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Predicting tensile and compressive mechanical properties of bimodal nano-aluminum alloys

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We present a new analytical model for predicting the tensile and compressive mechanical properties of bimodal nano-aluminum alloys. The model relies on simple material variables that show a Hall–Petch-like grain size dependence including a newly defined ductility parameter which can be used with the Hollomon equation to allow for the prediction of failure stress and strain. When the model is applied to bimodal nano-aluminum alloys, the results show excellent agreement with the experimental observations.

Keywords: Aluminum alloys; Nanocrystalline metal; Analytical methods; Mechanical properties

Bimodal metallic nanomaterials are a recent development in powder metallurgy (PM) techniques that combine grains of significantly different sizes [1,2]. In bimodal alloys, a high-strength nanocrystalline (NC) phase, produced by cryomilling, is mixed with a highly ductile coarse-grained (CG) powder to produce attractive materials having both high strength and good ductility. To date, the most widely reported mechanical data is for bimodal materials of aluminum (Al), and these materials can form the basis for even higher-strength trimodal alloys, which combine nanoparticle (NP) ceramic reinforcements in the NC phase [1–5]. There is, however, no means of predicting mechanical properties such as yield strength (σ_y), maximum stress and failure strain ($\varepsilon_{failure}$) for these bimodal materials. In the present work, an analytical model has been developed that describes these properties based on the grain size dependence of several material properties and the assumption that the stress–strain behavior of the material can be described by the Holloman equation [6]. The model is then applied to experimental results of both tensile and compressive tests of Al-5083 bimodal materials tested in the longitudinal direction, as sufficient data exists for these materials and they exhibit advanced mechanical properties that cannot be achieved in similar monolithic alloys [2].

Since the bimodal materials are composed of mixtures of two identical phases of the same alloy, the only substantial difference between the phases is the grain size. It will be shown that many of the material properties necessary to determine the mechanical properties can be described by a "rule of mixtures" behavior, such that any property, P, depends on the properties of the CG and NC phases (P_{CG}) and P_{NC}, respectively), and the volume fractions of each phase (f_{CG} and f_{NC}) through $P = f_{CG}P_{CG} + f_{NC}P_{NC}$. These properties include yield stress (σ_y), strain-hardening exponent (n) and a newly defined ductility parameter (A) that will be addressed later. σ_y depends on the strengthening mechanisms that are active in the material. In multiphase materials, such as precipitation-hardened alloys or metal-matrix micro- and nanocomposites, there is a significant difference in the properties of each phase. However, for the bimodal alloys processed by the PM technique, strengthening mechanisms that rely on differences between the two phases, such as coefficient of thermal expansion strengthening and modulus mismatch strengthening, are not likely to affect the yield strength of the mixture. Although Orowan strengthening is intrinsic to metallic alloys, it is unlikely that there is a significant strength difference between the CG and NC phases. Therefore, grain boundary (i.e. Hall–Petch) strengthening remains the primary mechanism actively influencing the strength of the bimodal material.

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To predict the maximum stress and strain to failure for the biomodal materials in our model, it is assumed that (i) the stress–strain behavior in the plastic regime can be described by the classical Hollomon relation [6], and (ii) the material fails at the ultimate tensile or compressive stress (UTS or UCS). An analysis of the experimental data sets [1–5] shows that the second assumption appears to be generally valid in the case of Al-based nano-alloys as failure occurs very near the maximum stress and there is little unstable deformation. When the failure stress ($\sigma_{t-\max}$) considerably deviates from the UTS in other alloy systems, the model can be applied to predict the UTS. It is also assumed that the true yield strain (ε_{t-y}) can be linearly approximated from the yield stress and the elastic modulus, Y. Given the above approximations, the strain-hardening exponent, n, is described by Eq. (1), where $\sigma_{t-\max}$ and $\varepsilon_{t-\max}$ are the true maximum stress (i.e. UTS or UCS) and strain to failure, respectively:

$$n = \frac{\ln \sigma_{t-\max} - \ln \sigma_{t-y}}{\ln \varepsilon_{t-\max} - \ln \varepsilon_{t-y}}. \tag{1}$$

To predict the failure stress and strain, a newly defined ductility parameter, A, serves as the failure criteria in this model. This ductility parameter is defined as the area under the $\ln \sigma_t$ vs. $\ln \varepsilon_t$ curve (where σ_t and ε_t represent the true stress and true strain, respectively) between the yield stress and maximum (i.e. failure) stress as described by the following equation:

$$A = \frac{\ln \sigma_{t-\max} + \ln \sigma_{t-y}}{2}(\ln \varepsilon_{t-\max} - \ln \varepsilon_{t-y}). \tag{2}$$

The strain to failure ($\varepsilon_{t-\max}$) can be determined from Eq. (3), which is a rearrangement of Eq. (2) and makes use of the relation that $\ln \sigma_{t-\max} = \ln \sigma_{t-y} + n \ln(\varepsilon_{t-\max}/\varepsilon_{t-y})$. When Eq. (3) is solved for a positive root, $\varepsilon_{t-\max}$ is then a function of the true yield stress (σ_{t-y}) and strain (ε_{t-y}) as well as n and A according to Eq. (4).

