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Processing-Microstructure-Property Relationships I

Thursday AM

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MICROSTRUCTURE MODELING OF MAGNESIUM ALLOYS FOR ENGINEERING PROPERTY PREDICTION

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Abstract

Magnesium alloys have found increasing application in the transportation industry due to their low weight and high strength. However, wider application is hindered by limited ductility. Microstructural features, such as porosity, brittle eutectics, and grain size, can significantly influence the macroscopic response of a component. These features can vary widely throughout a component. Our approach to studying the microstructures influence on bulk properties begins with measuring microstructural features in different regions of a component. These measurements are used to create statistically equivalent, 3D synthetic samples of the microstructure. The synthetic microstructures are meshed using finite elements and used to simulate the response and investigate the influence of specific features. We will demonstrate how the digital microstructure samples are generated, how variations in microstructural features influence the bulk properties, and how this methodology can be used to predict component performance and optimize processing.

Introduction

Magnesium alloys are finding increasing applications in lightweight vehicles because Mg and its alloys are the lightest metallic structural materials. High strength and low density make Mg alloys prospective alternatives to aluminum alloys. However, Mg's limited ductility presents a critical hurdle to more wide spread use. It is well established that microstructural features such as amount and distribution of porosity, grain size, and brittle eutectic phase and precipitates can significantly influence the ductile of Mg alloys. Unfortunately, these features vary spatially throughout a casting and from specific alloy to alloys. The specific casting process used and the processing parameters can also influence the final microstructure.

The characteristic microstructure of high-pressure die-cast (HPDC) AM series alloys consists of α-Mg dendrite cells and a divorce eutectic of α-Mg and β-$Mg_{17}Al_{12}$ [1,2]. Intermetallic Mn-rich particles are also observed. Some of the α-Mg dendrite cells found in the center of a casting prematurely solidified in the show sleeve and carried into the die. This results in a bimodal distribution of dendrite cells sizes between those formed in the sleeve and in the die [2].

The microstructure closer to the die walls consists of a very finer dendrite cell size, approximately 5-7 μm, with little to no porosity observed. This "skin" region results from higher cooling rates and exhibits higher strength and ductility compared to the interior [3,4]. The dendrite cells in the interior are 10s of μm in diameter depending on processing parameters with externally solidified cells being the largest.

A third region has been observed in some castings. A porosity segregation zone (PSZ) is sometimes observed between the skin and interior regions consisting of one or more bands of high porosity that follow the contours of the die [1,2,5]. The PSZ has a negative effect on the strength and ductility of the casting and is thought to be linked to processing parameters. Dahle et al. have developed a model for prediction when and where the PSZ forms based on casting parameters [6].

The Al content of Mg alloys leads to changes in the microstructure morphology. Dahle et al. [5] shows that low Al content alloys, i.e. 1% by weight, have globular, equiaxed dendrite cells. Increasing the Al content to 5%, results in pools of eutectic beginning to form between the dendrite cells. By 9\% Al, the dendrite structure is fully formed with eutectic between the dendrite arms. Even the slight increase in Al from AM50 to AM60 results in an increased volume fraction of the β-phase.

Porosity is also observed in HPDC Mg alloys. The bulk porosity level is often reported and used to model ductility and fracture. However, Weiler et al. [7] and Lee et al. [8,9] have suggested that the areal fraction of pores along the fracture surface and largest pore volume mater more than the bulk value. Weiler et al. utilize a critical local strain model [10-12] with the areal fraction of porosity to model plastic instability resulting from internal necking due to the reduced cross section area. This was used to calculate the fracture strain. This method requires testing samples to calibrate the material parameters used to describe the bulk response of the Mg alloy as well as x-ray imaging to determine the porosity distribution and largest pore volume.

