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Criterion function for predicting freckles in CMSX-4 during directional solidification

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Abstract. In the present work the impact of curvature effects on freckle formation in CMSX-4 during directional solidification was modelled and simulated. Modelling work is based on a four-step criterion function for predicting freckles. First, only surface elements are taken into account. Second, critical cross-sectional areas are identified where freckle formation is possible. As a new aspect, third, curvature effects are taken into account for predicting freckles in radiation shadow. Fourth, the Rayleigh number is calculated based on a permeability function of dendrite arm spacing and fraction of liquid. In the thus identified areas sufficient thermo-solutal convection takes place to initiate freckle formation. With the new model freckles can only appear in areas where the thermal temperature profile is concave, that is, at locations where the temperature gradient is positive against the surface normal. The present model was tested simulating step samples. For that, the individual parts of our industrial Bridgman furnace were input and joined in one FEM model. The thermal results clearly show concave solidus isothermal at the shadow faces of the step sample in the cluster. Freckles are predicted at the corresponding locations. When comparing simulated freckle formation with experimental findings, good correlation was found. Furthermore, we could predict both the transition length that occurs when the cross-sectional area increases stepwise and the run length when the cross-sectional area is reduced.

1. Introduction

Directionally solidified or single crystal castings of superalloys are characterized by their excellent high temperature properties. However, the production of defect-free components is more problematic with increasing component size. Typical structural defects are particularly freckles, which are observed as aligned chain-like small defect grains predominantly at the outer surface of thick-walled casting areas. Because of the negative influence of freckles on the life of the components, this structure defect is usually a discard criterion and should therefore be avoided. The solidification of nickel based superalloys is characterized in that the interdendritic residual melt is enriched with the light elements Ti and Al, while the heavy elements W and Re are depleted. This lower density results in interdendritic upward convection in the mushy zone. From broken and melted off dendrites the chain-like freckles are formed. So far, three important impact factors of freckle formation are known: (1) the chemical composition, that is, alloys with high contents of T, Al, W, and Re show increasing probability of freckles; (2) the size of the castings, freckles occur primarily in thick-walled castings rather than in thin-walled; (3) the solidification parameters, a low temperature gradient and a slow rate of solidification promote freckles formation.

2. State of the art

Freckles appear under certain conditions, primarily at the surface of directionally solidified castings on what is referred to as the *surface effect*. Copley et al. [1] report that in directional solidification virtually all freckles found occur at the external surface of the castings. Thus when it comes to freckle formation, a critical cross-sectional size of the component must be achieved, which refers to the so-called *size effect*. In thin sections freckle formation does not occur. For this purpose a minimum cross-sectional area A_0 and a diameter D_0 is defined. From the local geometry the equivalent diameter $D_{eq} = 4\ A\ /\ U$ is calculated, wherein A is the local cross-sectional area and U is the circumference. From this, the critical diameter criterion for freckles formation derives as follows:

$$I_D = D_{eq} / D_0 \tag{1}$$

Ramirez and Beckermann [2] investigated correlations of freckle formation depending on material and process based on different Rayleigh number definitions. Auburtin [3] examined freckle formation in directionally solidified rods made of the three superalloys (Waspaloy, Mar-M247, CMSX-4). In his research, he developed a modified Rayleigh based criterion that incorporates the anisotropy of the mushy zone, permeability and gravity to describe the influence of process parameters, and the angle of the growth front on freckle formation. This is known as the *process and material effect*. He assumes that the thermo-solutal convection takes place either perpendicular or parallel to the primary dendrites:

$$Ra_x = F_x /(\eta D / K_x^2) \qquad \text{and} \qquad Ra_z = F_t /(\eta D / K_{tx}^2)\,. \tag{2}$$

The driving force for freckle formation is given by:

$$F_x = g\ (d\rho / dT)\ G_F \sin(\alpha) \quad \text{and} \quad F_Z = g\ (d\rho / dT)\ G_F\,. \tag{3}$$

For the modified Rayleigh criterion of Auburtin the parameter set in table 1 was used. Viscosity and thermal diffusion constant were assumed to be concentration- and temperature-independent in the solidification range. The critical specific change in density that results in the formation of freckles was determined experimentally with 30 kg/m^3/K. By microprobe measurements on quenched samples the concentration profiles could be determined and transformed into density profiles by weighted averaging. By inserting these parameters in equations 2 and 3, the Rayleigh numbers can be simplified as follows:

$$Ra_x = 4.62 \cdot 10^{-15} G_F (G_L V)^{-2.75} \sin(\alpha) \quad \text{and} \quad Ra_Z = 3.64 \cdot 10^{-14} G_F (G_L V)^{-1.32}. \tag{4}$$

