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Modelling of microstructural effects on the mechanical behavior of ultrafine-grained Nickel using crystal plasticity finite element model

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ABSTRACT

In this contribution, a crystal plasticity finite element model (CPFEM) is revisited to study the microstructural influence on macroscopic mechanical behavior of ultrafine-grained (UFG) Nickels processed by two different powder metallurgy methods: Hot isostatic pressing (HIP) and spark plasma sintering (SPS). In addition, a modified Hall–Petch relationship is used at the grain level to investigate both grain size and oxide phase dependence of UFG materials mechanical behavior. Within the framework of small strain hypothesis, grain scale simulations of the UFG face centered cubic (FCC) Nickel are performed by applying the CPFEM accounting for the experimental grain orientation data at the integration points. A good agreement between experimental and numerical results is achieved.

1. Introduction

The interest in the development, investigation and applications of nanocrystalline (NC) and UFG materials, with average grain size typically below 1 µm, is due to their superior mechanical strengths compared to their conventional coarse-grained (CG) counterparts. Bulk NC/UFG materials can be synthesized in two essentially different ways. The first one is the "top-down" approach, where the bulk CG materials are refined by severe plastic deformation (SPD) (Dubravina, Zehetbauer, Schafler, & Alexandrov, 2004; Kapoor, Kumar, Mishra, Huskamp, & Sankaran, 2010; Krasilnikov, Lojkowski, Pakiela, & Valiev, 2005; Segal, 1995; Valiev, Islamgaliev, & Alexandrov, 2000, 2006) or by large plastic deformation such accumulated roll bonding (ARB) (Kamikawa, Tsuji, Huang, & Hansen, 2006; Tsuji, Ueji, & Minamino, 2002) and dynamic plastic deformation (DPD) (Dirras et al., 2012). The second way for producing ultrafine-grained materials is the so-called "bottom-up" approach. Samples are assembled from individual atoms or nanoparticles (Atkinson & Davies, 2000; Bui, Dirras, Ramtani, & Gubicza, 2010; Billard, Fondère, Bacroix, & Dirras, 2006; Champion, Bernard, Guigue-Millot, & Perriat, 2003; Sanders, Youngdahl, & Weertman, 1997).

The relation between the microstructure and the mechanical properties of NC/UFG materials are expected to be of great interest for the scientific community. Indeed, microstructure characteristics of the processed materials show a strong

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influence on the mechanical behavior. Almost studies published in the literature show that the grain size refinement is one of the principal reasons for increasing the flow stress of bulk NC and UFG materials. The effect of grain size on the flow stress of materials can be expressed by the empirical Hall–Petch relationship (Hall, 1951; Petch, 1953). It is generally accepted that for conventional polycrystals with micrometer-sized grains, the yield stress is proportional to the inverse square root of the mean grain size, i.e., $\sigma = \sigma_0 + kD^{-1/2}$, where σ is the yield stress, σ_0 is the friction stress, k is a constant referred to as Hall–Petch slope and D is the mean grain size. For "top-down" processed materials, the effect of intense shear or large plastic deformation results in a material containing high dislocations density and high fraction of low angle boundaries (LAGBs) compared to materials processed by other processing techniques, containing essentially high angle grain boundaries (HAGBs). In such a case, the study of the grain size effect on the flow stress is not simple because both the dislocation density and LAGBs also contribute on the strengthening of materials (Kapoor et al., 2010; Krasilnikov et al., 2005). In the work of Bui, Pham, and Fafard (2013), the microstructure and mechanical properties of drawn conventional 6063-O tubes at different cross-sectional reductions using variable wall thickness tube drawing process were investigated in details. The calculated contribution of the dislocation density to yield stress varies from 59 to 90 MPa for the deformed materials at cross-sectional reductions from 11.6% to 36%. These experimental studies showed that the traditional Hall–Petch relationship does not describe well the grain size dependence of the flow stress of NC/UFG materials because of intrinsic features. Indeed, the yield stress of such materials has at least two strengthening components: the first one is the Hall–Petch strengthening due to HABGs and the second one is the strengthening due to intrinsic features. In the cases of "bottom-up" approach, the materials, consolidated at elevated temperature from nanopowders, exhibited a low dislocation density, a thermally stable microstructure, and a random texture. For such microstructures suggest that the yield stress has mainly one strengthening component due to HAGBs. It follows that the grain size dependence of the flow stress can be explained solely by the classical Hall–Petch relationship. It should be noticed that, in some cases, other intrinsic features such as the dislocation substructures or the presence of a fine dispersion of oxide phase can contribute to the strengthening of UFG and NC materials (Bui et al., 2010; Bui & Pham, 2011; Billard et al., 2006; Gubicza, Dirras, Szommer, & Bacroix, 2007). For instance, Bui et al. (2010) studied the strengthening behavior of UFG Nickel having grain size in the range of 0.25–5 μm processed from nanopowders using SPS technique. The authors found that the fine-grained microstructure and the presence of a NiO phase were the principal strengthening factors in as-processed bulk materials. For a computed flow stress of about 1022 MPa, the maximum strengthening component due to the presence of the oxide phase was about 635 MPa.

