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THERMAL STRESS AND CRACK PREDICTION

OF INVESTMENT CASTS ALLOYS

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Abstract

Deformation and cracking of cast parts due to thermal stresses and hindered shrinkage are frequent casting defects. Whereas the numerical simulation of mold filling and solidification are already state of the art, applications of a thermal stress analysis are rarely found. The present study reveals how a combined thermo-mechanical model can be used for the investment casting process by optimizing casting design and process parameters.

By means of the 3D-FEM-program CASTS, developed at the Giesserei-Institut, investigations were carried out to determine quantitatively the formation of thermal strains and stresses of intermetallic alloy based investment castings. To improve the accuracy of the stress prediction, a new unified constitutive model developed at the University of Illinois was applied which combines creep and plastic strain together. A relation between the local stress level and the tensile strength of the material was used to predict areas susceptible to cracking.

In order to validate the numerical analysis, various casting experiments accompanied the modeling investigations. The influence of notches in the casting geometry and mold preheat temperature on the cracking sensitivity was monitored during casting by a special electrical device and compared to simulated results. Cracking is less likely at slower cooling rate, such as found with a preheated mold. Such analysis may help to develop future guidelines to minimize the susceptibility to cracking of investment castings and to improve quality in other casting processes as well.

Introduction

Intermetallic γ-TiAl alloys represent a new material for high temperature applications in turbine and motor construction. These alloys have excellent high temperature properties, i.e. tensile strength, creep and oxidation resistance, resulting from their ordered atomic structure. Besides that, the γ-TiAl-based alloys offer a very low density compared to conventional Ni-based superalloys. Thus, alloys based on γ-TiAl are close to technical application. A suitable near-net-shape manufacturing method for γ-TiAl alloys is the investment casting process. Investment cast parts have excellent surface quality and high dimensional accuracy. However, the remarkable cracking sensitivity during cooling is a major obstacle for casting titanium aluminides [1-3]. In order to avoid such casting defects and to predict cracking sensitivity in complex shaped γ-TiAl cast parts, it is necessary to determine quantitatively the formation of thermal stresses and their dependence on the casting parameters. Therefore, numerical simulation was used as a viable tool for predicting crack formation in investment castings.

Numerical Procedure

Simulations were performed using the finite element software package, CASTS, which has been developed at the Foundry-Institute. This program enables coupled 3D-modeling of casting processes and can predict temperatures, stresses and microstructural evolution [3,4]. In this work, CASTS was used for a coupled thermo-mechanical analysis of investment castings. The model features a new unified constitutive model developed at the University of Illinois which combines creep and plastic strain. It also features special interface elements between contacting materials, that exhibit no volumetric extension.

Thermal Analysis

The thermal analysis takes into account various boundary conditions such as convection, insulation or radiation as well as the release of latent heat during solidification. All thermophysical properties are temperature-dependent. Initial temperature distributions may be set from previous calculations using a separate mold filling simulation. Heat flow between different materials is modeled by interface elements. A Gauss-Seidel algorithm solves the discretized Fourier equation of heat conduction. The calculated temperatures are input for the subsequent strain and stress simulation.

Strain and Stress Simulation

Thermal stresses are due to hindered shrinkage of the casting and inhomogeneous cooling conditions. Total strains and stresses are calculated incrementally, based on the time dependent temperature field. The stress simulation alternates between a global and a local level. The displacements $\{\delta\}$ at a time step t are calculated at the global level:

$$\left[K^t\right]\left\{\delta^t\right\} = \left\{R^t\right\}_{tot} = \left\{R^t\right\}_{ie} + \left\{R^t\right\}_{th} \qquad (1)$$

with K as the stiffness matrix and $\{R\}_{tot}, \{R\}_{th}$, $\{R\}_{ie}$ as total, inelastic and thermal force vectors. At time t the temperature-dependent values of. $\{R\}_{th}$ are easily calculated from the known temperature distribution:

$$\{R^t\}_{th} = \int_V [B]^T \{\alpha^t\}\{\Delta T^t\} dV \tag{2}$$

Here, $[B]$ is the strain-displacement matrix containing shape function derivatives and $\{\alpha\}$ contains the thermal expansion coefficient. $\{R\}_{ie}$ takes into account inelastic strains.

