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MODELING OF THE SLIP-TWINNING TRANSITION IN NANOCRYSTALLINE NICKEL AND NICKEL-TUNGSTEN UNDER SHOCK COMPRESSION

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Abstract. A constitutive description of the slip-to-twinning transition, based on the critical shear stress, is applied to determine the twinning transition pressures in nanocrystalline nickel and nickel-tungsten (13 at. %) under shock compression. The model predicts a critical transition pressure of 78 GPa in 30 nm Ni and 16 GPa in 10 nm Ni-W. These predicted results are in good agreement with laser shock experiments carried out on the same materials.

Keywords: Shock compression, laser shock, isentropic compression, nanocrystalline nickel.
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INTRODUCTION

The two most common mechanisms of plastic deformation in metals are slip (or dislocation motion) and deformation twinning; slip is by far more frequent than twinning. Slip involves the sliding of atomic planes past each other, whereas twinning is a process where a region of the crystal undergoes a homogeneous shear such that the original crystal structure is reestablished in a new orientation. Twinning generally occurs at low temperatures, high shear-loading rates, and in conditions where there are few slip systems available to accommodate plastic deformation. The aim of this contribution is to provide a constitutive description of the onset of twinning in nanocrystalline nickel and nickel-tungsten subjected to shock compression. The parameters affecting the twinning transition will be discussed, followed by modeling of the onset of twinning. Predictions of the model will be compared to experimental work carried out on the same material at the Lawrence Livermore National Laboratory by Wang et. al. [1, 2]

Temperature, strain-rate and grain-size effects

Despite the fact that dislocation activity is directly associated with the twinning phenomenon, dislocation motion is very sensitive to strain rate and temperature, whereas twinning is much less sensitive to these parameters [3]. In the analysis on the onset of twinning in nanocrystalline nickel and nickel-tungsten that follows, it is assumed that the twinning shear stress is insensitive to temperature, pressure and strain rate.

The slip behavior of Ni is modeled via the Zerilli-Armstrong constitutive description, which captures the essential physical phenomena:

$$\sigma_{slip} = \sigma_G + C_2\varepsilon^n \exp(-C_3T + C_4T \ln\dot{\varepsilon}) + k_s d^{-1/2} \qquad (1)$$

where, σ_G =48.4 MPa, C_2 =2.4 GPa, C_3=0.0028 K^{-1}, C_4 =0.000115 K^{-1}, and k_S =0.2 MN/m$^{3/2}$ [4]. The strain-hardening exponent n of the nc Ni samples was simply equated to 0 as determined by measurements carried out on the same material by Choi et al. [5]. The values of C_3 and C_4 used are those for copper since data on Ni was not available. Stress-strain plots of nickel with micrometer sized grains were utilized to establish C_2.

The dependence of shock pressure on strain rate for Ni, obtained through the Swegle-Grady relationship, is not available in the literature. As an approximation, the S-G description for copper is adopted since Al and Cu, both FCC metals, have a comparable strain-rate response to shock pressure even though the stacking fault energy of Al is much higher. Thus, the S-G relationship for Ni is given as follows [6]:

$$\dot{\varepsilon} = 7.84 \times 10^{-33} \times P_{shock}{}^{4} \qquad (2)$$

Both plastic strain by slip (and associated work hardening) and shock heating alter the flow stress of a material by slip processes and are incorporated into the computation. The pressure dependence on strain, determined from Rankine-Hugoniot equations and equations of state is expressed as follows [6]:

$$P_{shock} = \frac{C_0{}^2 (1 - e^{\varepsilon})}{V_o [1 - S(1 - e^{\varepsilon})]^2} \qquad (3)$$

The associated temperature rise in Ni as a function of shock pressure is given by the equation [6]:

$$T_{shock} = 8 \times 10^{-20} \times P_{shock}^{2} + 9 \times 10^{-10} \times P_{shock} + 301.5K \quad (4)$$

The effect of grain size on the twinning stress has been found to be greater than that on the slip stress for many metals and alloys [7]. A Hall-Petch relationship can, thus, be ascribed to the twinning stress:

$$\sigma_T = \sigma_{To} + k_T d^{-1/2} \qquad (5)$$

where k_T is the twinning Hall-Petch slope (higher than the k_S slope for slip), σ_{To} is the initial twinning stress assumed for a monocrystal $\left(\lim_{d \Rightarrow \infty} (d^{-1/2}) = 0 \right)$, and d is grain size. In the present modeling, it is assumed that k_T for nickel is approximately three times k_S [8].The twinning H-P slope was, thus, assumed to be 0.6 MN/m$^{3/2}$. Haasen [9] carried out tensile tests on mono-crystalline Ni and observed twinning at shear stresses of 250-280 MPa, which is equivalent to a normal stress, σ_{T_o}, of 500-560 MPa.

