Effect of the dendritic morphology on hot tearing of carbon steels

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Abstract. Hot tears form during solidification in the brittle region of the dendritic front. Most hot tearing criteria are based on solid and fluid mechanics, being the phenomenon strictly depending on the solid resistance to applied strains and on the liquid capability of filling the void spaces. Modelling both mechanisms implies the precise description of the dendritic morphology. To this scope, the theory of coalescence of the dendritic arms at grain boundaries of Rappaz et al. has been applied, in this work, to the columnar growth of carbon steels by means of a simple mathematical model. Depending on the alloy composition, solid bridging starts at solid fractions down to about 0.8 and up to above 0.995 (very low carbon). The morphology of the brittle region changes drastically with increasing carbon and adding other solutes. In particular, ferritic dendrites, typical of low carbon steels, tend to offer short and wide interdendritic spaces to the surrounding liquid making possible their complete filling, and few solid bridges; peritectic steels show the rise of austenite growing and bridging rapidly in the interdendritic spaces, preventing void formation; austenitic dendrites form long and narrow interdendritic spaces difficult to reach for the liquid and with a lot of solid bridges. Sulphur addition mainly acts in delaying the coalescence end, more markedly in ferritic dendrites.

1. Introduction
Hot tearing is a common defect, which develops during solidification because of the application of tensile strains to the material with poor ductility due to the presence of small liquid fractions.

The description of the physical mechanism of the hot tearing phenomenon as well as most of the hot tearing criteria [1-7] are based on the mechanical evolution of the solid bridges that counteract the applied strains till reaching a possible rupture, and the fluid-dynamics of the liquid that is sucked into the interdendritic spaces and is not always able to completely fill the void spaces opened by the strain action. Both the mechanical and the fluid-dynamic aspects require to know the morphology of the dendritic frame to be properly described.

Exploring more specifically the field of steel solidification, for which hot tearing is commonly recognized as a main problem [8-9], the microstructure of reference is undoubtedly the columnar dendritic one. The description of the morphology of the dendritic framework can be approached by first explaining the main characteristics of the columnar microstructure; strains form because of thermal gradients on average directed parallel to the dendrite growth direction and to the average columnar grain direction; as the applied strains tend to separate the columnar grains, the material develops mechanical resistance only at the onset of coalescence of adjacent grains.

Grain boundaries play an important role as they are weak sites because of the coalescence delay caused by the dendrites misorientation. Therefore they both determine the onset of mechanical resistance and are sites of strain accumulation and hot tearing formation.
2. Columnar dendrites

The first step to set up a model of the columnar dendritic morphology is to define a simplified geometry of the dendrites. At this scope, an upper paraboloid shape and a lower square parallelepiped one (figure 1) are assumed. The paraboloidal growth arrests when adjacent dendrites come in touch as soon as their diameter reaches the value of the primary dendrite arm spacing (PDAS). From that time on, the solidification proceeds towards the corners until they are fully solidified. The solid fraction at the first contact between adjacent dendrites is easily obtained in an approximated way, by dividing the area of the circle of diameter PDAS by that of the square of side length PDAS:

\[ f_{s\text{-touch}} = \pi \left( \frac{PDAS^2}{4} \right) (PDAS^2)^{-1} = \frac{\pi}{4} = 0.785 \] (1)

Figure 1. Simplified scheme of the columnar dendrite growth (PDAS: primary dendrite arm spacing, SDAS: secondary dendrite arm spacing).

Figure 2. Scheme for the calculation of the progression of the contact area.

The solid fraction given by equation (1) is better approximated for cells than for dendrites since, when the side branches of these last touch, there is still liquid within the dendritic frame, consequently the actual solid fraction should be lower. It is worth noting that the obtained value is very close to commonly accepted values of solid fraction of zero strength.

