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Title

Multi-scale thermomechanical simulation of solid-liquid interactions during solidification

Project management/-processing

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Task definition

The main focus of the work was the self-consistent multi-scale simulation of the solidification of Al-chill casting components, the modelling of quasi-incompressible phases (melt, amorphous phase of semi-crystalline polymers) in the calculation of effective mechanical properties of metals and polymers, and the further development of viscoplastic material laws for the complete solid-liquid range. For the calculation of the deformation of the forming microstructure during solidification by external forces, the mechanical modelling in the multi-phase field approach is further developed.

Procedure

For a multi-scale simulation of the solidification of a cup-shaped Al-chill casting, local thermal conditions, i.e. heat extraction rate and temperature gradient were extracted from a macroscopic thermo-mechanical casting simulation (TP B9) and used as boundary conditions for the mesoscopic microstructure simulation. In general, a different temperature gradient is calculated on the microstructure scale than on the macroscopic component scale. The development of the solid phase fraction calculated on the microstructure simulation and the associated release of latent heat were used in a renewed casting simulation for modelling the solidification interval, see Figure 1(a). These iterative simulation runs on the two length scales are carried out until a consistent description of the temperature curves on the micro- and macroscale is achieved. Previous simulations have shown that only a few (5) iteration steps are necessary to achieve this.

In order to model quasi-incompressible materials, mixed, stabilized finite elements have been implemented in the homogenization tool. The pressure stabilization is achieved by a double Gaussian integration [1]. Furthermore, the periodic boundary conditions are no longer represented by a penalty approach but by a master-slave projection algorithm.

When reformulating the viscoplastic material law for the coherent solid-liquid region [2], care was taken to ensure that the pressure-dependent term now varies continuously during the transition from a compression to a tensile state or vice versa.

For the further development of the phase field model in the direction of mechanics, a theoretical study was carried out in which a mixed stress-strain approach was investigated for the diffuse interface. This approach makes it possible to ensure both the mechanical equilibrium of the surface forces and the kinematic compatibility of the strain tensor at the interface.

Results

A first macroscopic casting simulation of the Al cup is carried out with an fS(T) curve (solid phase fraction) from a material database, which, however, does not take into account the local microstructure development in the component. This corresponds to the usual procedure for simulation at component level. Then followed a first local microstructure simulation (in our example in point A of the component, Figure 1a) with an initially estimated constant heat extraction rate (iter1).

