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Grain refinement under high strain rate impact: A numerical approach

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ABSTRACT

In this paper, the mechanical response of ultra fine grained metallic materials under high strain rate impact conditions is investigated by means of a finite element based numerical framework. A dislocation based viscoplastic model is used to predict the evolution of the initial fine grain microstructure (average grain size of 203 nm or 238 nm, depending on the material history) with impact deformation. A Taylor impact test is simulated in order to assess the validity of a numerical solution through comparison with experiment. It is shown that our model captures the essential features of the mechanical behaviour. A further grain refinement down to the average grain size of 140–160 nm is predicted by the simulations.

1. Introduction

Ultra fine grained (UFG) and nanocrystalline metallic materials exhibit enhanced mechanical strength, and for this reason a number of research projects have been devoted to finding new ways to fabricate them. Among the many methods that have been proposed, grain refinement by severe plastic deformation has proved to be very efficient and is becoming increasingly popular [1].

Recently, it has been shown that nanocrystalline microstructures (in the sense of the commonly accepted definition based on the grain size being below 100 nm) can be generated under high strain rate conditions [2]. However, the mechanisms responsible for this extreme grain refinement are still not fully understood.

A two-phase model suitable for UFG materials has been previously developed based on dislocation density evolution [3,4]. In the model, a dislocation cell structure is assumed to form under straining, and the dislocation cell walls and cell interiors are treated as separate "phases" obeying a rule of mixtures. A particular strength of this model is that the evolution of the dislocation cell size with deformation can be accurately predicted. It was also tacitly assumed [3,4] that the misorientation between neighbouring cells increases with strain, so that eventually the dislocation cells are converted to new, smaller size, grains. This model has been demonstrated to describe deformation behaviour under quasi-static loading conditions successfully, but it has not been applied to high strain rate deformation conditions as yet.

In this paper, we investigate the suitability of this dislocation based model for predicting the microstructure evolution at very high strain rates (in the subsonic range). In the first part of the paper, the model is briefly presented. The parameters of the material under investigation here, namely UFG copper, are then detailed. The procedure that has been followed to calibrate the model for the high strain rate regime is discussed. Once the material parameters are properly calibrated, numerical simulations under high strain rate conditions are performed. The Taylor impact test is selected to verify the model because it is a standard mechanical test for assessing the dynamic behaviour of materials. It is demonstrated that the model employed here can capture the essential features of the mechanical response of the impacted specimen in terms of its shape and the velocity of the free end of the specimen. Furthermore, the model applied to UFG copper pre-strained by equal channel angular pressing – a technique producing severe plastic deformation in the material [1] - predicts a further reduction in the grain size upon impact. Finally, the limitations of our current model are discussed and conclusions are drawn.

2. Constitutive model for ultra fine grained materials

Heavily deformed metals often possess a fine microstructure due to the formation of pronounced dislocation cell structures, which serve as a pre-cursor to a refined grain structure (with the continual reduction of its characteristic size [5]) or recrystallization.

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Therefore, the material may be idealised as a two-phase composite consisting of cell walls of high dislocation density and cell interiors which are relatively low in dislocation density. Based on this idealisation, a dislocation based model of severely deformed materials has been proposed [3,4]. In this section, we shall restrict ourselves to a general presentation of the main equations defining this model.

The material is assumed to be characterised by two scalar internal variables, namely the average dislocation densities in the two "phases" introduced above, which determine the total dislocation density ρ_{tot}. The average cell size d is assumed to scale with the inverse of the square root of ρ_{tot}:

$$d = \frac{K}{\sqrt{\rho_{tot}}}, \tag{1}$$

where K is a constant. Owing to the assumed two-phase structure of the material, ρ_{tot} can be expressed as a weighted sum of the average dislocation density in the walls, ρ_w, and that in the cell interiors, ρ_c. This rule of mixtures reads

$$\rho_{tot} = f\rho_w + (1-f)\rho_c, \tag{2}$$

where f is the volume fraction of the walls. The expression describing the evolution of f with strain used in the present work was suggested in Refs. [3,4] as an adaptation of the experimental data on OFHC copper [3]

$$f = f_\infty + (f_0 - f_\infty)\exp\left(-\frac{\gamma^r}{\tilde{\gamma}^r}\right), \tag{3}$$

where f_0 is the initial value of f, f_∞ is its saturation value and $\tilde{\gamma}^r$ describes the variation of f with the resolved shear strain γ^r (the inverse of $\tilde{\gamma}^r$ representing the rate of decay of f). This particular form of the volume fraction, with f_0 taken to be larger than f_∞, implies that the walls become sharper as the strain increases in the material and that this sharpening outstrips the concurrent increase in cell boundary area with cell size reduction.