To describe the dendrite morphology according to this simplified scheme, it is needed to express the extent of the contact area between adjacent dendrites, given along the dendrite transverse section by the geometrical parameter \( D_t \), of figure 2, given by:

\[ \frac{D_t}{z} = \frac{D}{z} \sin \alpha \] (2)

with:

\[ \alpha = \arccos \left( \frac{PDAS}{D} \right) \] (3)

The correlation between the geometrical parameter \( D \) (related to the curvature of the rounded corners of the transverse section as shown in figure 2, and the solid fraction \( f_s \), is obtained equating
this last to the ratio between the area of the transverse section at a given height and that of the dendrite square base:

\[ D = \left( \frac{f_s}{\pi} \right)^{\frac{1}{2}} 2PDAS \]  

(4)

3. Coalescence of the columnar dendrites

Contacting side branches of adjacent parallel dendrites belonging to the same grain coalesce immediately as soon as their mutual distance is of the same order of the interface thickness. Dendrites at the grain boundaries coalesce if the grain boundary energy is lower than the solid-liquid interface energy of the two initial surfaces [10]. For tilt grain boundaries it is required that the interface undergoes solidification undercooling (\( \Delta T_b = \) bridging undercooling) to balance the difference between grain boundary and interfaces free energies, before coalescence can start. \( \Delta T_b \), for pure materials, is derived balancing the sum of the free energies of the two solid/liquid interfaces and that of the interposed undercooled liquid, with the grain boundary free energy, per unit area [10]:

\[ \Delta T_b = \frac{\gamma_{gb} - 2\gamma_{sl} \delta}{\Delta s_f} \]  

(5)

with: \( \gamma_{gb} \)=grain boundary energy; \( \gamma_{sl} \)=solid-liquid interface energy; \( \Delta s_f \)=fusion entropy for unit volume and \( \delta \)=solid-liquid interface thickness.

The resulting expression relates the undercooling to the entropy of fusion of the liquid entrapped between the two grains. \( \Delta T_b \) increases as the difference between the grain boundary energy and the interface energy increases, and also as the entropy of fusion of the residual liquid decreases.

The grain boundary energy is function of the misorientation angle \( \theta \) according to the Read-Shockley relationship [11]:

\[ \gamma_{gb} = \gamma_{gb0}(1 - \ln\theta) \]  

(6)

The solid/liquid interface free energy has been derived for pure materials (Spaepen-Thompson) [12]:

\[ \gamma_{sl} = \frac{\alpha_m \Delta s_f}{(N V^{\frac{1}{3}})^{\pi}} \]  

(7)

where: \( \alpha_m \)=0.71 for bcc e \( \alpha_m \)=0.86 for fcc and hcp; \( N \)=Avogadro’s number; \( V \)=molar volume of the solid at the interface; and \( \Delta s_f \)=molar fusion entropy.

Body centred cubic and fcc or hcp lattices have different coefficients. The bcc lattice tends to develop a smaller solid/liquid interface free energy than the other two ones.

In the case of multi-component alloys the fusion entropy at each stage of the solidification accounts for the composition at the interface resulting from microsegregation and diffusion.

Modeling of the microsegregation and diffusion in the solid during the multi-component dendrite growth is used to derive the variables (values referred to the interface) needed for calculating \( \gamma_{sl} \): entropy of fusion from enthalpy of fusion, molar mass and volume. The density of the solid at the interface is derived through empirical relationships available on the literature as function of temperature and composition.

The model used in this work consists of two separate models, for microsegregation and coalescence; the first one provides input data to the second one. In this way, the reduction of undercooling due to back diffusion of solutes from the last liquid in the interface, is neglected.

Grain boundaries are modelled as they are sites where preferentially hot tearing forms because of the low mechanical resistance induced by the longer permanence of the liquid. The main features of the grain boundary morphology (figure 3) are provided by the bridging undercooling and the primary and secondary arm spacing as they influence the hot tearing tendency by determining shape and extension of the coalesced areas, and shape and extension of the liquid channels respectively. The former determine the solid resistance to applied strains, while the latter the volumes where the liquid
will not be able to flow. The possibility of tearing is higher for thin solid bridges forming at low solid fraction and small primary and secondary arm spacing. Therefore, tearing is favoured when bridging starts with low undercooling. The last liquid forms channels mainly located at the corners of the primary trunks. The critical region for hot tearing formation is where the local pressure drops below a minimum value. This region generates hot tearing porosity only above a minimum volume below which it becomes invisible (figure 4).