If one of the thus determined Rayleigh numbers exceeds the critical value $Ra^*(\text{CMSX-4}) = 10^{-8}$ according to Auburtin [3], freckles are formed. The criterion for freckle formation corresponds to:

$$I_{Ra} = Ra / Ra^*, \tag{5}$$

with $Ra = \max(Ra_x, Ra_z)$. By combination of the criterion for the critical cross-section and the Rayleigh number, a generalized criterion can be formulated as follows:

$$I = I_D \cdot I_{Ra} \tag{6}$$

Table 1. Parameters and physical data for the calculation of Rayleigh numbers.

parameter	value and unit	Description	Ref.
g	= 9.81 [m/s^2]	acceleration due to gravity	
D_T	= 9*10^{-6} [m^2/s]	thermal diffusivity	
η	= 4*10^3 [kg/ms]	dynamic viscosity	
f_L	= 0.5 at the location of freckles	fraction of liquid	
$d\rho/dT$	= 30 [kg/m^3/K]	specific density change	
G_L	process parameter [K/cm]	gradient at the growth front	
G_S	process parameter [K/cm]	gradient at solidus	
G_F	= 0.8 G_L + 0.2 G_S [K/cm]	gradient at location of freckles formation	
K_x	= 3.62 * 10^3 $f_L^{3.34}$ $\lambda_1^{0.699}$ $\lambda_2^{2.73}$ [m^2]	perpendicular permeability	[4]
Kz	= 3.75 * 10^{-4} f_L^2 λ_1^2 [m^2]	parallel permeability	[4]
λ_1	= 0.0015/(G_L* V)$^{0.33}$	distance between primary dendrites	[5]
λ_2	= 0.0004/(G_L * V)$^{0.42}$	dendrite arm spacing	[5]
V	= process parameter [m/s]	solidification rate	
α	= process parameter [°]	angle at the growth front	

3. Work carried out

The modified Rayleigh criterion of Auburtin [3] considers only the growth angle of the solidification front, the curvature has been neglected. In fact, the concave curvature and the associated *curvature effect* is a basic requirement for freckle formation on the surface, as shown by Ma et al. [6]. In the present study the curvature requirement was included in the modified criterion by a critical angle β which was defined between the surface normal of the cast component and the growth front. If $\beta > 90°$, we obtain a concave solid-liquid interface and freckle formation will occur. The overall model with the extension to the curvature requirement of the solidification front has been implemented as shown in figure 1.

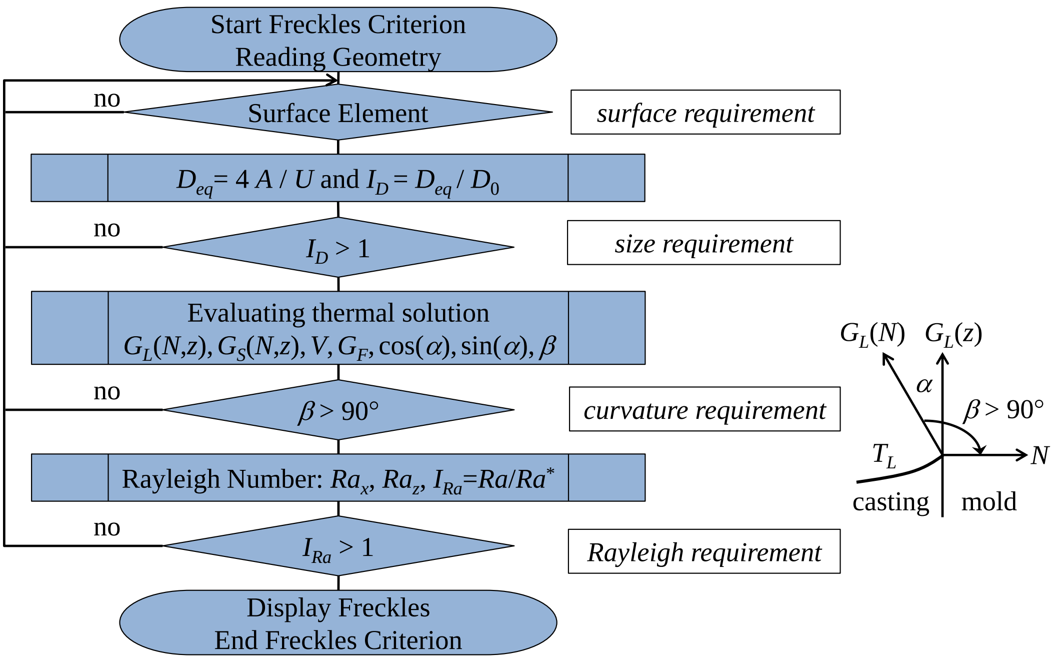

Figure 1. Flow chart for calculating the freckles criterion including curvature requirement.

