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# Crystal plasticity finite element analysis of ferritic stainless steel for sheet formability prediction

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## ABSTRACT

A crystal plasticity finite element analysis was conducted for predicting forming limits of a ferritic stainless steel. A virtual microstructure crystal plasticity finite element model, or a representative volume element (RVE), was developed, in which the behavior of grains was governed by a rate-dependent viscoplastic crystal plasticity model. To account for the variation in hardening of different slip modes, the model parameters of different slip modes in the bcc metal were obtained from the uniaxial stress-strain, longitudinal-transverse strains, and hydraulic bulge test data using an inverse method. A multi-scale framework, which combines the virtual microstructure models and the Marciniak-Kuczynski procedure, was developed and applied to the forming limit analysis of a ferritic stainless steel. Forming limits predicted using the combined slip mode compared well with the measurements when the  $\{110\}\langle 111 \rangle$  and  $\{112\}\langle 111 \rangle$  slip systems are operating and the  $\{123\}\langle 111 \rangle$  slip systems are inactive. The influence of the slip system activity on the yield criteria and forming limits is discussed.

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## 1. Introduction

Crystal plasticity offers tools for examining evolution of microstructure of polycrystalline materials during deformation by accounting for the underlying physics, or crystallographic slip. Moreover, the evolution of microstructure, which is linked to the mechanical properties, can be used to predict macroscopic behavior. With the development of efficient computational codes and hardware, crystal plasticity models are being widely used in many applications.

A common application of crystal plasticity is the analysis of deformation mechanisms. Guery et al. (2016) studied the slip activities of an austenitic stainless steel using in-situ microscopic digital image correlation measurements and crystal plasticity finite element method. Marchenko et al. (2016) studied the strain aging phenomena in  $\alpha$ -titanium using crystal plasticity simulation. In addition to dislocation glide, twinning and transformation are also considered in crystal plasticity analysis. Abdolvand et al. (2015) investigated deformation twinning using three-dimensional synchrotron X-ray diffraction and crystal plasticity finite element methods. Abdolvand and Wilkinson (2016) studied the effects of reorientation and twin shear

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transfer in twinning by conducting high-resolution electron backscatter diffraction experiments and crystal plasticity finite element simulations. Sun et al. (2016) incorporated twinning and transformation into the crystal plasticity constitutive model for representing the behavior of twinning-induced plasticity (TWIP) steel. Yu et al. (2014) studied martensite transformation mechanisms of NiTi shape memory alloy using crystal plasticity.

Another type of applications of crystal plasticity is the prediction of mechanical behavior using microstructure information. Zhang et al. (2016) calculated the initial yield surface of an aluminum alloy using high-resolution crystal plasticity simulations. Gawad et al. (2015) developed a hierarchical multi-scale framework to calculate the evolution of the yield surface using crystal plasticity virtual experiment. Eyckens et al. (2015) studied differential hardening of steel sheets using multi-scale crystal plasticity modeling. Erinoshio et al. (2013) employed the crystal plasticity finite element method (CPFEM) to represent polycrystal behavior and predict the ductility of ferritic steel. In CPFEM, the response of the microstructure is directly calculated in the finite element sense with a representative volume element (RVE).

When loading is not proportional and the amount of deformation is not marginal, the accuracy of phenomenological models in predicting mechanical behavior is often reduced because of microstructure evolution. The microstructure of the deformed state may vary significantly from that of the initial undeformed state based on which phenomenological models are usually established. Crystal plasticity models are expected to provide improved prediction under non-proportional loading because they can account for microstructure evolution such as the rotation of grain orientations and the development of dislocation patterns. A typical example is the localized necking in sheet metals. As a neck develops, the deformation in the localized region differs from that in the outer region. In addition, the amount of deformation is usually beyond the measurable range.

