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Constitutive Behavior of Nanocrystalline Bimodal Materials Postprint

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Date: 2023-03-18T00:00:00+00:00

Abstract

Nanocrystalline bimodal materials composed of micron-scale coarse-grained particles and nano-scale nanocrystalline particles exhibit not only high strength but also enhanced ductility. A new constitutive model for nanocrystalline bimodal materials is proposed based on Taylor strength theory and the Johnson-Cook model to investigate the influence of grain size and nanocracks on the constitutive and failure behavior of nanocrystalline bimodal materials, with numerical calculations conducted. The results indicate that model predictions show good agreement with experimental results. The computational results reveal that: in nanocrystalline bimodal materials, the nanocrystalline matrix provides high strength, while coarse grains effectively enhance material ductility; the presence of nanocracks does not cause failure but rather plays a positive role in strain hardening.

Full Text

Constitutive Behavior of Bimodal Nanocrystalline Materials

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Abstract

Bimodal nanocrystalline (BNC) materials composed of micrometer-sized coarse grains (CG) and nanometer-sized nanocrystalline grains (NG) exhibit both high strength and enhanced ductility. This paper proposes a new constitutive model for BNC materials based on Taylor strength theory and the Johnson-Cook model to investigate the effects of grain size and nano-cracks on the constitutive and failure behavior of these materials, with numerical calculations performed accordingly. The results demonstrate excellent agreement between model predic-

tions and experimental data. The calculations reveal that in BNC materials, the nanocrystalline matrix provides high strength while coarse grains effectively improve ductility, and the presence of nano-cracks does not cause failure but rather plays a positive role in strain hardening.

Key words metal materials, constitutive behavior, bimodal nanocrystalline materials, Taylor strength theory, Johnson-Cook model

Introduction

Nanocrystalline materials (with grain sizes below 100 nm) exhibit exceptional mechanical properties such as high strength and wear resistance due to their unique microstructure. However, the ductility of nanocrystalline materials decreases with reducing grain size, limiting their engineering applications. Over the past two decades, numerous methods have been proposed to enhance the ductility of nanocrystalline materials, among which constructing bimodal nanocrystalline materials—embedding micrometer-sized coarse grains in a nanocrystalline matrix—has proven effective. In such structures, the grain size distribution follows a statistical bimodal pattern, with the probability density function displaying distinct peaks. The nanocrystalline matrix provides high strength, while coarse grains improve ductility.

During the past two decades, extensive research has investigated the mechanical properties and deformation mechanisms of bimodal nanocrystalline materials, qualitatively confirming that bimodal grain size distributions enhance ductility. For instance, Wang et al. prepared bimodal nanocrystalline copper containing 25% coarse grains (by volume) that achieved 30% uniform elongation while maintaining high strength. Shen et al. produced bimodal nanocrystalline nickel via direct current electrodeposition, demonstrating high ultimate strengths of 1440–1916 MPa and ductility of 5.6%–11.3%, attributing the improved ductility to enhanced strain hardening capacity. Fan et al. studied the plastic deformation and fracture behavior of ultrafine-grained bimodal Al-Mg alloys, finding highly localized plastic deformation with fracture controlled by shear localization, void formation, and necking in tension. Han et al. investigated the deformation behavior of bimodal nanocrystalline 5083Al alloys, observing that tensile ductility increased while strength decreased with increasing coarse grain volume fraction, primarily due to crack bridging and delamination between nanocrystalline and coarse grain regions during plastic deformation.

Despite numerous studies on bimodal nanocrystalline materials, theoretical modeling and quantitative analysis remain limited. Ovid'ko et al. developed a theoretical model to study crack initiation in BNC materials but did not consider constitutive behavior or establish reliable constitutive relationships. Zhu et al. established two statistical models to investigate strength and ductility, showing that micro-cracks do not cause failure and that back stress from micro-cracks enhances strain hardening capacity, though their model did not address

crack propagation. The authors' research group previously developed a constitutive model based on strain gradient plasticity theory, but it did not consider nano-crack effects or fracture behavior. To thoroughly investigate the constitutive behavior and fracture performance of BNC materials, this paper establishes a new theoretical model combining Taylor strength theory and the Johnson-Cook plasticity model, comprehensively considering grain size distribution, coarse grain volume fraction, nano-cracks, and dislocation emission from crack tips to quantitatively describe the constitutive behavior and failure strain of BNC materials.

