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A multiscale simulation framework of the accumulative roll bonding process accounting for texture evolution

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ABSTRACT

The accumulative roll bonding process is one of the most prominent severe plastic deformation processes for obtaining sheet materials with ultra-fine-grained microstructures and high strength. The properties of such sheets differ significantly from those of conventionally rolled sheets. It is hence desirable to have a simulation framework that can accurately predict the material properties, including the evolving texture and anisotropy during processing. Here, we propose such a framework for *multiple pass* rolling using explicit finite elements and embedding the visco-plastic self-consistent (VPSC) polycrystal texture model for the material response. To facilitate multiple pass rolling, we propose a novel solution mapping scheme that transfers the material state from the deformed finite element mesh to a new one. Additionally, we implement a two-level parallelization scheme – with decomposition of the FE domain using message passing interface (MPI) and thread based parallelization of the material response using OPENMP – to ensure reduced simulation times. The predictive capabilities of the proposed framework are demonstrated by simulating the accumulative roll bonding of aluminum alloy AA5754 sheets. The simulations validate the working of the solution mapping scheme, and clearly show the development of a through thickness gradient of texture and anisotropy in the roll-bonded sheet after two passes.

1. Introduction

The adoption of new materials in the automotive, aerospace or energy sectors hinges ever increasingly on the possibility to reliably model their mechanical behavior during processing and under typical usage conditions, as well as their failure when subjected to catastrophic loading, e.g. during a car crash. Material models have therefore become an essential ingredient for the emerging discipline of *integrated computational materials engineering* (ICME), which promises to significantly shorten the materials development cycle [1]. For example, the integration of computational material models in the product design process as well as in manufacturing process simulation would allow engineers to explore new ways of optimizing the properties of a component through processing. The key for successful implementation of the ICME paradigm is the availability of material models which describe the multiple links among processing, microstructure, properties and performance in a multiscale modeling framework. However, for many innovative materials or processing routes reliable material models are not yet available. In particular, the *accumulative roll bonding* process to produce high strength metal sheets, e.g. for automotive applications, would profit from a reliable and robust material model to optimize the process parameters and describe the resulting microstructure and mechanical properties.

Among the various *severe plastic deformation* (SPD) processes, the *accumulative roll bonding* (ARB) process is most promising for achieving ultra-fine-grained (UFG) microstructures in metallic sheet materials. First proposed by Saito et al. [2], the ARB process is based on the principle of stacking two sheets of materials and subsequently feeding them to a rolling mill where the thickness is reduced by 50%. As the geometrical dimensions of the processed sheet remain more or less unchanged to the starting material, the process can be easily repeated. Both sheets are initially degreased and wire brushed to remove thick oxide layers; in the absence of such oxide layers and driven by large plastic strains, the stacked layers fuse at the interface to ensue good bonding properties. A detailed overview on the principles of ARB-processing and the properties of some processed materials is provided in Ref. [3]. A

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major advantage of the ARB process is that it can be easily integrated/adapted into existing industrial rolling trains without major modifications and can be scaled up to produce sheet materials with UFG microstructures on an industrial scale [4]. Furthermore, the ARB process offers numerous possibilities to tailor materials properties by producing laminated sheet materials [5–7], graded structures [8], particulate [9,10] or fiber reinforced composite sheet materials [11–13].

The repeated roll bonding of the sheets in the ARB process leads to substantial accumulation of plastic deformation resulting in a UFG microstructure. This UFG microstructure causes a significant increase—by almost a factor of two—in the strength of the material, in comparison to the coarse grained counterpart. Although this is generally offset by a decrease in ductility, it has recently been reported that application of ARB to low density sheet materials, like aluminum alloys, can result in both high strength and high ductility of the material [5] and has been attributed to room temperature strain rate sensitivity of the material (see also e.g. [14–16]).

The ARB process itself involves a multitude of parameters, e.g. rolling speed, friction between the rolls and the feedstock, number of rolling passes, and stacking and rolling direction, which can have a considerable effect on the properties of the roll bonded sheet. Although comparable to a conventional rolling process in principle, the role of such process parameters is either significantly enhanced or completely different in ARB due to the high thickness reduction and repeated stacking of roll bonded sheets in every pass. For instance, sheared surface layers (due to friction between the rolls and the feedstock) give rise to a characteristic through thickness strain gradient in the roll bonded sheet. With repeated cutting and stacking, the shear profile changes substantially [14], leading to different rates of microstructure evolution along the thickness of the sheet. Consequently, the number of rolling passes has a discernible effect on the through thickness strain gradient. The anisotropy in the roll bonded sheet is thus not just a function of texture/microstructure, but also the strain gradient and the number of rolling passes [17]. It is thus to be expected that the properties of ARB sheets differ appreciably from those of conventionally rolled sheets [18], and additionally, can significantly impact further applications (e.g. deep drawing) of the roll bonded sheet.