4. Calculated grain boundary features for the Fe-C system
The microsegregation and coalescence models have been applied to the binary Fe-C system for C ranging between 0.002 and 1 wt%, considering grain boundaries with fixed tilt angle and a fixed cooling rate of 1 K/s. Figure 5 shows where the lines start and end of coalescence lay with respect to the solidus and liquidus ones in the phase diagram and, for some compositions, the schematic representations of the dendrites in the style of figure 3, where the shapes of the dendrites and of their contacting and coalesced areas can be observed. It is noted how solid bridging, and the associated mechanical resistance, start at solid fractions as high as ~1 for low carbon content, going down to 0.8 for carbon content higher than about 0.3%. This behaviour can be mainly ascribed to the lower interface energy of ferrite with respect to austenite. The morphology of the brittle region changes drastically with increasing carbon, in particular: ferritic dendrites (low carbon) form short and wide interdendritic spaces easily filled by liquid with few and thick solid bridges; peritectic steels show the rise of austenite growing and bridging rapidly in the interdendritic spaces, preventing void formations in a way similar to eutectics growth; austenitic dendrites form long and narrow interdendritic spaces difficult to reach for the liquid and with a lot of weak solid bridges. Narrowing and elongating of the residual liquid volumes of austenitic dendrites can be partly attributed to the primary arm spacing decrease with increasing carbon content.
The different tendency shown by low and high carbon steels is explained in terms of physical behaviour at the grain boundaries (figure 6). Strains applied to low carbon steel dendrites accumulate in the disconnected grain boundary, which open forming wide spaces filled by liquid. Thick solid bridges, formed through sudden coalescence near to the solidus, break only when subjected to large strains. Differently, strains applied to high carbon steel dendrites are shared between grains and solid bridges in the grain boundaries, liquid flows in narrow channels and stops at solid fraction less than solidus, where thinner bridges can be easily broken at small strains.

The addition of other alloying elements changes both the solidification and the coalescence temperature ranges. Figure 7 shows how the addition of 0.02% of sulphur to the binary Fe-C alloy causes coalescence of ferritic dendrites starting at lower solid fractions, and lowering of the coalescence end temperature for all carbon contents, with a more marked effect for C<~0.2%. The deleterious effects of sulphur addition consist in favouring the formation of thin bridges and in
generating narrow liquid channels. The first is mainly due to the drop of the solidus line, the second one to the drop of the end of coalescence line. These effects are more marked in low carbon steels. The addition of other alloying elements changes both the solidification and the coalescence temperature ranges.

![Figure 7](image)

**Figure 7.** Comparison of the position of the start and end of coalescence lines with respect to the corresponding phase diagrams between the binary Fe-C system and after addition of 0.02% of sulphur.

5. Conclusions

The different tendency to form hot tears shown by Fe-C alloys is basically explained by the features of the dendrite solidification mainly expressed by the extension of the solidification range and the primary and secondary arm spacing. The effect of bridging undercooling is to weaken the grain boundary concentrating tensile strains in it. Bridging undercooling overlaps its effects to the basic cracking tendency simply due to solidification, introducing important differences depending on the lattice structure and the solutes concentration. Bridging undercooling embrittling action is mainly due to the elongation of the boundary characterized by thin solid bridges with low solid fraction, associated to low permeability to the liquid flow. No embrittling effect can be adduced only to the delay of the start of coalescence, since the possible gap formed by separating the two grains can be easily filled by the liquid. It can be concluded that the variable tendency to hot tearing of multicomponent steels is caused by the effects of the alloying elements on both solidification path and coalescence evolution.

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