1. Constitutive Model for Bimodal Nanocrystalline Materials

The BNC materials described in this paper consist of micrometer-sized coarse grain regions embedded in a nanocrystalline matrix. Based on literature, coarse grains are dispersed within the nanocrystalline matrix. The actual grain structure and distribution in fabricated BNC materials are complex and difficult to describe mathematically. For simplicity, this model assumes uniformly distributed coarse grains in the nanocrystalline matrix, as shown in [Figure 1: see original paper]. Taylor strength theory is applied to describe the constitutive behavior of BNC materials.

1.1 Taylor Strength Theory

According to Taylor strength theory, strain hardening in materials originates from dislocation slip in both coarse and nanocrystalline grains, with flow stress expressed as:

$$\sigma_{\text{flow}} = M\alpha\mu b\sqrt{\rho}$$

where α , μ , and M are the Taylor constant, shear modulus, and Taylor factor, respectively; b is the Burgers vector; and ρ represents the total dislocation density in both coarse and nanocrystalline grains. Through a simple rule of mixtures:

$$\rho = f_{NG}\rho_{NG} + f_{cg}\rho_{cg}$$

where f_{NG} and f_{cg} are the volume fractions of nanocrystalline and coarse grains, respectively, and ρ_{NG} and ρ_{cg} are the corresponding dislocation densities. In dislocation-controlled plastic deformation mechanisms, the density of statistically stored dislocations is determined by dislocation emission and annihilation. Based on the Kocks-Mecking model and Capolungo model, the relationship between dislocation density and plastic strain is:

$$\frac{d\rho}{d\varepsilon_p} = \frac{k}{d} - \psi\rho$$

where ε_p is plastic strain; ψ is a proportionality factor; d represents grain size (coarse grain size when calculating ρ_{cg} , nanocrystalline grain size when calculating ρ_{NG}); and k is a material constant.

1.2 Effect of Nano-Cracks on Constitutive Behavior

During plastic deformation of BNC materials, numerous cracks nucleate in grain boundary regions of the nanocrystalline phase, as shown in [Figure 2: see original paper]. These cracks increase the number of dislocations piled up at grain boundaries, significantly enhancing the back stress effect on flow stress in the nanocrystalline phase. Therefore, considering crack effects on dislocation motion, the back stress influence must be incorporated into the elastoplastic constitutive relationship of the nanocrystalline phase by adding a back stress term to the flow stress, modifying Equation (1). Accounting for nano-crack effects, the flow stress becomes:

$$\sigma_{\text{flow}} = M\alpha\mu b\sqrt{\rho} + \sigma_{\text{back}}$$

where σ_{back} is the back stress arising from dislocation accumulation at grain boundaries emitted from nano-crack tips. The back stress caused by dislocation pile-up can be expressed as:

$$\sigma_{\text{back}} = \frac{N\mu b}{\pi L}$$

where N is the number of dislocations emitted from nano-crack tips. The authors previously developed a model investigating grain boundary sliding and dislocation emission from crack tips on the fracture toughness of nanocrystalline materials. When a cracked specimen is subjected to external loading, stress concentration occurs at the crack tip, causing dislocation emission and slip to grain boundaries where pile-ups form, generating back stress that significantly influences strain hardening in BNC materials.

The number of dislocations emitted from nano-crack tips is given by:

$$N = \rho_{\text{crack}}N^*$$

where ρ_{crack} is nano-crack density and N^* is the maximum number of dislocations emitted from a single crack tip. Literature defines crack density as:

$$\rho_{\text{crack}} = \rho_0(1 - \exp[-(\varepsilon_p/\varepsilon_0)^m])$$

where ρ_0 is reference crack density and m is a parameter. The critical stress intensity factor is:

$$K_{IC} = \sqrt{\frac{2E\gamma}{1-\nu^2}}$$

where γ is surface energy. The factor D related to grain size distribution can be expressed as:

$$D = \frac{d_{\max} - d_{\min}}{d_{\max} + d_{\min}}$$

where d_{\max} and d_{\min} are maximum and minimum grain sizes.