A number of studies on forming limit prediction using crystal plasticity have been published. Barlat (1987) used the Taylor/Bishop and Hill procedure to calculate the yield criterion and analyzed the effect of crystalline orientation on forming limits by using the Marciniak and Kuczynski. (1967) procedure, also known as the M-K approach. Later, crystal plasticity models were directly combined with the M-K procedure. These models can be classified in terms of the homogenization scheme used in the polycrystal. In a few of the works, the Taylor assumption was used (Zhou and Neale, 1995; Wu et al., 1997; Savoie et al., 1998; Kim et al., 2013), while in others, the viscoplastic (VPSC) or elastic viscoplastic (EVPSC) self-consistent method (Signorelli et al., 2009; Franz et al., 2009; Neil and Agnew, 2009; Wang et al., 2011) was used. The crystal plasticity approach has allowed the exploration of various effects of microstructure on the forming limit such as those of the slip systems (Inal et al., 2005; Serenelli et al., 2010; 2011), texture components (Wu et al., 2004; Yoshida et al., 2007), hardening laws (McGinty and McDowell, 2004), and loading history (Yang et al., 2010; Holmedal et al., 2008; Beyerlein and Tomé, 2007). Instead of using the above homogenization schemes, the CPFEM approach can be used for forming limit analysis. Because the equilibrium and compatibility conditions with neighboring grains are satisfied in CPFEM, it is expected to provide a more accurate prediction of the forming limits.

In order for crystal plasticity models to precisely describe the mechanical behavior under various loading conditions, the model parameters should be calibrated accurately. The material parameters may be obtained from finer scale simulations such as dislocation dynamics (Queyreau et al., 2009; Wang and Beyerlein, 2011) and molecular dynamics (Gilbert et al., 2011; Lim et al., 2015). A few parameters such as the critical resolved shear stress may also be obtained directly from tests on single crystals (Franciosi, 1983). However, the measurement or calculation of all the model parameters by independent tests or simulations is a practical challenge. Therefore, the inverse nonlinear optimization approach is more suitable to obtain the parameters of crystal plasticity models. In this approach, a set of parameters is calibrated numerically so that the constitutive model reproduces the measured macroscopic behavior, which is described in most studies by uniaxial stress-strain data (Herrera-Solaz et al., 2014; Yalcinkaya et al., 2008; Xie et al., 2004). In the inverse approach, however, the solution may not be unique, especially when constitutive equations are complex, the number of parameters is large, and the input data are limited. Therefore, providing additional experimental data such as longitudinal-transverse strain data under uniaxial loading conditions and stress-strain data under biaxial loading conditions are likely to improve the accuracy of constitutive models.

Body-centered cubic (bcc) metals exhibit a unique plastic behavior originating from a large number of slip systems. The slip trace analysis of single crystal specimens loaded in prescribed directions (Spitzig and Keh, 1970; Franciosi, 1983) revealed the operation of  $\{110\}\langle 111 \rangle$ ,  $\{112\}\langle 111 \rangle$ , and/or  $\{123\}\langle 111 \rangle$ , as well as certain higher index slip systems with high resolved shear stress. This can be explained partly by the fact that bcc metals do not have close-packed crystallographic planes. In addition, the breakdown of the Schmid law, or non-Schmid effect, is observed in bcc metals, especially at low temperatures (Christian, 1982). The non-planar core structure of  $1/2\langle 111 \rangle$ -screw dislocations are known to be responsible for the dependence of slip on stress components other than the resolved shear stress (Ito and Vitek, 2001; Gröger et al., 2008). Moreover, the influence of various factors, such as base metal properties, alloying elements, temperature, and strain rate, on slip renders the analysis of deformation mechanisms complicated. The determination of crystal plasticity parameters of bcc metals should therefore be carried out carefully, especially if the constitutive model is to be applied to complex problems such as forming limit predictions.

In this study, a crystal plasticity finite element analysis was conducted for predicting forming limits of a ferritic stainless steel. A virtual microstructure crystal plasticity finite element model and a rate-dependent viscoplastic crystal plasticity model, which will be used to reproduce the mechanical behavior of the material, are introduced. The procedure for obtaining hardening parameters for different slip modes using an inverse method is presented. The development of a multi-scale framework, which combines the virtual microstructure models and the M-K procedure, is explained. Finally, the forming

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