In view of the aforementioned aspects, it is desirable to have a computational framework to simulate and understand the ARB process in order to obtain optimized process parameters, so as to avoid trial-and-error experimental setups. To date, most studies on ARB processed materials have been experimental investigations to understand both the process and the enhanced properties of the roll bonded sheet, as evident in the references mentioned above. By contrast, few computational studies can be found in the literature; these studies have been limited to understanding individual aspects of the ARB process. For instance, texture evolution which plays an important role during ARB has been the subject of a few numerical investigations. Heason and Prangnell [19] performed EBSD and X-ray measurements on a roll bonded AA1100 sheet, and analyzed the evolution of texture using the Taylor [20] full constraints model with simple and idealized textures. A similar study was performed on AA3003 by Pirgazi et al. [21], but by using the ALAMEL model [22]. In contrast to the idealized deformation paths assumed in the previous two studies, Li et al. [23] used realistic strain histories to investigate the texture evolution in commercially pure aluminum by means of the ALAMEL model. Finite element (FE) simulations of a *single-pass* rolling process were employed to obtain the relevant strain histories; the FE simulations were calibrated to embedded pin experiments in order to reasonably estimate the shear deformation [24] seen in ARB processed materials.

A primary goal of this work is to establish a computational framework that enables the simulation of *multiple pass* ARB process, while simultaneously accounting for the change in texture and anisotropy of the material. The principal idea here is to obtain the structural response using a FE calculation, while the material response is obtained by "averaging" the constitutive behavior of individual crystals in a defined polycrystal. Such "averaging", termed generally as *numerical homogenization*, is now a well established technique to solve problems involving the micromechanical behavior of polycrystalline materials. An excellent review of such methods is provided in Ref. [25]. Although different flavors of such a multi-scale framework are available, all boil down essentially to two choices: (a) the polycrystal homogenization theory to be used [26], i.e. *full-field* or *mean-field* theory, and (b) implementation of the mesoscopic model within the multiscale analysis framework [22], i.e. whether the polycrystal model is to be *embedded* in the FE computation, or merely used in a *hierarchical* fashion.

Polycrystal homogenization theories can be broadly classified into two categories, viz. full-field and mean-field methods. Full-field methods provide a fairly accurate assessment of the intragranular stress and strain fields. Examples of such methods include the *crystal plasticity finite element method* (CPFEM) and *crystal plasticity fast Fourier transform* (CPFFT) method. CPFEM has been extensively used with artificial microstructures (e.g. [27–29]) as well as experimental microstructures obtained typically from EBSD measurements (e.g. [30–32]). The CPFFT method [33,34] is identical to CPFEM with one major difference – the governing equations are solved in the Fourier space. Although restricted to periodic microstructures in principle, a major advantage of CPFFT over CPFEM is the speed of computation [35]. The choice of such full field methods for numerical homogenization, however, necessitates the usage of FE^2-type methods (e.g. [36]), which would essentially result in lengthy computation times for multiple pass ARB simulations.

In what concerns the implementation of the numerical homogenization model within the multiscale analysis framework [22], choice must be made between *embedding* the model in the FE computation—i.e. interrogating the polycrystal model during each increment—and using it in a *hierarchical* fashion [37,38], where the parameters for a macro-scale (anisotropic) phenomenological yield criterion (e.g. [39,40]) are pre-computed by interrogating the polycrystal model. This choice, as a result, is clearly a decision on balancing accuracy and speed, since embedded models tend to be more accurate but less efficient (in terms of computational times) than hierarchical models. Nonetheless, it must be noted that adaptive sampling strategies (e.g. [41]) can be used in conjunction with embedded models to achieve results in shorter lead times.

The fundamentals of our computational framework lie in the aforementioned multiscale approach; we use a mean field homogenization model *embedded* in a FE computation. In particular, we use the viscoplastic self-consistent (VPSC) model of Lebensohn and Tomé [42] as our choice of the mean field model, since it has been widely used for many studies involving both cubic (e.g. [43]) and *hcp* (e.g. [44–46]) materials and is known to provide fairly accurate predictions of the texture and anisotropy [47,48]. The VPSC model is embedded in an explicit finite element framework using the commercial finite element software Abaqus. It must be pointed out that this embedded VPSC-FE model is not entirely new, and has been the subject of previous studies (e.g. [44,49,50]). However, such basic implementations are insufficient to overcome the challenges posed by the ARB process.

A primary challenge in simulating the ARB process – as seen from the discussion before – is the increase in number of elements, by a factor of two, with each ARB pass. Additionally, due to the