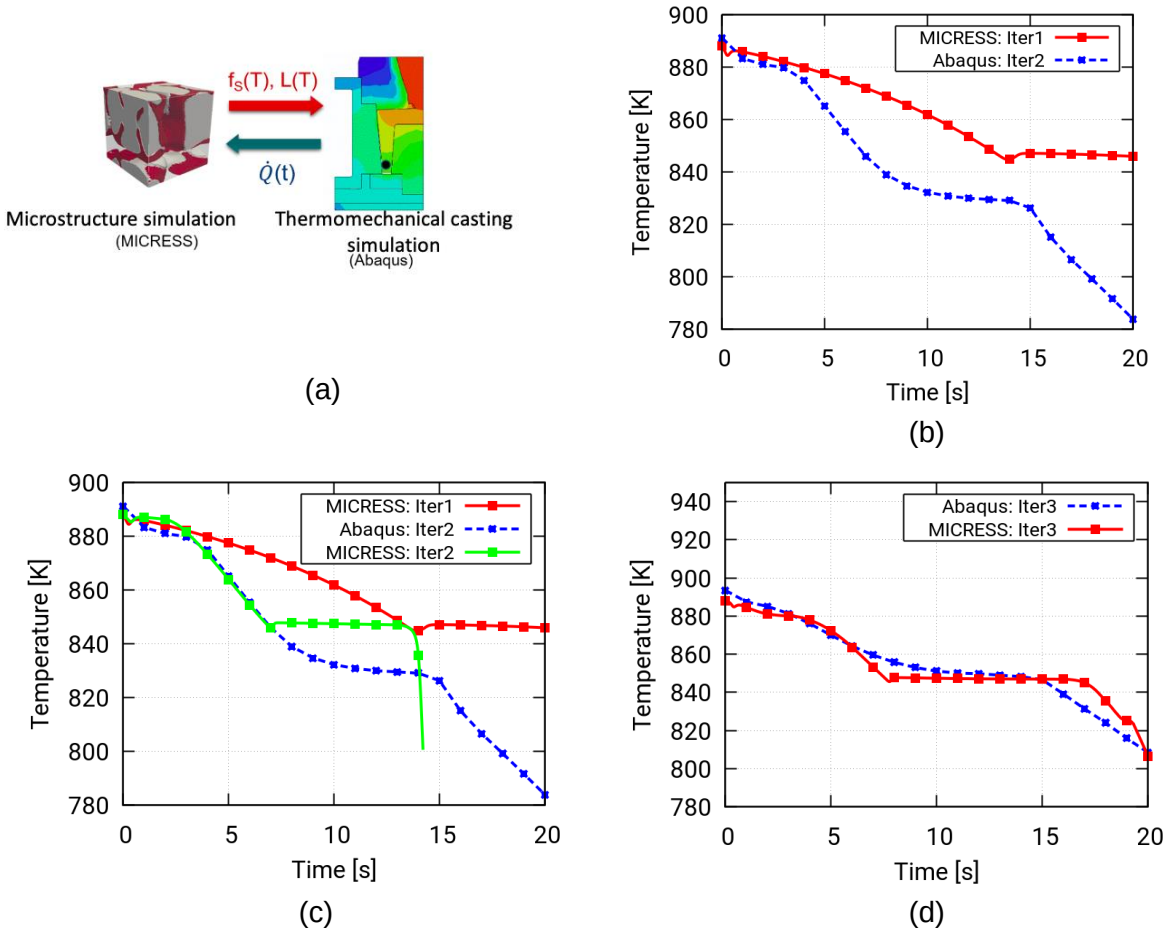

Figure 1: Representation of the iterative simulation on microstructure and component scale (a), and comparison of the local temperature curves (at point A) of the microstructure and casting simulation after the first (b), second (c) and third (d) iteration.

As can be seen in Figure 1b, the microstructure simulation leads to a temperature curve that deviates significantly from the cooling curve in the cup. The corresponding temperature-dependent curve of the solid phase fraction was then used in the second casting simulation (iter2) instead of the usual fS(T) curve from the database. By using the local heat draw rate from this casting simulation in the next microstructure simulation (iter2), the deviation between the temperature curves on the micro- and macroscale is already significantly smaller, in particular the total solidification time is already in good

agreement, see Fig. 1c. Already after the third iteration a consistent description of the temperature curves on both scales was achieved, Figure 1d.

To achieve a more precise prediction of the local mechanical properties in an injection molded polypropylene (PP) sheet, the existing multi-scale simulation of injection molding was improved in cooperation with the IKV [1, 3]. For a more precise representation of the quasi-incompressibility of the amorphous phase (= 0.499), mixed linear finite elements were implemented in the homogenization tool. Homogenization and localization calculations for a benchmark RVE of a composite material, epoxy resin with a glass sphere, have shown that the element variant P1+P1 is the most precise variant. Besides the pressure stabilization of type Li-He, this element variant is characterized by a linear displacement field enriched with volume bubble. This variant, in combination with the newly implemented master-slave projection algorithm for periodic boundary conditions, leads to significantly improved effective properties of the "cross-hatched" PP lamella on the nanoscale, as shown in Table 1. For comparison purposes, this table also lists the predictions with classical linear and quadratic elements in combination with the penalty approach for periodicity. The gain in precision for the calculated properties is due to the unrealistically high stiffness of the classical tetrahedra for quasi-incompressible phases, which leads to a strong reduction of the microscopic displacements on the RVE and the correction of the volume averaged Hooke Matrix (see Figure 2).

Element	Nodes	E_1	E_2	E_3	G_{12}	G_{13}	G_{23}
P1	40264	1750.2	1854.2	**8280.0**	513.8	687.0	602.8
P2	280678	1687.8	1790.1	**7486.3**	489.5	658.8	580.2
P1+P1	40264	1411.8	1798.1	**3958.7**	262.3	321.5	297.0

List 1: Effective elasticity and shear modulus [MPa] of the straight design of the "cross-hatched" semi-crystalline PP lamella.

On the next higher microscale, four different solidification structures were homogenized over the 3 mm thick cross-section of the PP stepped plate using the radial spherulite model. These are a coarser microstructure, initiated by thermal nucleation, and a fine microstructure, which is caused by athermal nucleation. In both microstructures, the boundary layer between the individual spherulites was shown separately once and not in a second variant.

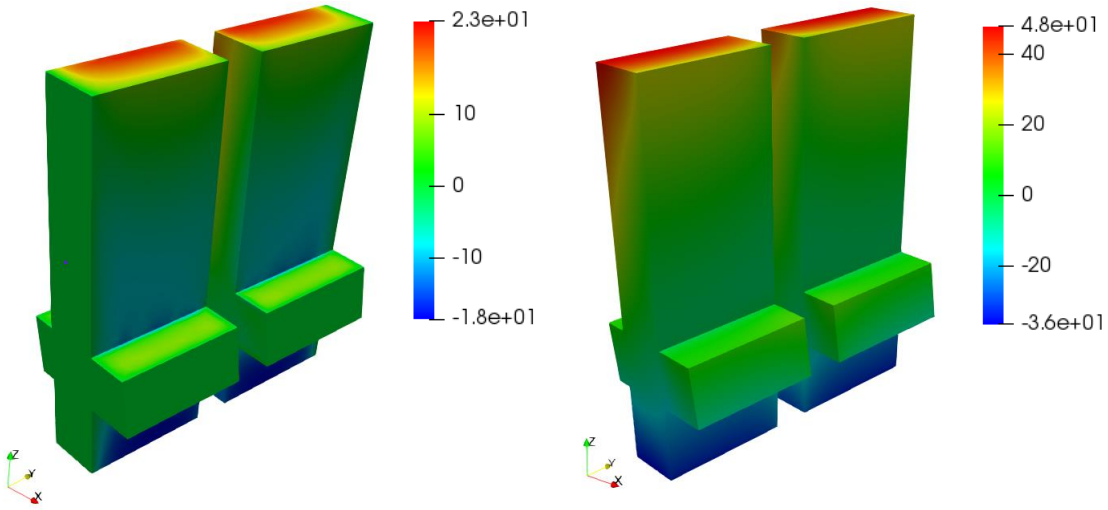

Figure 2: Microscopic displacements [nm] in the Ez direction of the crystalline phase of the cross-hatched PP lamellae under a load in the same direction. Left: linear P1 elements; right: mixed, stabilized P1+P1 elements.