The N^* in Equation (6) represents the number of dislocations emitted from a crack tip and sliding along one slip plane:

$$N^* = \frac{K_{IC}\sqrt{\pi r}}{2\pi\tau_{IC}\sin\theta} \left(\cos\frac{\theta}{2} + 1 \right)$$

where θ is the angle between dislocation emission direction and crack propagation direction, ν is Poisson's ratio, and r is dislocation core radius. Equation (10) shows that N^* depends on the critical stress intensity factor K_{IC} and θ . [Figure 3: see original paper] illustrates the relationship between critical stress intensity factor K_{IC} and θ . For simplicity, this paper considers only dislocation emission at $\theta = 70^\circ$, where K_{IC} reaches its maximum. According to literature, the relationship between maximum dislocation number N^* and grain size d is shown in [Figure 4: see original paper].

2. Johnson-Cook Model

The Johnson-Cook model comprises two components: a strength model describing material deformation under high strain rates and elevated temperatures, and a failure model establishing relationships between strain, strain rate, temperature, hydrostatic pressure, and fracture strain. As an empirical model with simple form and few parameters easily obtained through experimental data fitting, the JC model has been widely implemented in various dynamic finite element software packages.

The JC strength model takes the basic form:

$$\sigma = (A + B\varepsilon_p^n) \left[1 + C \ln \frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} \right] \left[1 - \left(\frac{T - T_r}{T_m - T_r} \right)^m \right]$$

where A is yield strength; B , n , C , and m are material constants; $\dot{\epsilon}$ is equivalent plastic strain rate; $\dot{\epsilon}_0$ is reference strain rate (taken as 1 s^{-1}); T is temperature; T_r is reference temperature (typically room temperature); and T_m is melting temperature. The three terms represent strain hardening, strain rate hardening, and thermal softening effects, respectively. Parameters A , B , and n can be obtained by fitting data from the second part of the model.

The JC failure model considers the effects of stress triaxiality, strain rate, and temperature on failure strain, proposing a linear incremental relationship between damage parameter D and equivalent plastic strain increment:

$$D = \int \frac{d\epsilon_p}{\epsilon_f}$$

where ϵ_f is failure strain. This indicates that damage accumulates linearly with plastic deformation, with failure occurring when D reaches 1. Failure strain is defined as:

$$\epsilon_f = [D_1 + D_2 \exp(D_3 \sigma^*)] \left[1 + D_4 \ln \frac{\dot{\epsilon}}{\dot{\epsilon}_0} \right] (1 + D_{5T}^*)$$

where D_1 - D_5 are material constants and P is hydrostatic pressure. For simplicity, the current model neglects temperature rise (thermal softening) and assumes constant external loading, giving $d\sigma^*/d\epsilon_p = 0$. Thus, failure strain simplifies to:

$$\epsilon_f = \frac{D_1 + D_2}{1 + D_4 \ln(\dot{\epsilon}/\dot{\epsilon}_0)}$$

3. Results and Discussion

To further understand the constitutive relationships and failure behavior of BNC materials, numerical calculations were performed for nanocrystalline Cu-Ag composites using the proposed model. In this Cu-Ag material, silver serves as the coarse grain phase uniformly distributed in the nanocrystalline copper matrix. Model parameters are listed in .

3.1 Stress-Strain Curves

The constitutive and failure behavior of nanocrystalline Cu-Ag materials was predicted using Taylor strength theory and the Johnson-Cook model. The model first calculated the constitutive relationship, considering the effects of nanocrystalline matrix grain size and coarse grain volume fraction. With coarse grain volume fraction and grain size fixed at 20% and 2.5 μm , respectively, the constitutive relationship was determined and parameters were obtained through

fitting. For the Johnson-Cook model, when nanocrystalline grain size is 23 nm, n is 0.13; for the coarse grain part, n is 0.54 and d is 0.014.

[Figure 5: see original paper] shows the constitutive relationship for various nanocrystalline grain sizes. Material tensile strength increases with decreasing nanocrystalline grain size. For example, when grain size increases from 23 nm to 74 nm, strength decreases by 19.53%, demonstrating that strength improves through grain refinement. Simultaneously, ductility increases by 12.18% due to increased statistically stored dislocation density with larger grain sizes, though the modest size increase yields only slight ductility improvement. With coarse grain and nanocrystalline grain sizes fixed at 2.5 μm and 23 nm, respectively, the constitutive relationships for materials with different coarse grain volume fractions were calculated, as shown in [Figure 6: see original paper]. Tensile strength decreases with increasing coarse grain volume fraction. When coarse grain content increases from 10% to 30%, tensile strength decreases by only 2.44% while ductility increases substantially by 42.2%. These results demonstrate that in BNC materials, the nanocrystalline matrix provides high strength while the coarse grain phase enhances ductility, with increasing coarse grain fraction significantly improving ductility at minimal strength cost. All constitutive curves exhibit distinct hardening stages, consistent with uniaxial tensile test results for BNC materials. In coarse grains, larger intergranular distances provide fewer obstacles to dislocation slip, making dislocation motion easier and enabling greater dislocation accumulation, thereby contributing to enhanced ductility.

