated model building and editing tools enable you to construct, visualize, and manipulate molecular structures and key thermodynamic inputs. Design based on experiment alone cannot explore as much of the complex compositional landscape of metal alloys. BIOVIA Materials Studio offers a single environment for the calculation of thermodynamic phases of metal alloy mixtures in-silico and prediction of the microstructure solidification and grain growth.

In summary, BIOVIA Materials Studio PhaseField enables metallurgists to explore the evolution of microstructures in novel multicomponent alloys through simulations of solidification and grain growth. These calculations allow scientists to understand how to control the microstructure to maximize alloy performance. Additionally you can use the 3D microstructure as input for FE-RVE models that will be used to create homogenized materials models for engineering level simulations or to predict the grain composition (fractions of each phase) as a function of solidification conditions.

Key Features

- Solidification
- Grain growth
- TTT diagram

Running Jobs

- All BIOVIA Materials Studio PhaseField jobs are run in the background through the Pipeline Pilot Connector freeing up the BIOVIA Materials Studio client for other research.
- All BIOVIA Materials Studio PhaseField jobs can be submitted to remote high performance computation servers and make use of parallel computing.



Figure 5: A simulation of dendritic growth during diffusion-controlled peritectic transformation in carbon steel over first 4 seconds of solidification (blue = liquid, purple = d-ferrite, red = g-austenite)

LEARN MORE

REFERENCES

- OpenPhase http://openphase-solutions.com 1.
- Steinbach, I Phase-field models in materials science, 2. Modelling and Simulation in Materials Science and Engineering vol. 17 issue 7 (2009) pp: 073001 https://doi.org/10.1088/0965-0393/17/7/073001
- Steinbach, I. Why Solidification? Why Phase-Field?. JOM 3 65, 1096-1102 (2013) https://doi.org/10.1007/s11837-013-0681-5
- 4 A Monas et al Dual-scale phase-field simulation of Mg-Al alloy solidification 2015 IOP Conf. Ser.: Mater. Sci. Eng. 84 012069 https://doi.org/10.1088/1757-899X/84/1/01206

Our **3D**EXPERIENCE® platform powers our brand applications, serving 11 industries, and provides a rich portfolio of industry solution experiences.

Dassault Systèmes, the **3DEXPERIENCE** Company, is a catalyst for human progress. We provide business and people with collaborative virtual environments to imagine sustainable innovations. By creating 'virtual experience twins' of the real world with our **3DEXPERIENCE** platform and applications, our customers push the boundaries of innovation, learning and production.

V. R **3D**EXPERIENCE

Dassault Systèmes' 20,000 employees are bringing value to more than 270,000 customers of all sizes, in all industries, in more than 140 countries. For more information, visit www.3ds.com.



Americas Dassault Systèmes 175 Wyman Street Waltham, Massachusetts 02451-1223 แรล

Europe/Middle East/Africa Dassault Systèmes 10, rue Marcel Dassault CS 40501

France

Dassault Systèmes K.K. ThinkPark Tower 2-1-1 Osaki, Shinagawa-ku, 78946 Vélizy-Villacoublay Cedex Tokyo 141-6020 Japan

Asia-Pacific