

# THERMAL MECHANICAL MATERIALS MODELING FOR IMPROVED MANUFACTURING PROCESSES

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In manufacturing processes such as hot metal forging, materials are simultaneously exposed to elevated temperature and subjected to severe mechanical straining. As such, material microstructure will constantly be evolving through the process and the ability to model microstructure evolution is the key to predict material properties and responses. In this paper, a combined modeling, experiment and numerical simulation approach to improve the understanding of the manufacturing process of a high-pressure gas reservoir is demonstrated. Presentation will highlight significant modeling, experiment and numerical simulation issues encountered and how have these issues been resolved.

**Keywords:** forging, microstructure evolution, thermal/mechanical modeling and experiments

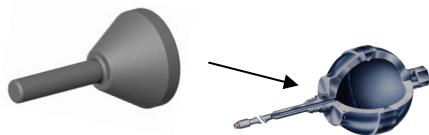
## 1 Introduction

The purpose of this paper is to provide an overview of the science-based thermal/mechanical materials modeling activities at Sandia National Laboratories, California. Sandia/California has been engaged in the development of high performance computing based predictive modeling and simulation capabilities in support of the Science-Based Stockpile Stewardship Program of the U. S. Department of Energy. Of particular interest is the development of constitutive models that can efficiently and accurately predict material responses under severe environments. Our philosophy is to include required physics in our models and validate the models through both laboratory and field scale experiments. Through the combination of constitutive model development, high performance computing based numerical simulation and experiment validation, we seek to establish a predictive simulation capability. This development process is demonstrated through a gas reservoir manufacture problem that involves metal forging. Under elevated temperature and severe mechanical straining, material microstructure will constantly be evolving and the ability to model the evolution process is the key to predict material properties and responses. Recrystallization and grain growth are important features of the microstructural evolution during high temperature plastic deformation of metals. Hot-working metal processes, such as multi-stage forging, require accurate control/prediction of these features to assess the quality of the process and to estimate the material properties of the final product. In

this paper, a constitutive model based on elasto-viscoplasticity is presented that simulates the evolution of Recrystallization. Laboratory experimental capabilities were shown to characterize material properties as well as provide data for model validation. Numerical simulation and comparison between calculated and measured results are shown to optimize the design of the manufacturing process.

## 2 Problem statement

Sandia mission requirements include the production of steel reservoirs, Figure 1, to store hydrogen, tritium and deuterium gases under high pressure. One of the design parameters involves gas diffusion over time that can potentially result in degradation and possible fracture of the vessel material. It is important that the manufacturing process produce optimal material properties to inhibit the gas diffusion process. Only two steels (304L SS and 21-6-9 SS) have been proven to survive the long-term harsh hydrogen/tritium environments. Unlike automotive and aerospace steel forgings, these steels cannot be heat treated to raise strength after forging. Increased strength levels need to be achieved through warm-work during forging.



**Figure 1:** Schematic of a gas reservoir

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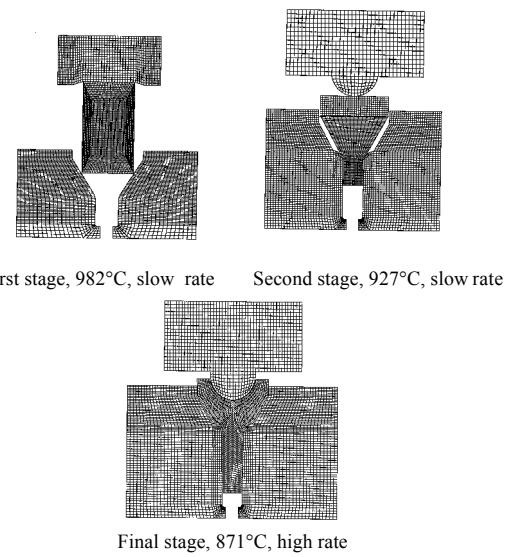
Material state requirements lead to strict specifications on the grain size and grain flow, minimum and maximum values of yield strength, and minimal spatial variation in yield strength.

A combined constitutive modeling, experimental mechanics and computational simulation approach have been developed to tackle this problem. A brief description is presented below and references are provided for those who are interested in more detailed information.

