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나노결정 알루미늄의 기계적 거동 (II): 모델링

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Mechanical Behavior of Nanocrystalline Aluminum (II) : Modeling

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Abstract

The responses of nanocrystalline aluminum powder of different grain sizes, was modeled Using, Khan, Huang, and Liang (KHL) viscoplastic model including bi-linear Hall-Petch type, based on experimental measurements. Correlation of strain-rate-dependent stress responses for different grain sizes were in good agreement with the experimental results.

Key Words : Nanocrystalline Aluminum, Dynamic Viscoplastic Response, Split-Hopkinson Bar, Constitutive Modeling, Modified Hall-Petch Relation

1. Introduction

The strength of micro- and nanocrystalline metallic materials have been mainly modeled [1-2] by classical Hall-Petch relation expressed as follows:

$$\sigma_Y = \sigma_0 + \frac{k}{\sqrt{d}} \qquad (1)$$

where σ_Y is the yield stress, and σ_0 is the friction stress needed to move individual dislocations. k and d are a constant and the grain size, respectively. Thus, the yield stress increases linearly with the decrease of grain size. The predicted grain size dependence of the stress-strain curves were in reasonable agreement with experimental results.

When the Hall-Petch relation is used for materials with only nano-size grains, an anomaly may be encountered; namely negative intercept on stress axis if this linear relationship is extrapolated to relatively large grain regimes (micro-size or larger). Khan *et al.* [3] Bonetti *et al.* [4] for aluminum and Lloyd [5], in case of aluminum-nickel alloy, observed that the slope of the curve in the coarse-grain-size regime is smaller than that in the fine-grain-size regime, and is similar to the present observation for pure aluminum. Gray *et al.* [6] observed similar Hall-Petch slopes for fine-grained Cu and Ni, and observed that these slopes are greater than those of the corresponding polycrystalline materials. This deviation may be attributed to the changes in deformation mechanism. The deformation mechanisms for micro-size or larger grains are established to involve dislocations and/or twinning. In the nano-range, the deformation mechanism is believed to be due to either grain boundary sliding, or twinning [7]. The negative intercept of a single Hall-Petch slope not only leads to poor correlation of the yield stress but also to a negative friction stress that is physically unreasonable.

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In this investigation, based on a comprehensive response over a wide range of strain rates from nanocrystalline aluminum powders [3], a modified Khan, Huang, and Liang (KHL) viscoplastic model from previous works [1-2] is proposed. This new model includes bi-linear Hall-Petch relation that resolves the negative intercept anomaly. This model is correlated and compared with the experimental results. It includes the grain size, temperature, and strain-rate dependency of the flow stress as a function of the effective plastic strain.

2. Constitutive Model for Viscoplastic Response

In order to model the viscoplastic stress response using a bilinear Hall-Petch relation, the KHL model was modified [1-2]. The original model used for materials with grain size in a macro range, is expressed as follows [8]:

$$\sigma = [A + B(1 - \frac{\ln \dot{\varepsilon}}{\ln D_0^p})^{n_1} (\varepsilon^p)^{n_0}](\frac{\dot{\varepsilon}}{\dot{\varepsilon}^*})^C (\frac{T_m - T}{T_m - T_r})^m \quad (2)$$

where σ is the flow stress and ε^p is the plastic strain. T_m, T, T_r are melting, current, and reference temperatures in Kelvin, respectively. $D_0^p = 10^6$ s^{-1} is an arbitrarily chosen upper bound strain rate in most applications and $\dot{\varepsilon}^* = 1$ s^{-1}. $\dot{\varepsilon}$ is the current strain rate. A, B, n_1, n_0, C and m are material constants. Since the constant A is closely related with the yield stress, this term was modified earlier for nanocrystalline materials by Khan *et al.* [1], where A was replaced by the conventional Hall-Petch relation as given by equation (2).

$$a_0 + \frac{k_0}{\sqrt{d}} \quad (3)$$

This modification, however, had limited application when the grain size was nano-meter range [1]. In order to extend the application to grain size in micro-meter and larger range, this term was appropriately replaced by a bilinear approximation.