3.2 Effect of Nano-Cracks on Constitutive Behavior

The influence of nano-cracks on the constitutive relationship and dynamic strain hardening of BNC materials was investigated. Nano-cracks alter stress and strain fields, with crack tip stress concentration causing dislocation emission that slides to grain boundaries forming pile-ups, generating the back stress in Equation (1). Calculation results are presented in [Figure 7: see original paper], showing that back stress has negligible effect on yield strength but positively influences dynamic strain hardening.

3.3 Comparison with Experimental Results

To validate the theoretical model, nanocrystalline bimodal Cu-Ag materials were prepared by high-temperature and high-pressure sintering. Copper and silver powders with average grain sizes of 20 nm and 5 μm were mechanically mixed for 4 hours, then sintered at 5 GPa and 700°C. The XRD spectrum of the sintered specimen is shown in [Figure 8: see original paper], from which the nanocrystalline matrix grain size was calculated as 47.18 nm. Microstructure and morphology are shown in [Figure 9: see original paper], confirming that copper and silver did not form intermetallic compounds, satisfying the required bimodal distribution.

Uniaxial tensile tests were conducted on the nanocrystalline bimodal Cu-Ag

materials to validate the theoretical predictions. [Figure 10: see original paper] compares theoretical and experimental results, demonstrating excellent agreement in yield strength and work hardening rate. This confirms that the proposed theoretical model can effectively describe the constitutive and fracture behavior of BNC Cu-Ag materials.

Conclusions

1. The strength of nanocrystalline bimodal Cu-Ag materials increases with decreasing nanocrystalline grain size. Ductility increases while strength decreases with increasing coarse grain volume fraction. Nano-cracks do not cause premature failure; the back stress they generate positively affects dynamic strain hardening.
 2. Theoretical predictions using the proposed model show excellent agreement with experimental results, demonstrating its capability to describe both constitutive behavior and fracture behavior of bimodal nanocrystalline materials.
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References

1. Y. G. Liu, J. Q. Zhou, D. Hui, A strain-gradient plasticity theory of bimodal nanocrystalline materials with composite structure, *Composites Part B*, 43, 249 (2012)
2. V. L. Tellkamp, A. Melmed, E. J. Lavernia, Mechanical Behavior and Microstructure of a Thermally Stable Bulk Nanostructured Al Alloy, *Mater. Trans. A*, 32, 2335 (2001)
3. S. Billard, J. P. Fondere, B. Bacroix, G. F. Dirras, Macroscopic and microscopic aspects of the deformation and fracture mechanisms of ultrafine-grained aluminum processed by hot isostatic pressing, *Acta Mater.*, 54, 411 (2006)
4. U. F. Kocks, H. Mecking, Physics and phenomenology of strain hardening: the FCC case, *Prog. Mater. Sci.*, 48, 171 (2003)
5. L. Capolungo, C. Jochum, M. Cherkaoui, J. Qu, Homogenization method for strength and inelastic behavior of nanocrystalline materials, *Int. J. Plast.*, 21, 67 (2005)
6. C. C. Koch, D. G. Morris, K. Lu, A. Lnoue, Ductility of nanostructured materials, *MRS Bull.*, 24, 54 (1999)
7. G. He, J. Eckert, W. Loser, L. Schultz, Novel Ti-base nanostructured-dendrite composite with enhanced plasticity, *Nat. Mater.*, 2, 33 (2002)