$$\{R^t\}_{ie} = \int_V [B]^T [D] \{\Delta\varepsilon^t\}_{ie} dV \tag{3}$$

where $[D]$ is the matrix of elastic constants. The inelastic strain increment vector $\{\Delta\varepsilon\}_{ie}$ can be calculated on a local level by integrating the inelastic strain rate vector $\{\dot{\varepsilon}_{ie}\}$:

$$\{\Delta\varepsilon^t\}_{ie} = \int_{t-\Delta t}^{t} \{\dot{\varepsilon}_{ie}(\varepsilon, \sigma, T)\} dt \tag{4}$$

A unified constitutive law calculates inelastic strain rate in the γ-TiAl depending on the current local temperature T, the stress, σ, and the microstructure, as represented by the total strain, ε_{tot}:

$$\dot{\varepsilon}_{ie} = h_1\left(1 - 0.098\, e^{-\left(\frac{\varepsilon_{tot}}{0.7}\right)^{1.4}}\right) e^{h_2 T}\left(\sigma - h_3 \operatorname{sgn}\sigma + h_4|\sigma|\right) \tag{5}$$

The values of the constants h_1, h_2, h_3 can be found in [5]. To integrate the non-linear equation system (eq. 4) a two level iterative scheme developed by Lush [6] has been used. The successful application of this approach for steel continuous casting processes has been shown by Zhu [7]. To optimize the integration, this scheme reduces the set of equations to integrate to only the scalar effective strain $\bar{\varepsilon}$ and effective stresses $\bar{\sigma}$. Using the Prandtl-Reuss equations for plastic flow, the multicomponent strain vector can be derived:

$$\{\Delta\varepsilon^t\}_{ie} = \frac{3}{2}\Delta\bar{\varepsilon}_{ie}^{t} \frac{\{\sigma'^{\,t-\Delta t}\}}{\bar{\sigma}^{t-\Delta t}} \tag{6}$$

where σ' is the deviatoric stress tensor. Knowing both forces, eq. (1) is solved with a preconditioned conjugate gradient algorithm.

In order to take the mechanical interactions between the mold and casting into consideration, a new gap/contact approach was developed which employs the same interface elements that are used in the temperature calculation. A detailed description can be found in [8]. Unlike other methods, the mold is not assumed to be rigid.

This approach simplifies the appropriate setting of mechanical boundary conditions with contact. At each time step and for each interface node, the algorithm checks whether a gap between mold and cast part exists or whether local contact forces have to be accounted. Closing and opening of adjacent interface nodes is controlled by manipulating the global stiffness matrix. Whereas classical procedures like the penalty-method or the use of Lagrange multipliers may lead to numerical problems, this approach is numerically stable and accurate, although it increases the required computation time by up to 30 %. An example of the agreement between the results using this method and experiments is shown in figure 1.

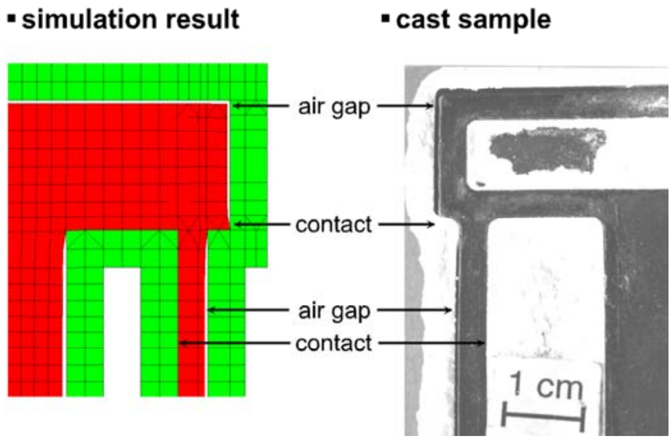

Figure 1: Predicted air gap / contact zones between the ceramic shell and investment casting (left) are compared with a cast sample shown with the mold partially removed (right).