It was found from the experiments [3] that, yield stress (σ_Y) vs. inverse square root of grain size ($d^{-0.5}$) data for nanocrystalline aluminum are approximated by a single Hall-Petch relation with negative intercepts on the stress axis; the correlation with experimental data is very poor. Similar pattern is observed for nanocrystalline iron [1], although with a small positive magnitude of intercept in this case. This pattern is not appeared for nanocrystalline iron but can be found for nanocrystalline aluminum [3], Al-6Ni [4], Cu, Ni [5], and Ni [9]. The experimental data clearly suggests a bilinear approximation. Therefore, bi-linear type Hall-Petch relation is introduced:

$$\alpha_1 + \frac{\beta_1}{\sqrt{d}} \quad \text{for} \quad 0 \le d^{-0.5} \le d^{*-0.5} \quad (4)$$

$$\alpha_2 + \frac{\beta_2}{\sqrt{d}} \quad \text{for} \quad d^{*-0.5} \le d^{-0.5}$$

where d^* is a reference grain size at which the yield stress starts to increase appreciably. α_1, α_2, β_1 and β_2 are constants determined from the linear regression of yield stress (σ_Y) vs. inverse square root of grain size ($d^{-0.5}$) data. In this investigation, expression shown in equation (3) was included in KHL model by replacing yield stress term (A) to predict viscoplastic stress response of the nanocrystalline materials. The modified KHL model given by:

$$\sigma = (a + \frac{k}{\sqrt{d}})[1 + \frac{B}{a}(1 - \frac{\ln \dot{\varepsilon}}{\ln D_0^p})^{n_1} (\varepsilon^p)^{n_0}](\frac{\dot{\varepsilon}}{\dot{\varepsilon}^*})^C (\frac{T_m - T}{T_m - T_r})^m \quad (4)$$

The model now allows the grain size to influence both the yield stress and work hardening at different strain rates. The constant B has been replaced by B/a ($\equiv B^*$) so that the model reproduces original expression mathematically, as the grain size d becomes very large.

3. Results and Discussion

In order to a set of material constants, non-linear least squares calculation was performed to optimally correlate the multiple data sets for a grain size of 60 nm at strain rates of 1 s^{-1} and 0.0001 s^{-1}, and 40, 50, 60, 80 nm at a strain rate of 0.0001 s^{-1} for nanocrystalline aluminum [3]. The refined material is shown at the presentation. The modified constants are due to the extension of the model to include variation in work hardening due to different grain size. Correlated curves for various grain sizes of nanocrystalline aluminum are shown in the presentation. In most cases, the correlations are in good agreement with the measured data. Furthermore, dynamic data using Split-Hopkinson bar were predicted based on the material constants determined from the refined correlation. Although the high strain rate loading invokes adiabatic deformation, this was neglected in the prediction since only the small deformation was involved such that the heat generation due to high-speed plastic deformation may be considered small. Predictions of dynamic response for nanocrystalline aluminum with the modified KHL model are shown in the presentation. Considering that the measurement at the earlier stage of the Split Hopkinson Pressure Bar test usually includes errors due to non-balance of forces on the two faces of a specimen, and the thermal softening due to heat generated during plastic deformation was neglected in the calculation, the agreement with experimental results is considered reasonable.

4. Conclusions

In order to avoid negative or excessively low friction stresses in the prediction of nanocrystalline aluminum, an unconventional bi-linear Hall-Petch relation was introduced. This expression gave a good correlation with experimental observation [3], as compared to the conventional Hall-Petch relation in the entire range of grain sizes. This bi-linear expression was implemented into the KHL model in order to correlate the viscoplastic stress response of nanocrystalline aluminum. The stress responses from the quasi-static loading under different grain size and strain rates were compared with other experimental observations using material constants that were optimized by the nonlinear least-squares fit. The correlations and prediction were found to be in good agreement with experimental results.

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