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Surface & Coatings Technology

# Numerical analysis of highly reactive interfaces in processing of nanocrystallised multilayered metallic materials by using duplex technique

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### ARTICLE INFO

Article history: Received 15 April 2015 Revised 9 July 2015 Accepted in revised form 10 July 2015 Available online 16 July 2015

Keywords: Nanocrystallised multilayered materials Finite element modelling Stainless steel Oxidation Interfaces Multilevel analysis

# 1. Introduction

The remarkable enhanced mechanical properties, such as high yield and ultimate strength, hardness and superplasticity of nanocrystalline and ultrafine-grained metals and alloys, with mean grain size lower than 100 nm comparing to the analogous coarse grained metals attracted widespread interest in the last two decades [1–6]. However, a significant number of nanocrystallised materials exhibit significantly lower ductile properties than their coarse grained counterparts [7–9]. In order to obtain nanocrystallised structures many different techniques can be used. Refining the grain size through severe plastic deformation (SPD) is known to provide the processed material with novel properties. The potential application of such advanced materials as biomedical implants has been evaluated by investigating the effect of different grain sizes on a variety of cell-substrate interactions [10]. The refined to the nano-level grain surfaces are considered to have potential to alter absorption of proteins that mediate cell adhesion, control and enhance subsequent cell functions and tissue growth [11]. Normally, these techniques allow for modification only of the surface layer. The affected depth of the nanocrystallised surface layer in such materials is limited to several tens of micrometres [12,13]. For bulk materials, such limited volume fraction of the nano-grains is not sufficient for improvement of their mechanical properties and often it is the reason for rapid

# ABSTRACT

The behaviour of the highly reactive interfaces during the processing of nanocrystallised multilayered materials has been investigated in the present work. Conditions leading to the formation of strain localisations around the oxidised interfaces during the thermomechanical stage of the duplex processing route have been investigated using multilevel numerical analysis. The analysis is based on the finite element methodology and involved coupling of the macro level model representing the rolling of the multilayered metallic material at elevated temperatures with the meso level model representing the oxidised interface within the nanocrystallised material. The multilevel thermomechanical model has been applied for the analysis of the strain, stress and damage evolution around the oxidised interfaces for the different technological parameters. The analysis included verification of the modelling results with the available experimental material. The 316L stainless steel is considered in the investigation.

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saturation of the yield strength. This problem can be solved by increasing the volume fraction of the ultrafine grains within the material structure. Combining any of SPD techniques used for grain refining at the surface layer of the material with subsequent thermomechanical (TMP) processing allows for obtaining metallic materials with multilayered bulk structure and the increased volume fraction of the nano-sized grains. Such duplex techniques can be used to produce materials with enhanced yield and ultimate strength, while conserving an acceptable elongation to failure. As an example, the duplex process combining surface mechanical attrition treatment (SMAT) with co-rolling process at elevated temperatures has been described in details elsewhere [14]. The materials are joined in a bonding mill at elevated temperatures by rolling them together with the massive reduction that ranges from 50 to 80% in a single pass. The rolling temperature of about 550 °C was chosen for joining 316L stainless steel sheets to allow compromise between bonding at the interfaces and preservation of the grain refining achieved by SPD technique. However, interfacial oxidation during the subsequent TMP processing and impurities deposited on the surface results in bonding imperfections. It has been shown that the interfacial oxidation can lead to the formation of discontinuous oxides or a continuous oxide layer at the interfaces (Fig. 1) [15].

One of the reasons of such behaviour could be weakening of the scale-metal interface at higher temperatures. The discontinuous oxides distributed along the interface influence the material flow during the co-rolling stage of the duplex process and can also influence the micro-structure development around the interfaces. It will inevitably have an

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Fig. 1. Optical micrographs of the cross section of 316L steel samples illustrating formed discontinuous (a, b) and continuous (c, d) oxide layers at the interface after nanocrystallisation and subsequent hot rolling. ND – normal direction; RD – rolling direction.

impact on the final material properties. In other words, formation and behaviour of the oxide scale at the interfaces takes its own role in the microstructure development during the processing of such multi-layered metallic materials. However, the underlying processes explaining the co-operative relationship between formation and failure of the oxide scale and microstructure development around the interfaces are not clearly understood. The aim of this work is to investigate the conditions leading to the formation of the strain localisations around the oxidised interfaces of the multilayered structures depending on different technological parameters. The available experimental evidence has been interpreted by using computer simulation based on the multi-level finite element (FE) analysis involving modelling of strain and stress evolution around the interfaces and analysis of the damage initiation highlighting the main trends in interface behaviour.

## 2. Experimental prerequisites

The grain refining mechanism during the SPD process of different metallic materials has been widely investigated in recent years [16]. It is believed that dislocation activities, mechanical twinning and dynamic recrystallization are responsible for the grain refining down to the nano-level. The dislocation mechanism operates in metals that contain large number of slip systems with high stacking fault energy (SFE) [17]. The coarse grains are subdivided into smaller ones by formation of high density dislocation walls and dislocation tangles followed by grain rotations. The twinning mechanism occurs in metals characterised by low SFE and associate with less slip systems [18]. According to this mechanism, the coarse grains are initially divided by mechanical twins followed by further refining through the formation of dislocation arrays, dislocation walls and tangles at high plastic deformation. The dynamic recrystallization mechanism is observed in metals that exhibit lower recrystallization temperature [19]. Nanocrystalline structure forms at the metal surface layer through this mechanism when the process temperature is high enough for recrystallization. The mentioned refining mechanisms are typical for single-phase alloys. However, advanced alloys used in modern industry normally contain multiple phases showing complexities of the refining mechanisms leading to nanocrystalline structure compared with single-phased systems. It has been found that cementite can be dissolved into the ferrite matrix in addition to the grain refining of both the ferrite and cementite phases during SPD [20].

Several processing techniques have been developed to produce bulk nanocrystalline materials over the last years apart from SPD of bulk metals. Among them are consolidation of ultrafine powders [21], ball milling and consolidation [22], electrodeposition [23] and crystallization of amorphous precursors [24]. The term "crystallization" is usually used for liquids or amorphous phases undergoing a phase transition known as solidification. The transformation can lead to the formation of nano-crystals in the liquid or amorphous matrix. However, the term "surface nanocrystallization" by SPD becomes widely applied in the relevant scientific literature nowadays [25,26]. At present, SMAT is considered as the most effective method, among the currently available SPD methods, for refining surface microstructure of bulk metals and alloys [25]. The technique has been successfully applied to a variety of metallic materials, such as pure metals, steels and alloys to achieve such high grain refinement of the surface layer [27].

TEM investigations combined with X-ray study of 316L austenitic stainless steel, which is material characterised by low SFE, subjected to SMAT revealed the chain of micro events leading to the formation of nanoscale grains at the surface layer [14,15,28]. The strain generated in the surface layer during such treatment is non-uniform exhibiting gradient distribution. The microstructure observation at various depths provided information on the mechanisms of grain refinement. Unidirectional parallel mechanical twins with high dislocation density were observed at about 200 µm depth leading to the formation of the twin-matrix alternative lamellar structure. The dislocations formed walls inside the micro-twins and some were arranged into planar arrays. At about 50 µm depth, as the strain increases, twin-twin intersection occurred to sustain the deformation, the phenomenon supposed to be associated with generation of nano-grains. The different twin systems are activated probably due to multidirectional repetitive loading as it takes place during SMAT. Thus, the initial coarse grains

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