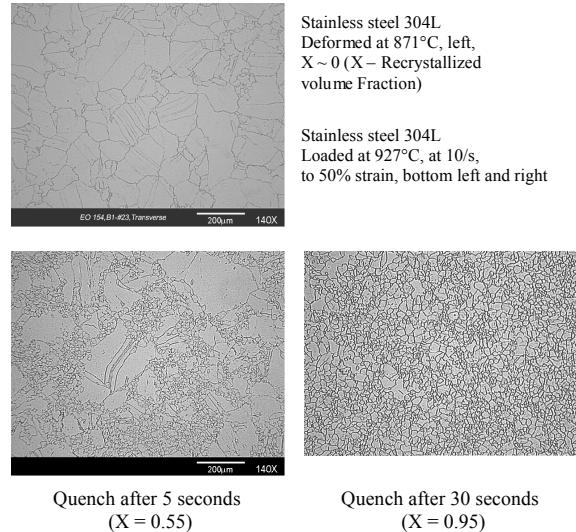
### 3 Constitutive Model Development

A typical three-stage forging process for production of stainless steel gas reservoirs is shown in Figure 2. Desired material characteristics need to be achieved during the forging process. However, microstructure evolution under combined mechanical deformation and heating and quenching can replace the strained grain structures with a new, strain-free set of grains. This process is known as recrystallization. In this case, recrystallization is detrimental and needs to be accounted for in order to attain the specified material strength levels. Figure 3 provides both a qualitative view as well as a quantitative measure of the microstructure evolution during forging.

Sandia has been developing elasto-viscoplasticity based models to describe the temperature- and rate-dependent finite deformation of metals [1-3]. These models have been applied to study metal forging with varying degrees of success [4]. Recently, an enhanced Evolving Microstructural Model of Inelasticity [5] that incorporates the capability to model static and dynamic recrystallization [6] has been published. Some results will be presented in Section 5 to demonstrate model capabilities. Because of space limitations, details of the model description will not be given here. Interested readers are referred to the above references for more information.



**Figure 2:** A three-stage forging process



**Figure 3:** Microstructure evolution during forging

### 4 Experimental Mechanics Program

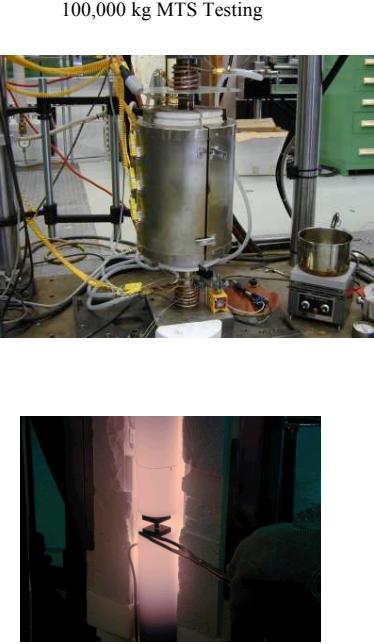
Accuracy of constitutive model predictions relies on materials properties measured from well-characterized experiments. Simulations must also be validated against experimental data to establish model applicability to the specific class of problems. Thus, a combined elevated temperature and large deformation experimental program has been developed to support the forging modeling and simulation effort. Because of the necessity to characterize the material behavior to large strain levels, compression experiments were chosen rather than tension experiments.

Although large strains are achievable in compression, frictional effects at the interface between the specimen ends and the test fixtures must be minimized to achieve a uniformly strained specimen, which yields meaningful material data. Minimizing friction includes designing a specimen with a grooved end surface geometry along with selecting an appropriate lubricant for the test temperature. This proper combination will allow the end material to radially expand during the axial straining of the specimen. Figure 4 shows original and deformed specimens that exhibit uniform expansions.



**Figure 4:** Uniform straining compression specimens

Compression tests at temperatures between room temperature and 1000°C were conducted in a three-zone resistance heated clamshell type oven. Specimens were heated by induction heating, utilizing a graphite susceptor surrounding the specimen to transfer the energy. Uniform heating over the entire specimen length was found to be critical for producing good results. The test set-up is shown below in Figure 5.



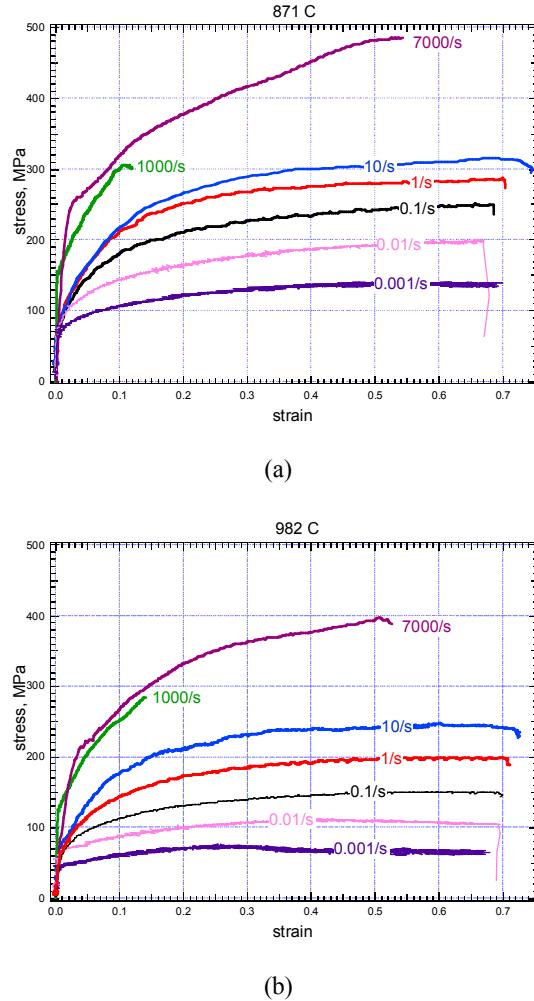
**Figure 5:** Heated Compressive Testing Set-up

