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A multi-scale self-consistent model describing the lattice deformation in austenitic stainless steels

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ABSTRACT

Differently oriented grains within a polycrystalline material exhibit different micro-mechanical lattice responses for a given macroscopic stress due to the local elastic and plastic anisotropy. A physical understanding of the lattice deformation mechanism during plastic flow is still lacking. In this study, a three-dimensional multi-scale self-consistent model is developed to examine the micro-mechanical deformation behaviour of F.C.C. polycrystalline austenitic stainless steels under uniaxial tensile loading at ambient temperature. The model is formulated in a crystal based plasticity framework and takes into account the detailed kinematics of dislocation slip and its influence on the evolution of the dislocation distribution on different crystallographic planes of individual grains within a polycrystalline material. The effect of athermal solute strengthening is also incorporated. Predictions of the microscopic lattice response developed within individual grains are compared with various available experimental results obtained using neutron diffraction (ND). There are significant differences in the way in which the lattice strain evolves with macroscopic strain obtained by different groups. This is explained in terms of the variation in initial residual stress state in the samples tested by these different groups.

1. Introduction

For metallic polycrystalline materials like austenitic stainless steels, the macroscopic deformation is dependent on the microscopic behaviour of each individual grain. Given an applied loading history, the local elastic and plastic anisotropy of differently oriented grains within the polycrystal leads to a variation in the micro-mechanical lattice response, whose evolution will depend on the detailed anisotropic flow, hardening and recovery laws for different slip systems in the body. The development of the local mismatch between grains during plastic deformation will lead to the accumulation of intragranular residual stresses, which has a considerable effect on damage development within the material (Clausen et al., 1998, Daymond and Bouchard, 2006). Therefore, understanding the local micro-scale variation between different grains or lattices plays an important role in assessing and improving the performance of such materials.

In recent years, the non-destructive neutron diffraction (ND) technique has been extensively used to measure the *in situ* evolution of micro-scale lattice strains for different subsets of grains within a range of polycrystalline materials during macroscopic deformation (Clausen et al., 1998, Daymond and Bouchard, 2006, Neil et al., 2010, Chen et al., 2014, Li and O'Dowd, 2011). It captures the change of spacing of lattice planes, thus measuring the elastic response, whose evolution depends on the micro-plastic response of each grain. Clausen et al., (1998), Daymond and Bouchard, (2006), Li and O'Dowd, (2011) have used constitutive models and/or finite element analysis to simulate the relationship between the behaviour of individual grains and that of the polycrystalline aggregate to predict and understand the micro-scale behaviour of such materials. However, to date, no previous studies have systematically compared the model prediction with micro-scale ND measurements to identify the dominant lattice deformation mechanisms.

Among the constitutive models that have been proposed or developed to predict the elastic-plastic behaviour of polycrystalline materials, self-consistent models have been used and/or developed extensively, which employ solutions of the classical Eshelby inclusion problem to homogenize the polycrystal (Eshelby, 1957, Mura, 1982), where each individual grain is regarded as an ellipsoidal inclusion embedded in a macroscopically homogeneous equivalent medium. Typical examples of such models can be traced back to the models proposed independently by Kroner (1961) and Budiansky and Wu (1962) (the K.B.W. model), and Hill (1967, 1965, 1966). The difference between these two types of models has been discussed by Hutchinson (1970). The K.B.W. model employs the solution for a plastically deforming inclusion (grain) within an elastic matrix and does

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not fully consider the plastic interactions between each grain in a polycrystal, while Hill's model adopts an incremental self-consistent scheme by taking into account the change of instantaneous or tangent moduli for the polycrystal to capture the elastic–plastic interaction. This may require the solution for an anisotropic inclusion embedded in an anisotropic medium, whose properties can change with time. Limited analytical solutions are available for the general anisotropic problem and numerical methods are generally required to solve the governing equations (Li and Dunn, 1998). In practice, extensions of Hill's approach self-consistent generally assume an equivalent isotropic medium (e.g. Berveiller and Zaoui, 1978). The advantage of the K.B.W. modelling approach is that the properties of the effective medium used in the solution of the inclusion problem do not change as the body deforms, i.e., it retains the same elastic properties, and if there is a random distribution of grain orientations, the elastic response is macroscopically isotropic. This greatly simplifies the analysis, which can be undertaken entirely analytically. Further, Hill (1967, 1965, 1966) and Hutchinson (1970) have also combined the self-consistent approach with a crystal plasticity framework and a simplified dislocation slip mechanism to characterize the hardening behaviour of each grain. However, all these models lack consideration of detailed evolution of dislocation structure associated with slip processes in individual grains, thus the work hardening behaviour is only reflected in an empirical way.