In addition to the experimental studies, numerical modeling is another important and useful tool to interpret the relation between the microstructure and the mechanical properties of NC/UFG materials. Much of the understanding of the micromechanisms operation during the inelastic deformation of NC/UFG materials has been obtained from large-scale molecular dynamics (MD) (Schiotz & Jacobsen, 2003), microstructure based models (Borodachenkova, Barlat, Wen, Bastos, & Grácio, in press; Zhu & Lu, 2012) and elastoplastic self-consistent (EPSC) methods published in the past few years. The self-consistent approach-based models were generally coupled with the specific local constitutive behavior of grain to study microstructure influence, i.e., grain size (Berbenni, Favier, & Berveiller, 2007; Raeisinia & Sinclair, 2009; Ramtani, Bui, & Dirras, 2009; Weng, 1983), coupled effects of grain size and crystallographic textures (Nicaise, Berbenni, Wagner, Berveiller, & Lemoine, 2011), twin (Clausen, Tomé, Brown, & Agnew, 2008; Lebensohn & Tomé, 1993b), grain boundary (Jiang & Weng, 2004), porosity (Barai & Weng, 2008), oxide phase (Bui & Pham, 2011), and damage (Lebensohn, Solas, Canova, & Brechet, 1996) on the macroscopic mechanical properties of materials. The grain size distribution and the value of mean grain size represent the key parameters in characterizing the nature of microstructure formed through metal forming process. Several models proposed in the previous researches take into account the law of Hall (1951) and Petch (1953) at grain level for studying the effects of the mean grain size/grain size distribution on strengthening of initial state materials. A first micro–macro modeling considering grain size effect has been proposed by Weng (1983) who considered a Hall–Petch-type equation with a mean grain size at the slip system scale. Among the earliest works to study the effects of grain size distribution to yielding is that of Kurzydlowsky (1990). This work used a polycrystalline model based on the Hall–Petch equation to predict yield stress. The results showed that as the width of the log-normal grain size distribution increases, the slope of the Hall–Petch plot decreases. In all of the above-mentioned works, the initial microstructure used as an input file was considered as a non-deformed microstructure with a slight dislocation density. In the work of Bui and Pham (2011), the experimental investigation showed a content of oxide phase dominated in ultrafine-grained materials. The calculated contribution of the oxide phase to strength was about 219 MPa. The generalized self-consistent approach proposed by Jiang and Weng (2004) for investigating the yield stress of NC materials, was reformulated following an incremental small strain scheme. The authors modified the Hall–Petch relationship at grain level of a generalized elastoplastic self-consistent model by introducing an additional part parameter for studying both grain size and oxide phase dependence of mechanical behavior of NC/UFG materials. In the work of Bui et al. (2013), an elastoplastic self-consistent model, proposed by Hill–Hutchinson (Hill, 1965; Hutchinson, 1970), was revisited for investigating the microstructure dependence of the mechanical behavior of deformed materials. They used the modified Hall–Petch relationship proposed in Bui and Pham (2011) for studying both grain size and dislocation dependence of deformed materials behavior.

An advantage of MD and EPSC methods is lower computational costs relative to finite element (FE) method. However, the MD and EPSC methods are at present not suitable for carrying out simulations of deformation and failure under conditions similar to those under which physical experiments on nanocrystalline materials are carried out (Kadkhodapour, Ziaei-Rad, & Karimzadeh, 2009). In the past years, the crystal plasticity FE model was one of the effective methods to study the