$$\ln \frac{\varepsilon_{t-\max}}{\varepsilon_{t-y}} = \frac{2A}{2 \ln \sigma_{t-y} + n \ln \frac{\varepsilon_{t-\max}}{\varepsilon_{t-y}}} \tag{3}$$

$$\begin{aligned} \varepsilon_{t-\max} &= \varepsilon_{t-failure} \\ &= \varepsilon_{t-y} \exp\left(\frac{-\ln \sigma_{t-y} + \sqrt{(\ln \sigma_{t-y})^2 + 2nA}}{n}\right). \end{aligned} \tag{4}$$

The failure stress ($\sigma_{t-\max}$) can be predicted using the same assumptions as listed above and is also a function of σ_{t-y} and ε_{t-y} as well as n and A given by the following equation:

$$\begin{aligned} \sigma_{t-\max} &= \sigma_{t-failure} \\ &= \sigma_{t-y} \exp(-\ln \sigma_{t-y} + \sqrt{(\ln \sigma_{t-y})^2 + 2nA}). \end{aligned} \tag{5}$$

As stated above, in bimodal nano-alloys, the properties of the material are dominated by grain size dependency and as such: (i) the grain sizes of each phase must be measured or determined, and (ii) the grain-size-dependent behavior of σ_{t-y}, n and A must be described. For Al-5083 materials, average grain sizes were not reported and have therefore been back-calculated using the experimental yield stress and the published Hall–Petch parameters [5]. Based on σ_y of the unimodal CG material reported in Ref. [4], the average diameter of the CG phase was determined to be 127.6 μm. Using the experimental data in Refs. [2–4], it was found that σ_y varies linearly with f_{CG} for materials containing 30 vol.% or greater of the CG phase and can be accurately described by the rule of mixtures if the grain size of the NC phase is ~90 nm. However, there is a definite non-linearity in the trend of σ_y vs. f_{CG} for materials containing less than 30 vol.% CG. Given that the only difference between the two phases is the grain size, it is likely that the non-linearity is the result of an increase in the grain size of the NC phase, D_{NC}. In materials with low CG vol.%, the contiguity of NC phases increases and this increased contact will allow more efficient coarsening of this phase. Figure 1a shows the D_{NC} and D_{CG} variations as a function of CG fraction, f_{CG}, based on Refs. [2–4]. D_{NC} values were back-calculated assuming that (i) the CG phase has a diameter of 127.6 μm and does not coarsen (based on the fact that there is no non-linearity in the CG-rich region of the σ_y versus f_{CG} curve); (ii) the rule of mixtures determines the σ_y behavior; and (iii) σ_y of the NC material is described by the Hall–Petch relation. From Figure 1a, D_{NC} can be empirically determined by $D_{NC} = D_{NC-\min} + (D_{NC-\max} - D_{NC-\min})\ \exp(\frac{-f_{CG}}{f^*_{CG}})$ using the appropriate values for the maximum and minimum NC grain diameters, $D_{NC-\max}$ and $D_{NC-\min}$, and the critical volume fraction of CG phase, f^*_{CG}, from Table 1. $D_{NC-\min}$ was determined to be 91.3 nm using the back-calculated grain size of the NC phase in the range of 30–100 vol.% CG. $D_{NC-\max}$ was determined to be 145.9 nm from the reported yield stress of the unimodal NC material using the Hall–Petch parameters for Al-5083 [5]. Because the same sample material was used for both tension and compression, D_{NC} and D_{CG} in the compression tests are assumed to be the same as in the tensile test. The Hall–Petch data for compression was determined from a plot of compressive σ_y vs. $D^{-1/2}$ for the unimodal NC and CG materials as reported in Refs. [1,3]. Using the rule of mixtures, the NC contribution to A and n can be back-calculated. Figure 1b shows the dependence of A and n on $D^{-1/2}$ for the material tested in tension, where the solid lines in Figure 1b indicate the trend lines of A and n as a function of $D^{-1/2}$ using linear regression. The strain-hardening exponent clearly follows a Hall–Petch-like dependence on grain size described by $n = n_o + K_n/\sqrt{D}$, where n_o and K_n are the strain-hardening exponent for an infinitely large grain and the corresponding Hall–Petch constant, respectively. Moreover, the ductility parameter, A, also clearly follows a Hall–Petch-like grain size dependence. Similar behavior was exhibited by samples in compression, and based on the regression lines for both tension and compression, the Hall–Petch parameters in Table 1 (A_o, K_A, n_o and K_n) were determined. Based on this analysis, it is possible to calculate A and n for each phase and use the rule of mixtures to determine A and n for any combination of f_{NC} and f_{CG}. Having determined σ_{t-y}, A, and n, Eqs. (4) and (5) can be used to predict the failure stress and strain.

Based on the model parameters in Table 1 and the empirical expression of D_{NC}, Figure 2 shows the rule of mixtures predictions for A and n (dotted lines) as a