Casting Experiments

To validate the numerical analysis, several casting experiments were performed. The alloy TiAl48Cr2Nb2 (at.-%) was chosen because this material is very sensitive to thermal stresses, which often lead to casting defects. The cracking sensitivity of investment cast γ-TiAl parts was investigated by varying the preheat temperature of the mold. This greatly varies the cooling rate, a critical casting parameter.

Temperatures were measured with thermocouples placed in the casting in order to determine reliable cooling curves to calibrate the numerical simulation of the temperature distribution. Figure 2 reveals a satisfying agreement between the measured cooling rates, and those simulated using an estimated, temperature dependent heat transfer coefficient between casting and ceramic mold. This is important for the accuracy of the subsequent stress calculations, due to the strong temperature dependence of the mechanical properties.

The geometry of the experimental casting samples, shown in figure 3, was specially designed to evaluate the cracking sensitivity. It consists of six segments of different diameters. Each segment has a sharp notch, which serves as a predetermined cracking point. The enlarged diameters separate the segments from each other, so guarantee a hindered shrinkage of the casting. Hence, longitudinal stresses are built up in the casting during cooling. If the stresses exceed the ultimate tensile strength, the segments crack apart. In order to monitor the formation of cracks in the segments, each of the enlarged diameters is supplied with an electric contact. By measuring the direct voltage, crack formation and growth during cooling can be observed either as a slow decrease (crack initiation) or a sharp drop of voltage (complete separation). The casting experiments were carried out in a centrifugal casting device using Yttria coated ceramic crucibles for melting.

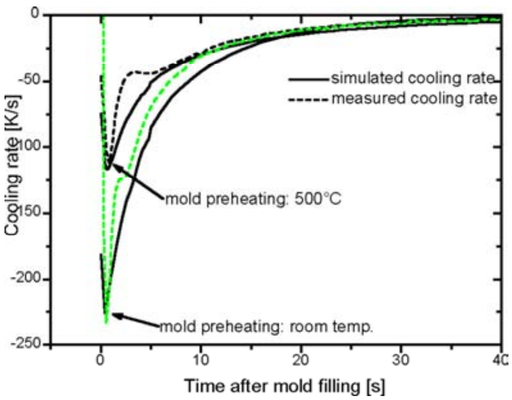

Figure 2: Comparison of various cooling rates measured in the casting between 5 and 6 ∅ mm segments (see figure 3) with numerical simulation results.

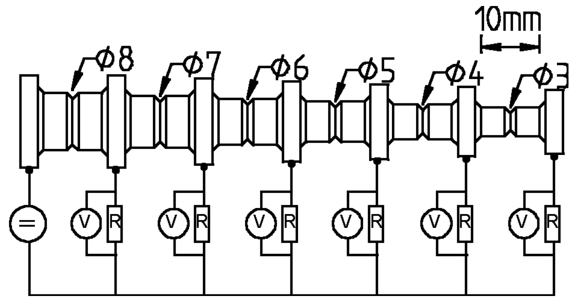

Figure 3: Sample geometry for the characterization of cracking sensitivity of γ-TiAl based alloys.

Model Validation

The casting experiments allow the validation of the results of the numerical simulation. Figure 4 shows a perspective view of the mesh of the sample geometry, created using an in-house package. Due to the symmetry of the casting, the mesh is reduced to a quarter of the original shape in order to reduce computing time. The resulting geometry, shown in figure 4, includes both the casting and ceramic shell mold, and is described by 8984 nodes, 6560 volume elements, and 1405 interface elements. Real castings have features with great variations in wall thickness, so the cooling is highly inhomogeneous.