The additional effect of the curvature now allows also the prediction of shadow effects in freckle formation. For this purpose, the geometry of a cluster mold was created linking six step samples. Also the industrial Bridgman furnace, in which the experiments were carried out, was entered in its geometry and the individual components were linked together. The overall model consists of chill plate, cast metal, shell, lower / upper heater, inner / outer baffle, cooling, insulation and wall material. The materials used have been provided with the appropriate thermo-physical data and the initial (cast metal and shell 1430°C), boundary (upper heater 1480°C, lower heater 1500°C, chill plate, and cooling 20°C) and run-time conditions (velocity of withdrawal 1mm/min) adapted to the experiments carried out. In the simulation model CASTS, that Laschet et al. [7] described in detail, the cast component is withdrawn in the cooling zone with a fixed withdrawal velocity, calculating the view factor matrix for each lowering step. Through the view factor matrix the radiation exchange among surfaces is calculated taking account of the variation due to the withdrawal. In this way the temperature profile impacted by shadow effects can be taken into account. The temperature field determined from this simulation is evaluated in the extended criterion function for freckle formation regarding temperature gradients and solidification conditions.

4. Results

The basis for the prediction of freckles in the present model is the geometry of the sample and the temperature result through processing the sample in the Bridgman furnace. For studying the influence of geometry changes on freckle formation sample geometries were used with varying cross sections. The gradation of the cross-section is 1.5mm and the step length 25mm. Figure 2 shows one example in a sectional view along the centre line of the xz-plane of the temperature field of a cluster of step samples after 5010s at a constant drawing rate of 1mm/min. The isothermal lines for liquidus are drawn in green and for solidus temperature in blue. It is clearly seen that under the chosen process conditions the solidification front is far ahead of the baffle. For each withdrawal step, the view factor matrix is recalculated. This shows the prediction of radiation shadows as they exist in the centre of the cluster. This can be recognized on the slope of the solidus isothermal lines towards the middle of cluster. For the outer step samples the concave curvature of the solidus isotherms into the direction of the centre of the cluster can be seen. We can also see that the liquidus isothermal line spreads at the corners where the cross-sectional area increases. Due to the Reynolds and the new curvature requirement no freckles will appear at corresponding locations.

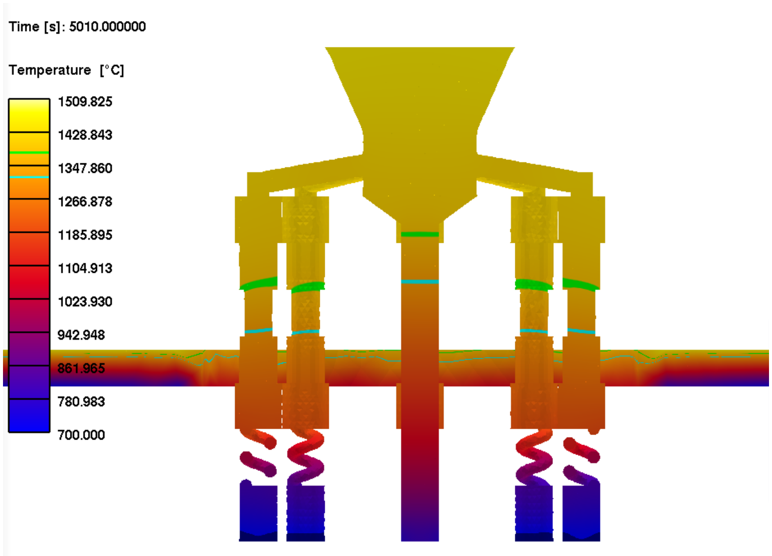

Figure 2. Temperature field during the withdrawal of a cluster of samples with levels for liquidus and solidus isothermal lines.

