## ELASTO VISCO-PLASTIC MODEL OF STEEL SOLIDIFICATION WITH LOCAL DAMAGE AND FAILURE

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**ABSTRACT:** A Nonlinear elastic visco-plastic thermo-mechanical steel microstructure model is coupled with a Gurson-Tvergaard-Needleman (GTN) model to predict local damage and failure in the columnar solidification zone of a steel casting. The new model operates on two scales - a unit cell grain model of micro-scale in the columnar zone as well as a macro-model tensile specimen to map observations with experiments. The model aims to investigate inter-granular embrittlement at intermediate temperatures during solidification processes. This embrittlement occurs due to pro-eutectoid ferrite film formation and precipitation of inclusions at the prior-austenite grain boundaries. This behavior of the unit cell is then mapped onto macro-model tensile specimens to measure reduction in ductility. The effect of ferrite film and temperature are studied by calculating the micro-strains, macro-strains and void fractions at which cracks begin to form during the continuous casting process.

**INTRODUCTION**: Steel is an important engineering material which is subject to defects and embrittlement at elevated temperatures. Although thermo-mechanical analysis using computational models has been applied as a powerful tool to predict stress and deformation during steel processing, little previous work has been done to predict steel ductility.

**PROCEDURES, RESULTS AND DISCUSSION:** The model developed in this work to predict steel ductility has two different scales – a micro-scale grain model capturing the microstructural behavior and a macro-model capturing necking behavior during a tensile test [Cardoso 1995]. The grain model represents the columnar microstructure as a honeycomb of regular hexagons, as shown in Fig.1. The unit cell modeled includes three grain boundaries intersecting at the triple point and parts of the three regular hexagonal grains, which gives a rectangular shape to the unit cell. The preliminary isothermal model presented here solves the standard mechanical equilibrium equations, with total strain decomposed into elastic and inelastic (plastic) components [Koric 2006].

The dimensions of the grain model are based upon grain size measurements from experiments and equating the area of the grain to that of a circular grain of the same diameter as the grain size measurement. To account for the effect of ferrite films formation, the grain boundary region is assumed to be composed entirely of pro-eutectoid alpha ferrite while the grain matrix region consists of prior austenite and alpha-ferrite. The phase fractions are obtained from the Fe-C phase diagram at the temperature of interest. The temperature dependent mechanical constitutive model for the austenite is based on the formulations by Kozlowski [Kozlowski 1992], while the mechanical model of alpha ferrite is based on the power law formulation [Zhu 1993]

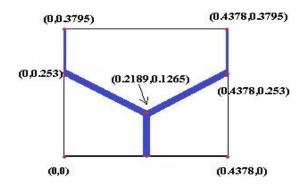
An experiment based strain rate is used as input to both these models to get the plastic behavior relationship of the two phases as shown in Fig 2. The behavior of the ferrite film is the same as

the ferrite phase while the grain matrix is assumed to have properties similar to a composite of austenite and ferrite, the individual compositions of each phase being determined from the phase diagram and volume fractions of the film region at the grain boundary and the rest of the grain. The plastic strength of the composite grain matrix is based on the rule of mixtures [Krock 1963] of particle reinforced composites where the equivalent strength of the grain matrix is the average of the upper and lower bound strengths. The Gurson-Tvergaard-Needleman (GTN) model [Needleman 1987] of ductile fracture is used to model the fracture in the grain matrix as well as the grain boundary region due to nucleation and growth of voids. The parameters in the Gurson model (q1, q2, q3, initial void fraction, void nucleation distribution- mean and SN, were taken according to [Alegre 2000]. The volume of nucleated voids parameter was changed to 0.04 in the grain boundary region, (0.004 in the grain matrix).

The grain model is subjected to a uniaxial strain along the horizontal direction while the top and bottom surfaces can deform naturally, but are enforced to remain straight by using appropriate boundary conditions to maintain the repeating nature of the unit cell. This deformation results in an equivalent plastic strain contour as in Fig.3 where there is strong concentration of plastic strain in the grain boundary region typical of ductile fractures. The homogenization technique is used to establish an overall stress vs. strain relationship of the unit cell as shown in Fig.2. This relationship is then used as the constitutive relation in the macro-model of a tensile test. Thus, using this hierarchical multi-scale method, information based on homogenized stress from the grain scale model is passed to the macro-model through the flow curves of Von Mises plasticity but not vice versa. This technique can be further expanded in future work with semi-concurrent multiscale methods where information is passed from fine scale to coarse scale and vice versa. To simulate the experimental conditions of the tensile specimen [Alegre 2000], properties at a constant temperature of 800°C and a strain rate of 10<sup>-3</sup> sec<sup>-1</sup> are used. The behavior of the unit cell obtain from the procedure described above is then used to define the plastic strength of the actual tensile specimen modeled based on the experiment. The equivalent plastic strength at failure of 0.39 is used to define the onset of failure of the tensile specimen. The macro-model tensile specimen subjected to a uniaxial load fails at a 29% engineering macro-strain which corresponds to a 31% reduction in area which compares with 20% reduction in area reported in the experiment.

To further validate the model, the entire "micro-macro model" methodology was repeated with no ferrite films and uniform composition in the entire grain. This resulted in no stress concentration in the grain boundary region and absence of embrittlement, with close to the expected ~100% reduction in area before failure at the neck. The micro-macro model is alos applied at a higher temperature of 870°C with the same grain boundary fraction, increased the austenite fraction (according the Fe-C phase diagram). This resulted, as expected at a higher temperature, in a higher-strength grain matrix relative to the grain boundary, resulting in more strain concentration and failure at only 7% applied engineering macro-strain in the tensile specimen and a reduction in area of just 7%

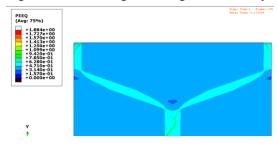
In conclusion, a micro-structure methodology has been developed to analyze hot ductility of steel using a micro-macro model approach. The model roughly matches measurements in lab experiments. Ferrite networks cause large drop in ductility explaining the lower ductility seen in the two-phase region. The effect of temperature on ductility matches observations where a decrease in temperature causes an increase in the ductility from 7% to 31%. The hierarchical multiscale model is ready to investigate embrittlement during manufacturing processes such as continuous casting.



140 Grain Model Ferrite 120 Composite grain (800C -80%Fer/20%*F* Results Grain model results (800C-80%Fer/20%A 100 Stress (MPa) 80 Max stress 60 Max Void fraction of 0.2 20 Eq. Plastic Strain of 0.39 0.1 0.2 0.3 0 Inelastic Strain (absolute)

Fig1. Schematic of grain and grain boundary

Fig2. Strength of phases and Grain model



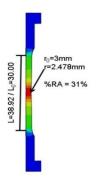


Fig3. Plastic Strain Contours in Grain Model

Fig4. Plastic strain contours on Tensile specimen at failure

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