Analytical physical dislocation models, e.g. dislocation network models, have been proposed (Mclean, 1968, Evans and Knowles, 1977) to characterise the hardening and/or recovery behaviour, by capturing the evolution of the dislocation structure during plastic or creep deformation. These models consider the dislocation structure of a deformed crystalline solid as a complex three-dimensional array of dislocation links arranged in a network, where a dislocation link is defined as the dislocation segment between two pinning points. A given grain will contain a distribution of link lengths. Among the extensions, models originally proposed by Lagneborg and Forsen (1973) and Ostrom and Lagneborg (1976) investigated for the first time the detailed evolution of the distribution of link lengths from a physical description of the glide motion of mobile dislocation links. Such a distribution is frequently described by an instantaneous distribution function (Ostrom and Lagneborg, 1976, Lagneborg and Forsen, 1973, Ardell and Lee, 1986, Ajaja, 1986, Shi and Northwood, 1993a, Lin et al., 1989). A typical distribution was derived by Wang et al. (1992), assuming that different slip systems uniformly orientate in three-dimensional space and all configurations are equally probable, which also minimizes the total entropy. However, such a distribution function only considers a static structure without any external stress. Further, all previous dislocation link length models have allowed the existence of links with infinite length in the network, which is physically unrealistic. Most importantly, previous evolution laws of the distribution function have not distinguished between different dislocation structures on different crystallographic planes, thus the hardening or recovery behaviour described by these models was simplified to be isotropic, i.e. the same for all slip planes, which has been confirmed to be inappropriate by recent dislocation dynamics (DD) simulations (Alankar et al., 2012, Groh and Zbib, 2009, Madec et al., 2003).

Alternatively, for the detailed dislocation interactions and slip motion, the fast-developing field of dislocation dynamics (DD) has proven to be a valid computational approach to study the mechanics of dislocation interactions and their effects on crystal level deformation and has thus provided a valuable link between crystal defects and the macroscopic response of a crystal (Ramasubramaniam et al., 2007, Gaucherin et al., 2009, Zbib et al., 1998, Van der Giessen and Needleman, 1995, Deshpande et al., 2003). This framework requires (1) a set of prescribed mobility rules for dislocations to slip and (2) randomly distributed sources to generate dislocations and continue the plasticity, such as Frank-Read source (Van der Giessen and Needleman, 1995, Benzerga et al., 2004) or jogs and closed dislocation loops as reviewed by Zhou et al. (2010) (in some three-dimensional studies the sources are naturally created during multiplication). Despite the development of DD models in both two-dimensional and three-dimensional directions, most of these works has focused on single crystals, since a common drawback of these models is the vast computational resources required to solve the elastic field of each dislocation segment, especially for three-dimensional problems (Gaucherin et al., 2009, Groh and Zbib, 2009). This may retard its application to polycrystals, which also requires the solution of a large number of boundary problems such as the reaction between dislocations and grain boundaries. However, DD simulations provide a useful qualitative tool to help characterize important parameters in analytical crystal plasticity models (Groh and Zbib, 2009, Devincre et al., 2006, Alankar et al., 2012). Here, we aim to establish an analytical polycrystal model in which the deformation laws and evolution of dislocation structure are guided by classical models of dislocation mechanics and are consistent with recent DD simulations.

In the present work, a multi-scale self-consistent model is established by incorporating the athermal part of a dislocation link length model into the crystal based plasticity and self-consistent framework. For the interaction between individual grains, we simply take the assumptions of the K.B.W. model, i.e. purely elastic interaction, to avoid the issues associated with an anisotropic medium and the choice of tangent moduli. The present model is an extension of previous self-consistent and dislocation link length models by considering: (1) the distinction between the self- and latent hardening behaviour in terms of different evolution processes of the dislocation distribution on different crystallographic planes of individual grains; (2) athermal solute strengthening and its effect on the plastic response; (3) the influence of the plastic mismatch strains between grains on the microscopic lattice response. The model is used to evaluate the lattice deformation of polycrystalline austenitic stainless steels under uniaxial tensile loading at ambient temperature. *In situ* neutron diffraction measurements, both parallel (axial) and perpendicular (radial) to the loading direction, published by different groups are compared and explained using the newly developed model.

The layout of the paper is: Section 2 describes in detail the framework of the multi-scale self-consistent model. Section 3 briefly outlines the neutron diffraction technique and presents experimental results obtained by different groups. Section 4 outlines the comparison between the model prediction and the available data in terms of the evolution of both lattice strain and residual lattice strain during uniaxial tensile loading. In this section the influence of an initial residual stress state on the measured results is explored. The results and lattice deformation mechanisms are discussed in Section 5 followed by concluding remarks in Section 6.

2. Formulation of the athermal self-consistent model

The athermal self-consistent model proposed in this paper consists of three sub-models, which describe the response from the macro- to the micro-scale, namely: continuum, crystal plasticity and dislocation link length models. In this section, we start from the last of these, with the principal concern on the kinematics of the slip processes and the evolution of microstructure on different crystallographic planes within each individual grain of the polycrystal. The continuum and crystal plasticity model for a polycrystalline aggregate have been presented in our previous work (Hu et al., 2013, Hu et al., 2015) and will only be briefly described later in this section.