To validate the simulation results, we come back to the results published by D. Ma et al. [6]. Freckles result, as mentioned, preferably on the sample surface. This work showed (cf. Figure 3d), that when an abrupt change in cross section occurs, the continuity of the surface is broken, and freckle formation supportive conditions have to rebuild on the upper level. In a cross-sectional widening the freckles on the lower end can arise only when a sufficient "support zone" was established. In this support zone are sufficient segregation and density inversion to allow convection, which then leads to freckle formation above the transition length. In the case of a cross-sectional reduction there exists already a large interdendritic mushy zone below the new surface. Freckles may appear on the new interface immediately.

The freckles criterion indicates the relative percent for exceeding the critical Rayleigh number and diameter in calculations. In the case of the CMSX-4 alloy used, the critical Rayleigh number is 10^{-8}, which is exceeded by up to 25% according to the prediction in figure 3. Well predicted is the effect of the transition length, which can be seen on the steps with cross-sectional enlargement. Conversely, the results also show clearly that a run length exist before the necking. The model revised to curvature effects clearly shows the maxima of the freckle formation in good agreement compared to the experiments. Before the introduction of the curvature requirement for freckle formation, freckles were predicted over the entire circumference of the sample (cf. figure 3a), whereas now only in the shadow zone a freckle probability is predicted (b-c), which is much more consistent with the experimental observations (d). The discrepancies in the level of freckle probability before (a) and after implementation of the curvature requirement (b-c) are due to minor errors corrected alongside.

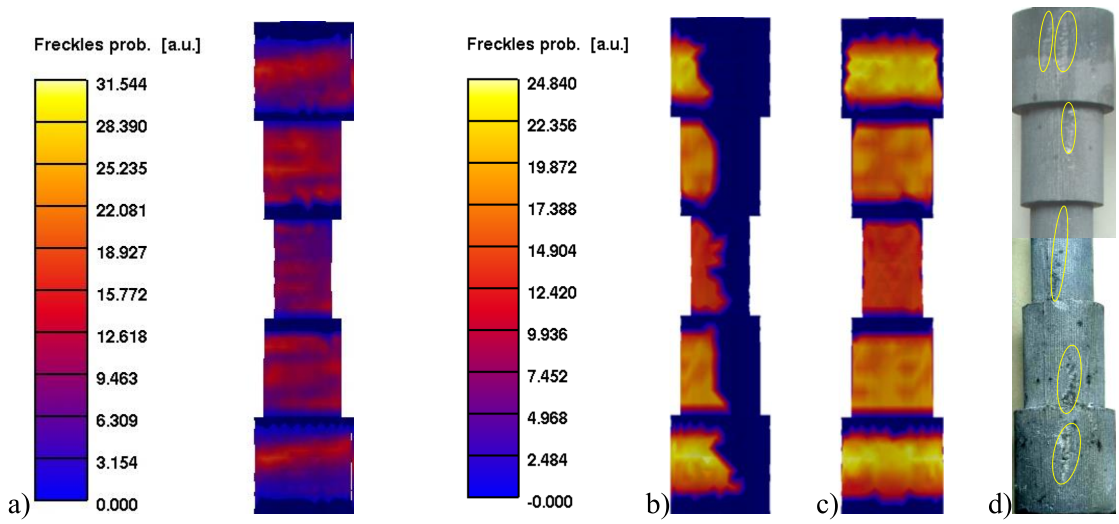

Figure 3. Freckle prediction based on the model described above, a) not taking and b) taking into account the new curvature requirement showing transition lengths with increasing or decreasing cross sections, c) view of the shadow side and d) comparison with experiment by Ma et al. [6].

5. Summary and conclusions

The proposed modified model for freckle formation of Auburtin was implemented numerically and extended to curvature effects in this work. Thus, there is a four-step approach to freckle formation: surface requirement, size requirement, curvature requirement, and the Rayleigh requirement. The model was compared with results of experimental castings. With the developed model, it was possible to predict the freckles that occur exclusively on the shadow side. Furthermore, the already known transition lengths when widening the cross-section as well as the run lengths when reducing the cross-section of the specimen have been predicted. The run lengths can also be seen in the experimental results to some extent. If the material-specific characteristics of an alloy are well known, critical zones in the cast component can be predicted with the extended model on the basis of the process parameters without much computational effort. It thus provides a practical approach for predicting freckles. As a new aspect, Ma et al. [6] observed freckles also at edges of samples with rectangular cross sections. This together with internal freckles that have also been seen in their study should be integrated with the prediction. Also surface structures have been varied and quantified with respect to freckle formation by Ma et al. [8], which is a point of future interest for modeling and simulation.

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