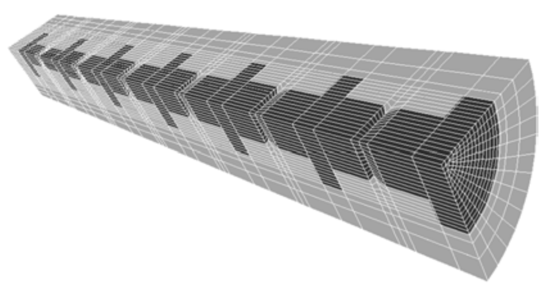

Figure 4: Mesh of the sample geometry.

Because the material properties are strongly dependent on temperature, the risk of cracking can not be evaluated by examining only the level of stress built up in the casting. In order to better account for the temperature dependence, a cracking criterion was used to evaluate the results of the temperature and stress simulation together. The cracking criterion is defined as the ratio between the calculated maximum principal tensile stress σ(t) and the corresponding temperature dependent tensile strength R_m of the material at that point in the casting:

$$C_{crack}(t) = \frac{\sigma(t)}{R_m(T)} \cdot 100\% \tag{7}$$

Reliable high temperature strength data are scarce in the literature. In this work, the ultimate tensile strength was estimated over a wide temperature range, figure 5. The stress calculation also requires Young´s Modulus and thermal expansion data. These thermo-mechanical properties were measured for temperatures up to 1350°C [10], and estimated above that, as given in figure 6. Poisson´s ratio was assumed to be temperature independent according to [11] and was set to 0.24.

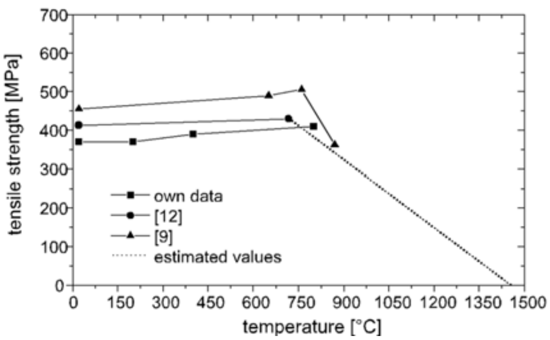

Figure 5: Temperature dependence of the ultimate tensile strength of γ-TiAl alloys for the calculation of the cracking criterion, based on data measured at the Foundry-Institute.

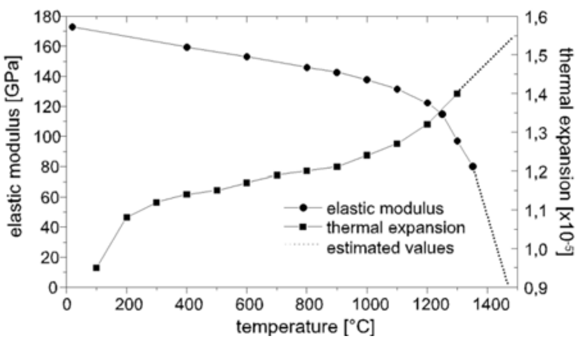

Figure 6: Young´s Modulus and thermal expansion of alloy TiAl48Cr2Nb2 (at.-%) showing their dependence on temperature. Data above 1350˚C were estimated.

Results and Discussion

Casting experiments and simulations were performed for different mold preheating temperatures. As previously described, electric contacts allowed the monitoring of crack formation and growth in the sample geometry during cooling. The results in figure 7 show that the higher cooling rates associated with a non-preheated mold promote crack formation. All segments up to ∅ 6mm crack completely in the non-preheated mold, figure 7a. As mold preheating temperature is increased, the sample geometry can be cast completely crack free, figure 7b.

