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# Strain rate effect of high purity aluminum single crystals: Experiments and simulations

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ABSTRACT

In order to study the strain rate effect on single crystal of aluminum (99.999% purity), aluminum single crystals are fabricated and subjected to uniaxial compression loading at quasi-static and dynamic strain rates, i.e., from $10^{-4}\,s^{-1}$ to $1000\,s^{-1}$. The orientation dependence is also investigated with single slip or multi slip. The stress–strain curves of pure Al single crystals along two orientations and at different strain rates are obtained after measuring initial orientation using the Laue Back-Reflection technique.

Crystal Plasticity Finite Element Method (CPFEM) with three different single crystal plasticity constitutive models is used to simulate the deformations along two orientations under various strain-rates. The classical and two newly developed single crystal plasticity models are used in the investigation. The simulation results of these models are compared to experimental results in order to study their abilities to predict finite plastic deformation of single crystalline metal over a wide strain rate range.

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## 1. Introduction

Most metals used in engineering are polycrystalline, which are aggregates of single crystals (grains). In many models for polycrystal metals, mechanical behavior of a polycrystalline has been viewed as the collective behavior of grains and their interactions with each other. Therefore, a physical-based modeling of polycrystals involves understanding, quantifying, and predicting the constitutive behavior of the constituent single crystal grains.

It is important to investigate the deformation responses of high purity single crystals both experimentally and numerically to gain further insight into deformation mechanisms of crystalline materials, since high purity single crystals eliminate the effect of grain boundary, grain interaction (single crystal), second phase particles and even solute atoms (high purity). This study only focus on FCC structures, so it should be noted that the following review only concerns FCC as well.

The study of the physics of single crystal plasticity can be traced to the early 20th century (Taylor, 1934). It has been established that crystalline materials deform plastically by the crystallographic slips of dislocations on discrete slip systems. Therefore, the plastic deformation of a single-crystal material point is the sum of the crystalline slips in all the activated slip systems. Plastic slip of a slip system only occurs when the resolved shear stress (driving force of slip) onto a crystallographic plane reaches a critical value (critical resolved shear stress, or CRSS) in the direction of slip. Depending on the relative orientation of the crystal lattice to the loading axis, it is possible that only slip system is active (single slip mode). The slip mode in which more than one system is active is called multislip (slip mode in this study denotes the activation of single or multiple slip systems of the same slip system family of FCC, it should not be confused with the activation of different slip system

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families as in BCC and HCP). Single crystals deformed by different modes (single or multislip) usually show different mechanical behavior and microstructure evolution. The CRSS of a slip system is a function of plastic strain and usually increase due to the material hardening caused by plastic deformation. Three conventional stages of hardening have been found for FCC single crystal deformation in the early studies: stages I or easy glide, stage II characterized by a much higher, linear hardening and stages III with a decreasing hardening. Late stage IV, V and VI have been identified at large strains (Argon and Haasen, 1993; Les et al., 1996, 1997; Mecif et al., 1997). The existence and extent of each stage depend on many factors such as the initial crystal orientation, temperature and strain rate and the type and purity of metal. In low to intermediate strain, while the well-defined three stages are typical of pure single crystal copper, most investigations of single crystal aluminum revealed a small or no stage I (Hosford et al., 1960; Howe et al., 1961; Bell and Green, 1967). The number of investigations in which high strain rates are attained is far smaller for single crystal than for polycrystal specimens (Lindholm and Yeakley, 1965; Ferguson et al., 1967; Edington et al., 1968). It is important to note that physically, the slipping and hardening of each slip system are the result of dislocation movement, density evolution and interaction.

Crystal plasticity (CP) theory and modeling are based on the aforementioned deformation mechanism of crystallographic slip, i.e., the plastic deformation of single-crystal material point is the sum of the shear of slip systems.

Taylor (1938) established a quantitative description of plastic deformation in single crystals based on crystallographic shearing. Rice (1971) and Hill and Rice (1972) developed a general finite deformation elastic–plastic framework for analyzing the deformations of rate independent single crystals. Later Peirce et al. (1982, 1983) presented a rigorous constitutive theory for rate dependent material response.