In order to evaluate the variation of the dislocation densities in the walls and in the cell interiors, the evolution equations for these two quantities are required. Based on the possible reactions involving dislocation density nucleation, interaction and annihilation, a set of two differential equations was derived [3,4]:

$$\dot{\rho}_c = \alpha^* \frac{1}{\sqrt{3}} \frac{\sqrt{\rho_w}}{b}\dot{\gamma}^r - \beta^* \frac{6\dot{\gamma}^r}{bd(1-f)^{1/3}} - k_0\left(\frac{\dot{\gamma}^r}{\dot{\gamma}_0}\right)^{-1/n}\dot{\gamma}^r\rho_c, \tag{4}$$

$$\dot{\rho}_w = \frac{\sqrt{3}\beta^*\dot{\gamma}^r(1-f)\sqrt{\rho_w}}{fb} + \frac{6\beta^*\dot{\gamma}^r(1-f)^{2/3}}{bdf} - k_0\left(\frac{\dot{\gamma}^r}{\dot{\gamma}_0}\right)^{-1/n}\dot{\gamma}^r\rho_w. \tag{5}$$

In the above equations, a Taylor-type assumption was made [3,4]: the shear strain rate $\dot{\gamma}^r$ is considered to be the same in the cell walls and the cell interiors.

The first term on the right-hand side of Eqs. (4) and (5) corresponds to the generation of dislocations due to the activation of Frank–Read sources. The parameters α^*, β^* and k_0 are numerical constants, b is the magnitude of the Burgers vector. The loss of cell interior dislocations to cell walls where they are 'woven in' is accounted for by the second term in Eqs. (4) and (5).

Finally, the last (negative) term in each of the evolution equations represents the annihilation of dislocations leading to dynamic recovery in the course of straining. The dislocation annihilation is associated with cross-slip of screw dislocations or climb of edge dislocations. The reference shear rate $\dot{\gamma}_0$ and the exponent n have a different meaning and different temperature dependence for these two processes. For the cross-slip controlled dynamic recovery, n is inversely proportional to the absolute temperature T [3,4]:

$$n = \frac{B}{T}, \tag{6}$$

where B is a constant, which depends on the stacking fault energy of the material.

In the context of finite element simulations, the mechanical behaviour of the material is specified through a constitutive model that relates the equivalent (von Mises) stress and the equivalent plastic strain rate. The equivalent stress can be taken as the sum of two terms:

$$\sigma = \sigma_1 + \sigma_2. \tag{7}$$

In this equation, σ_1 represents a strain-independent contribution to the stress that originates from the resistance to dislocation glide ('friction') not related to dislocation–dislocation interactions. This stress may be estimated from the yield stress of the undeformed material [6]. The second term in Eq. (7), σ_2, originates from dislocation–dislocation interactions and is strain-dependent.

We further define the resolved shear stress τ^r associated with the dislocation–dislocation interaction part of stress, σ_2, and the shear strain rate $\dot{\gamma}^r$ in terms of σ_2 and the equivalent von Mises strain rate $\dot{\varepsilon}$ via the Taylor factor M:

$$\tau^r = \frac{\sigma_2}{M} \quad \text{and} \quad \dot{\gamma}^r = M\dot{\varepsilon}. \tag{8}$$

As with the dislocation densities, the resolved shear stress is obtained by applying a rule of mixtures:

$$\tau^r = f\tau^r_w + (1-f)\tau^r_c, \tag{9}$$

where the subscripts w and c in the resolved shear stress refer to the cell walls and cell interiors, respectively.

The quantities τ^r_w and τ^r_c may finally be expressed in terms of the dislocation densities in the cell walls and cell interiors through:

$$\tau^r_w = \alpha G b\sqrt{\rho_w}\left(\frac{\dot{\gamma}^r}{\dot{\gamma}_{0,S}}\right)^{1/m}, \tag{10}$$

$$\tau^r_c = \alpha G b\sqrt{\rho_c}\left(\frac{\dot{\gamma}^r}{\dot{\gamma}_{0,S}}\right)^{1/m}, \tag{11}$$

where G is the shear modulus, α is a constant, $1/m$ is a strain rate sensitivity parameter and $\dot{\gamma}_{0,S}$ is a reference shear rate. Similarly to n, the temperature dependence of m is taken to be inversely proportional to the absolute temperature:

$$m = \frac{A}{T}, \tag{12}$$

where A is a numerical constant. Eqs. (10) and (11) were initially proposed for the case of deformation with moderate (quasi-static) strain rates, and extending their use – with the model parameters determined on the basis of quasi-static tests – to the dynamic loading conditions to be considered here implies that the same deformation mechanisms still apply. Obviously, the model is not applicable for extremely high strain rates when the velocity of gliding dislocations is no longer controlled by their interactions with localised obstacles but is rather governed by the phonon drag.

The set of equations presented in this section define macroscopic constitutive behaviour on the basis of physical mechanisms operating at the dislocation scale. Apart from the advantage this approach provides with regard to the simplicity of the architecture of the model and the ease of interpretation of the model parameters, a further benefit lies in its ability to predict the evolution of the microstructure (represented by the dislocation density and cell/grain size) with strain.

A tacit assumption in this model is the existence of an established dislocation cell structure. Strictly speaking, this means that this approach is only valid for dislocation cell forming materials that have already undergone a sufficient amount of straining for