8. M. Dao, L. Lu, R. J. Asaro, J. T. M. D. Hosson, E. Ma, Toward a quantitative understanding of mechanical behavior of nanocrystalline metals, *Acta Mater.*, 55, 4041 (2004)
9. Y. Wang, M. Chen, F. Zhou, E. Ma, High tensile ductility in a nanostructured metal, *Nature*, 419, 912 (2002)
10. L. L. Zhu, S. Q. Shi, K. Lu, J. Lu, A statistical model for predicting the mechanical properties of nanostructured metals with bimodal grain size distribution, *Acta Mater.*, 60, 5762 (2012)
11. I. A. Ovid'ko, A. G. Sheinerman, Ductile vs. brittle behavior of pre-cracked nanocrystalline and ultrafine-grained materials, *Acta Mater.*, 58, 5286 (2010)
12. L. L. Zhu, S. Q. Shi, K. Lu, J. Lu, A statistical model for predicting the mechanical properties of nanostructured metals with bimodal grain size distribution, *Int. J. Plast.*, 30, 166 (2012)
13. Y. G. Liu, J. Q. Zhou, D. Hui, A strain-gradient plasticity theory of bimodal nanocrystalline materials with composite structure, *Composites Part B*, 43, 249 (2012)
14. S. Billard, J. P. Fondere, B. Bacroix, G. F. Dirras, Macroscopic and microscopic aspects of the deformation and fracture mechanisms of ultrafine-grained aluminum processed by hot isostatic pressing, *Acta Mater.*, 54, 411 (2006)
15. V. L. Tellkamp, A. Melmed, E. J. Lavernia, Mechanical Behavior and Microstructure of a Thermally Stable Bulk Nanostructured Al Alloy, *Metall. Mater. Trans. A*, 32, 2335 (2001)
16. B. Q. Han, E. J. Lavernia, F. A. Mohamed, Mechanical properties of nanostructured materials, *Rev Adv Mater Sci*, 9, 1 (2005)
17. B. Q. Han, J. Y. Huang, Y. T. Zhu, E. J. Lavernia, Strain rate dependence of properties of cryomilled bimodal 5083 Al alloys, *Acta Mater.*, 54, 3015 (2006)
18. B. Q. Han, E. J. Lavernia, Z. Lee, S. Nutt, D. Witkin, Deformation behavior of bimodal nanostructured 5083 Al alloys, *Metall. Mater. Trans. A*, 36, 957 (2005)
19. Y. G. Liu, J. Q. Zhou, D. Hui, A strain-gradient plasticity theory of bimodal nanocrystalline materials with composite structure, *Composites Part B*, 43, 249 (2012)
20. H. P. Klug, L. E. Alexander, *X-ray Diffraction Procedures: For Polycrystalline and Amorphous Materials*, 2nd ed., Wiley, New York (1974), p. 625
21. Y. G. Liu, J. Q. Zhou, D. Hui, A strain-gradient plasticity theory of bimodal nanocrystalline materials with composite structure, *Composites*

- Part B, 43, 249 (2012)
22. D. N. Zhang, Q. Q. Shangguan, C. J. Xie, F. Liu, A modified Johnson-Cook model of dynamic tensile behaviors for 7075-T6 aluminum alloy, *J. Alloys Compd.*, 619, 186 (2015)
 23. H. Y. Zhan, G. Wang, D. Kent, M. Dargusch, Constitutive modelling of the flow behaviour of a β titanium alloy at high strain rates and elevated temperatures using the Johnson-Cook and modified Zerilli-Armstrong models, *Mater. Sci. Eng., A*, 612, 71 (2014)
 24. M. Wang, L. Lei, Nanosintering mechanism of MgAl₂O₄ transparent ceramics under high pressure, *Mater. Chem. Phys.*, 123, 529 (2010)
 25. H. P. Klug, L. E. Alexander, *X-ray Diffraction Procedures: For Polycrystalline and Amorphous Materials*, 2nd ed., Wiley, New York (1974), p. 625
 26. Y. G. Liu, J. Q. Zhou, D. Hui, A strain-gradient plasticity theory of bimodal nanocrystalline materials with composite structure, *Composites Part B*, 43, 249 (2012)
 27. M. Wang, L. Lei, Nanosintering mechanism of MgAl₂O₄ transparent ceramics under high pressure, *Mater. Chem. Phys.*, 123, 529 (2010)
 28. H. P. Klug, L. E. Alexander, *X-ray Diffraction Procedures: For Polycrystalline and Amorphous Materials*, 2nd ed., Wiley, New York (1974), p. 625
 29. Y. G. Liu, J. Q. Zhou, D. Hui, A strain-gradient plasticity theory of bimodal nanocrystalline materials with composite structure, *Composites Part B*, 43, 249 (2012)

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