Following the single crystal visco-plasticity modeling framework laid out by Rice (1971), and Hill and Rice (1972), the kinematic deals with the geometrical aspect of deformation without considering the stresses. It assumes a multiplicative decomposition of the deformation rate into elastic and plastic parts. The velocity gradient tensor can be related to the scalar shear rates of all the slip systems. The kinetics (or flow rule) determines the shear strain rate of a system at a certain applied resolved shear stress and a microstructure state. In the classical phenomenological approach, one "strength" for each slip system is used as the internal state variables (ISV) to represent the state of material. Conventionally, a power law was used as the flow rule (Hutchinson, 1976). More realistic flow rules based on the physics of thermal activation were also used by Nemat-Nasser et al. (1998), Balasubramanian and Anand (2002), Hansen et al. (2013), and other researchers. The hardening law refers to the evolution equations of slip system strengths as the material hardens with plastic deformation.

The framework and kinematics are the same for all crystal plasticity models that are based on the deformation mechanism of crystallographic slip. The classical phenomenological model uses strengths of slip systems as internal state variables and a power law as the flow rule. Considering that the slipping and hardening of each slip system are the results of dislocation movement, evolution and interaction, models based on the dislocation density have been proposed by many authors. The simplest type is to use a scalar (total) dislocation density for each slip system as ISV (Tabourot et al., 1997; Kocks and Mecking, 2003; Beyerlein and Tomé, 2008; Lee et al., 2010). More physical and advanced models includes those that separate the mobile and forest dislocations (Kubin and Estrin, 1990; Barlat et al., 2002; Austin and McDowell, 2011; Hansen et al., 2013), those that separate the edge and screw dislocations (Arsenlis and Parks, 2002; Alankar et al., 2009), those that consider the development of the dislocation densities in cell walls and grain interiors (Estrin et al., 1998; Roters et al., 2000; Tóth et al., 2001) and those consider the geometrically necessary dislocations (GND) in addition to the scalar statistically stored dislocations (SSD) (Ma and Roters, 2004; Ma et al., 2006a, 2006b; Gurtin, 2010).

It is worth mentioning that as the complexity of models increases, the number of parameters that need to be identified also increases and it is usually more difficult to perform the numerical simulations.

Combining crystal plasticity with finite element method, Crystal Plasticity Finite Element Method (CPFEM) is popular. CPFEM is a powerful simulation tool as it combines the FEM's ability of solving complicated boundary problem and CP's ability of taking the microstructure and deformation mechanisms into account. The FEM serves as the boundary problem solver, while at each integration point the material constitutive model is based on crystal plasticity theory.

The first CPFEM simulation was performed by Peirce et al. (1982). With the increase of computation power, CPFEM simulations have been extended from simplified 2-D setups with two or three slip systems for single crystal (Peirce et al., 1982) and polycrystal (Harren et al., 1988; Harren and Asaro, 1989) to 3-D setup with the all the 12 slips system for FCC (Becker et al., 1991) and complex grain arrangements. A recent comprehensive review of CPFEM is done by Roters (2010).

There are small scale and large scale CPFEM regarding the scale of volume a material point represents.

In small scale CPFEM simulations, the size of the finite element mesh is equal to or smaller than the grain size. In such cases, one integration point represents a single crystal (a part of a grain), so the single crystal plasticity model serves directly as the constitutive model. With such sub-grain resolutions, heterogeneity of deformation with a single crystal is taken into account (Zhang et al., 2009; Lee and Chen, 2010; Saito et al., 2012; Mayeur et al., 2013; Rossiter et al., 2013; Sabnis et al., 2013; Ardeljan et al., 2014; Knezevic et al., 2014) as well as the influence of grain boundaries and free surfaces (with special treatments of mesh at/crossing GB and free surface).

Large scale CPFEM refers to simulations with more than one crystal assigned to one integration point and the number of grain is usually large enough to study the average behavior of the material such as the texture evolution. Usually, the deformation within each grain is assumed to be uniform. Homogenization schemes are needed to connect a material point (an integration point in the FEM) to each constituent grain (modeled by single crystal models). Commonly used homogenization schemes are iso-strain (Taylor, 1938), iso-stress (Sachs, 1928) and the self-consistent schemes (Kröner, 1959; Molinari et al., 1987; Lebensohn and Tomé, 1993; Knezevic et al., 2013a, 2013b ).

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