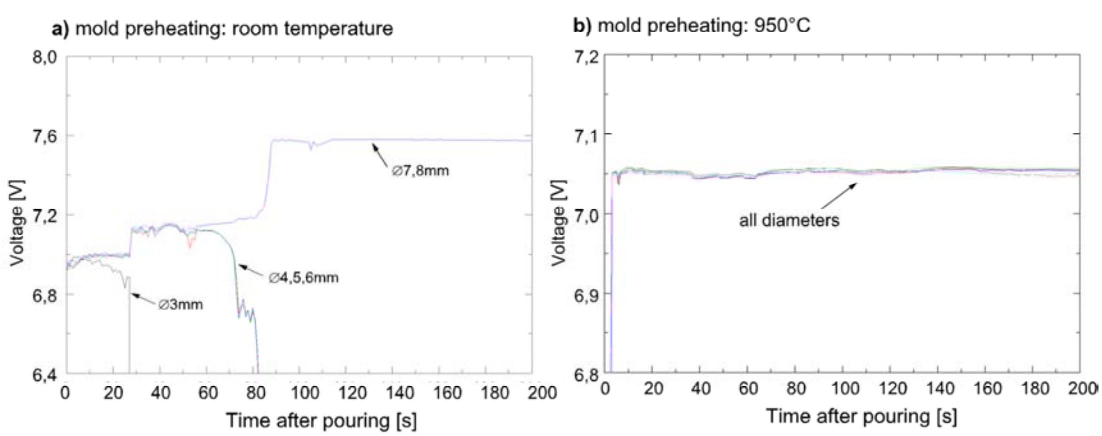

Figure 7: Monitoring of crack formation in the castings during cooling.

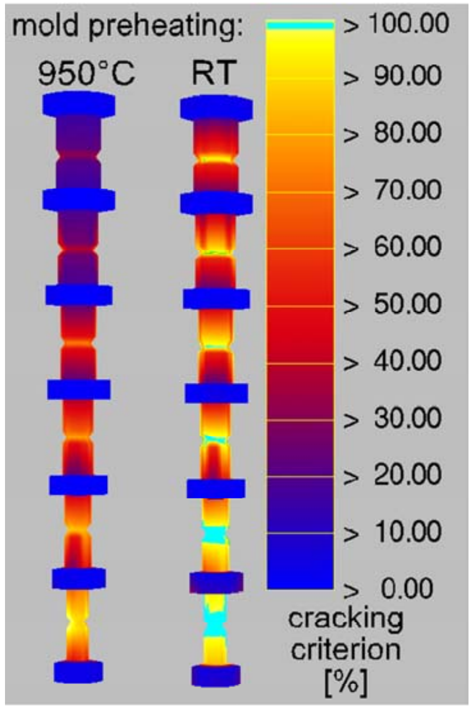

Figure 8: Calculated cracking criterion in the casting after complete cooling to ambient for different mold preheating temperatures: 950˚C and room temperature.

The temperature and stress distribution in the sample casting was then calculated for the two different mold preheating temperatures. The simulation results in figure 8 show the maximum value of the cracking criterion reached at each point in the casting after cooling to room temperature. The simulations predict lower residual stresses and lower cracking criterion values for the higher mold preheat. This is due to the slower, more homogeneous cooling. The maximum stresses in the castings can be found around the notches. For the high cooling rates encountered in the smaller segments, these stresses may reach or even exceed the ultimate tensile strength of investment cast γ-TiAl [3],[12]. With slower cooling rates, the risk of cracking is less. Figure 8 shows a reasonable agreement between the calculated results for the cracking criterion and the formation of actual cracks monitored in the castings during cooling.

Conclusions

The results of this work confirm that numerical simulation provides a useful tool for predicting the temperature, stress, and most importantly, the risk of crack formation, during casting and subsequent cooling. Specific findings from the simulation of γ-TiAl castings revealed that cracking is less likely at slower cooling rates, such as found with a preheated mold. Yet, the quantitative accuracy of the calculated results can be improved. The predicted stresses may be overestimated because the formation of cracks is neglected within the calculation. Reliable thermomechanical and thermophysical data for elevated temperatures up to the solidus temperature are rarely be found in the literature. Since the behavior of the material at high temperatures strongly influences the whole calculation, such data needs to be extended.

Acknowledgments

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