Figure 3 shows the variation of the mean effective modulus of elasticity and shear for the four different microstructure variants over the plate cross-section. The comparison with the experimentally determined mean modulus of elasticity and its confidence interval shows that the athermal variant without boundary layer provides the best description of the modulus of elasticity. This variant also provides the largest mean shear modulus. Only when it becomes possible to image the real interface thickness of approx. 300 nm in the microstructure simulation spherosim and to smooth its surface, the variant with boundary layer becomes interesting for the property prediction.

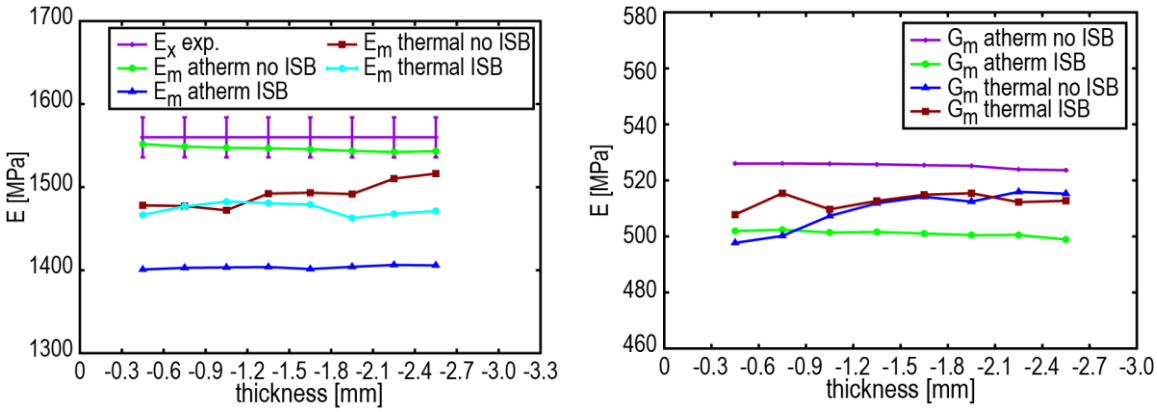

Figure 3: Variation of the effective mean elastic (left) and shear moduli (right) over the plate thickness for a simulated microstructure with a model for thermal or athermal nucleation taking into account / not taking into account a boundary layer (ISB) between the spherulites.

Summary and Conclsion

The developed iterative multi-scale approach takes into account the local microstructure development in macroscopic component simulation and provides a consistent calculation of temperature curves on macro and micro scale for gravity die casting of Al alloys. Thus, it is possible to consider the influence of alloy composition as well as different solidification morphologies (columnar, equiaxial, eutectic, grain size, ...) in the component simulation. The application of this iterative multi-scale approach for different casting forms, e.g. cup and F-sample (TP B9), will not only allow us to derive refined, microstructure-based effective material laws, but also to quantify the influence of local variations of the microstructure on the component precision (distortion, residual stresses). Effective viscoplastic flow curves of equiaxially and directionally solidified microstructures of the Al alloy A356 are to be determined by virtual tests and enable a refinement of the viscoplastic material models for the solid-liquid range.

The implementation of mixed, stabilized elements in the homogenization tool significantly improved the prediction of effective elastic properties of materials with quasi-incompressible phases, such as the amorphous phase of semi-crystalline polymers or the residual melt in the solid-liquid range. The next step is to generate new lamella designs with shorter or missing side arms for different degrees of crystallization across the component thickness and to determine their influence on the mechanical properties. Together with TP B4, the iterative multi-scale approach will also be applied to the solidification of semi-crystalline polymers.

Publication

[1] G. Laschet, H. Nokhostin, S. Koch, M. Meunier, Ch. Hopmann: „Prediction of effective elastic properties of a polypropylene component by an enhanced multiscale simulation of the injection molding process", Mechanics of Materials, under review, April 2019.

[2] G. Laschet, H. Behnken: "Thermo-elasto-viscoplastic constitutive laws for metallic alloys during their solidification", accepted for IOP Conference Series: Mat. Science & Eng., June 2019.

[3] G. Laschet, H. Nokhostin, S. Koch, Ch. Hopmann: "Microstructure dependent effective elastic properties of a polypropylene plate via a multiscale simulation of the injection molding process", Int. Workshop on Simulation Science, 8th-10th May 2019, Clausthal, Springer book of extended abstracts, May 2019.