Chawla et al. [13] have also explored how to include microstructural features in computational models. Serial section of 2070 aluminum composite containing SiC particles was conducted. A 3D geometric representation and finite element mesh was created from the series of images. The resulting model included the irregular shapes of the SiC particles. Commonly used simplifications for the SiC particles are a single cube or sphere in a continuum matrix. The complex geometric representation was compared to a single cube and a single sphere. The single sphere was shown to under predict the stress-strain response while the cube slightly over predicted the hardening response. The complex geometry matched the experimental response the closest and demonstrated the internal stress concentrations due to the sharp features of the SiC particles. This demonstrates the importance of actually representing the microstructure to capture the response of the material. However, having a single geometric representation is limiting and using serial sectioning to generating each new model is expensive and time consuming.

The various features of the AM series microstructure can be generally categorized into two types: intrinsic and extrinsic. Intrinsic factors include features intrinsic to the specific Mg alloy such as phase composition, grain size, morphology, volume fraction, and mechanical properties of the α-Mg matrix and eutectic β phase. Extrinsic factors come from the external processes applied to the alloy such as casting and heat treatment

processes and include: porosity, segregation, incomplete fill, hot tear, and cold shut. Combing a particular alloy and casting process result in a specific set of intrinsic and extrinsic features and in some cases flaws.

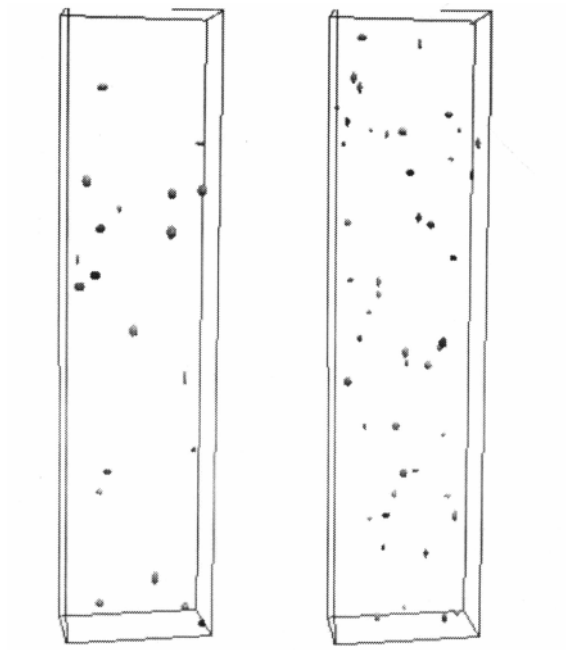
Computational analyses have been carried out to model the effect of extrinsic features such as porosity on the bulk ductility. However, previous work has focused on approximating the presence of pores and not on how the distribution of location and size influence the bulk response. Experimental observations have demonstrated that the amount of porosity as well as size and distribution vary throughout a casting and from casting to casting. The following work will outline a computational framework for samples containing random distributions of porosity for finite element analysis. First, the process for generating samples that are statistical equivalent to experimental observations is described. Next, the material models being utilized are described. Finally, results from preliminary finite element simulations are presented.

Generating Statistically Representative Samples

The exact microstructure of each casting is unique. Variation exists not only from sample to sample but throughout a single casting. As a result, reconstructing a microstructure from a single image from a single sample or even a handful of images from a single or multiple samples is extremely limiting. To combat this limitation a framework is created to generate unique representations that are statically equivalent to the target microstructure.

The current focus is how porosity affects the overall ductility of a sample. Weiler et al. [8] characterized the porosity of a series of samples cut from different regions of an AM60B high-pressure die-casting. Data collected includes number of pores, average pore volume, largest pore, volumetric porosity, density of pores, and average distance to the nearest pores. This information is used to generate a series of random samples containing pores that demonstrate the same parameters.