Typical results for 304L stainless steel as a function of temperature and strain rate is given in Figure 6. Clearly, stress-strain responses are temperature and strain rate dependent. The strain-rate dependence is similar at both temperatures; however, the strength is significantly lower at the higher temperature. These material characteristics need be captured by the constitutive model in order to predict material properties of forged parts and to improve the design of the forging process. See [7-8] for more details.

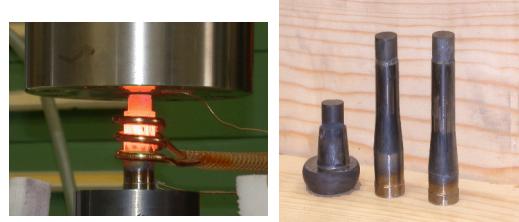
The experiment set up has also been applied to develop well-controlled laboratory scale experiments aimed to provide quantitative data for model validation purposes. Figure 7 presents an experimental configuration for a forging punch at temperature as well as specimen geometries for a validation experiment. Measurable quantities include temperature, forging force, residual material strength and microstructure. Refer to [4, 9, 10] for more descriptions and results.

## 5 Results and Discussions

The constitutive as described in Section 3 is used to analyze the three stage forging problem shown in Figure 2. Material constants in the model was determined from 304L stainless steel uniaxial compression at temperature



**Figure 6:** Stress-Strain Plot of 304L Stainless Steel as a Function of Strain Rate at (a) 871°C and (b) 982°C.

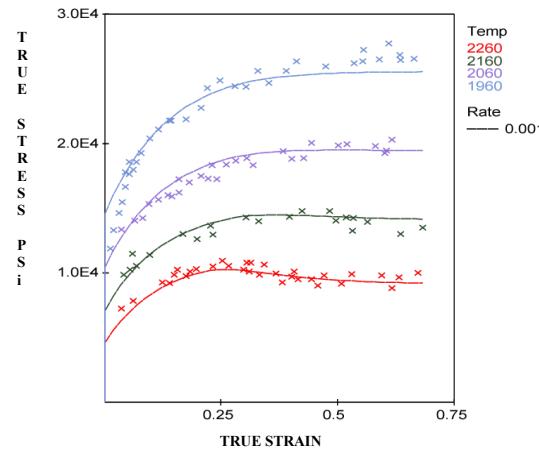


**Figure 7:** Controlled Laboratory Experiments Provide Quantitative Data for Model Validation.

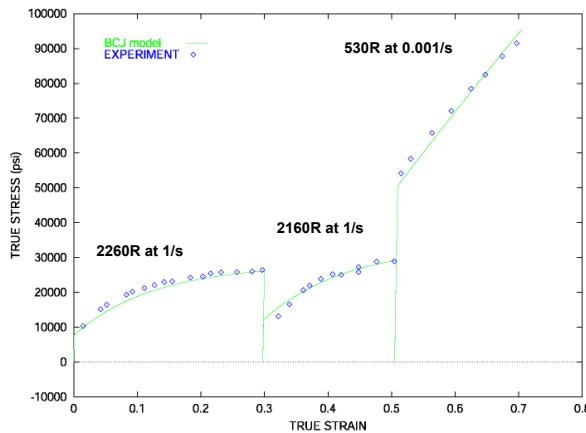
data measured using the experimental program in the previous Section. A typical data set for strain rate of 0.001/s at various temperatures and their correlation with calculations by the model is depicted in Figure 8. The model was able to represent the experimental data well. The data fit better at higher temperatures and larger strain levels. This is preferred for forging problems. Using model parameters determined from uniaxial compression data at a range of temperature and

strain rates, the model is applied to analyze the three stage forging problem in Figure 2. Stress versus strain history for the three-stage forging process has been measured and comparison between calculated and measured data is shown in Figure 9. Very good agreement between computed and measured data has been obtained. This indicates that the model has captured the essential physics of the problem. More in-depth discussions can be found in [3,4,9] and will not be presented here due to space limitations.

In summary, a microstructure-property based constitutive model has been developed to model the stainless steel forging process. Accompanying experimental capability has also been established to both characterize material properties and provide validation data. Very good agreement between computed and measured data for a three stage forging problem indicates the applicability of the model to this class of thermal mechanical problems.



**Figure 8:** Uniaxial Compression Model Data Fit.



**Figure 9:** Comparison between Model Calculation and Experimental Data for Multistage Forging.

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