Random samples of porosity are generated using the volumetric porosity and average pore volume as input parameters. Individual pores are randomly placed inside a bounding box and the porosity is calculated. This is repeated until the required porosity is reached. Pores are represented by ellipsoids. An ellipsoid is described by 2 equatorial radii a and b and a polar radius c. If a=b=c, the ellipsoid simplifies to a sphere. For simplicity, the equatorial radii are defined to be equal, meaning a=b. This leaves a and c to define each pore. The average radii are calculated to result in the average pore volume. For each pore added to the sample each radius is allowed to vary +/- 50% of the average radius value, resulting in various sized pores. If a pore intersects the bounding box or an existing pore, the pore is rejected. Once a sample is generated the porosity, average pore volume, and number of pores is reported and can be compared to the experimental observations. Figure 1 shows two samples generated using the same porosity of 5% and external dimensions of 3mm x 6mm x 25mm. Sample 1 contains 20 pores with an average pore volume of 0.18 mm3 while Sample 2 contains 48 pores with an average pore volume of 0.075 mm^3.



(a) (b)

Figure 1: Randomly generated samples with 5% porosity. (a) Sample 1 contains 20 pores. (b) Samples 2 contains 48 pores.

The geometries generated can then be automatically meshed for finite element analysis using tetrahedral elements. The result meshes conform to the pore surfaces. The interior of the pores is not meshed leaving voids.

Material Modeling

For the current analyses porosity is represented explicitly in the geometry while the details of the rest of the Mg microstructure are smeared out. The goal is to understand the influence of porosity parameters on the bulk ductility. Computational simulation provides the ability to isolate individual features for study. Future analyses will increase in complexity as additional features of the microstructure are added to the geometry.

$$\sigma = \sigma_{yld} + K\varepsilon^{n}_{p} \quad (1)$$

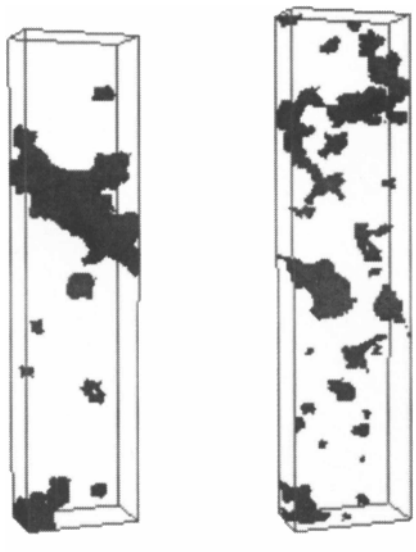
The Mg matrix is modeled using elasto-plasticity with isotropic hardening. The plastic flow stress follows the exponential form of Eqn. 1.

σ_{yld} represents the initial yield stress, ε_p is the plastic strain, K is the hardening coefficient, and n is the strain-hardening exponent. Standard values for Young's modulus, Poisson's ratio, and yield stress of 45 GPa, 0.25, and 125 MPa, respectively, are taken from available literature. The values of K and n reported by Shan et al. [4] of 467 MPa and 0.22 are also used.

Modeling Results

Using the material parameters in the previous section the samples shown in Figure 1 were subjected to simple tension was applied to each sample. The pores in sample 1 are primarily clustered in the upper portion of the sample while the pores in sample 2 are more

uniformly distributed throughout the sample. As seen in Figure 2, the clustering results in a clear stress concentration region where failure will occur while the more uniform distribution lacks a clear single path for failure.



(a) (b)

Figure 2: Location of failure stresses in samples containing 5% porosity.

Summary

Mg alloys have many intrinsic and extrinsic microstructural features that contribute to the bulk response of a casting. How these features effect the ductility is keep to improving the performance for lightweight automotive applications. Augmenting traditional experimental testing with computational simulation has been useful for isolating individual features and physical responses. Here we have outlined the process for generating a suite of unique digital samples for computational analysis focusing on specific microstructural features. This allows the variation seen in different regions of a casting and between castings to be captured. The effect of variation from sample to sample can be studied to determine the impact on the range of resulting property values.

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