Solid-solution strengthening and stacking-fault energy effects

Solid-solution strengthening and stacking-fault energy effects are incorporated into the slip-twinning model as a result of alloying with tungsten. The addition of solute atoms hinders the movement of dislocations, hence, creating a strengthening effect. Alloying also significantly reduces the stacking fault energy, γ_{SF}, as it alters the difference in the free energy between the HCP (stacking fault ribbon) and FCC structure and, therefore, the energy of the ribbon between two partials as well as their separation.

It is well-established in the literature that the twinning stress, τ_T, varies with stacking-fault energy. Venables [10] and Vöhringer [11] performed extensive analysis on the twinning stress for a number of alloys and found that it varies with the square root of the stacking-fault energy:

$$\tau_T = k \left(\frac{\gamma_{sf}}{G b_S} \right)^{1/2} \qquad (6)$$

where, k is a proportionality constant, G is the shear modulus, and b_S is the Burgers vector of a partial dislocation. Equation (6) has been incorporated into our analysis.

MODELING OF SLIP-TO-TWINNING TRANSITION

Nanocrystalline Nickel

In this analysis, it is assumed that the transition from slip to twinning occurs when the shear stress for twinning, τ_T, becomes equal to or less than the shear stress for slip, τ_S:

$$\tau_T \le \tau_S \qquad (7)$$

If one uses the same conversion parameters:

$$\sigma_T \le \sigma_S \qquad (8)$$

This is a reasonable approximation since both mechanisms are subjected to the same stress system at the shock front. It should be mentioned that the criterion described here is based on the critical shear stresses for slip and twinning; the pressure only enters insofar as it determines the shear stress and strain rate. Fig. 1 shows both the slip stress, σ_S, and the twinning stress, σ_T, as a function of pressure. The slip-twinning transition pressure for nickel having a grain size of 30nm was found to be ~ 78 GPa.

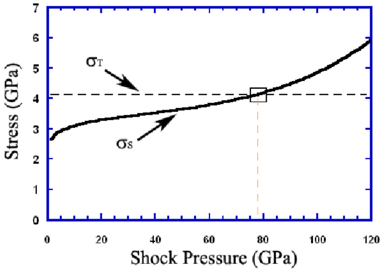

Figure 1: Slip and twinning stress vs. shock pressure for 30 nm nickel; twinning threshold ~78 GPa.

Nanocrystalline Ni-W, 13 at. %

Roth et al. [12]obtained the increase in yield stress in Ni as a result of alloying with different elements. They estimate that the flow stress of Ni increases from 100 MPa to approximately 450 MPa due to the addition of 13 at. % W. The expression for the predicted yield stress increment as the result of alloying is:

$$\Delta\sigma_{SS} = (\sum_i K_i^{1/m} C_i)^m \qquad (9)$$

where, m is 1/2 , K_i is the strengthening constant for solute i, and C_i is the concentration of solute i (for W, K_i =977 MPa at. fraction $^{-1/2}$). The effect of stacking-fault energy on the twinning stress is incorporated into the analysis through Equation (6). A k value of 6.8 GPa was estimated for nickel alloys. At 13 at. % tungsten content (that which is present in the nc Ni-W samples), the shear modulus and stacking-fault energy are 88 GPa and 52.5 mJ/m^2 (60% drop in *SFE*), respectively [13].

The Hall-Petch slope for Ni-W was estimated using yield strength data on Ni-W samples having grain sizes in the micrometer regime and micro-hardness measurements carried out on the nc Ni-W samples. A k_S value of 0.1 MPa/m$^{3/2}$ was estimated (k_T =0.3 MPa/ m$^{3/2}$). Just as in the case of pure Ni, a Hall-Petch behavior accounting for the effect of grain size on the twinning stress is adopted in predicting the critical twinning transition pressure in Ni-W (13 at. %):

$$\sigma_T = k\left(\frac{\gamma_{sf}}{Gb_S}\right)^{1/2} + k_{T_{NiW}} d^{-1/2} \qquad (10)$$

For Ni-13 at. % W, k =6.8 GPa, $k_{T_{NiW}}$ =0.3 MPa, γ_{sf} = 52.5mJ/m^2, G=88 GPa, b_S =0.249nm.

The temperature rise and strain associated with a given shock pressure are determined just as outlined in the case for pure Ni. The Z-A equation as a function of tungsten content is obtained by adding the solid-solution term into the athermal component of stress. The strain hardening exponent, n, for the nanocrystalline Ni-W samples was again equated to 0 [5]. The predicted twinning transition pressure for nc Ni-W, 13 at. %, having a grain size of 10 nm, illustrated in Fig. 2, is equal to 16 GPa.

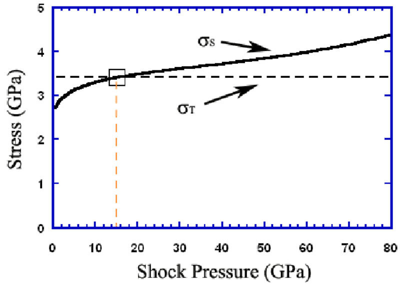

Figure 2: σ_S and σ_T vs. shock pressure for Ni-W (13. at. %), G. S. ~ 10nm, twinning transition ~ 16 GPa.

The twinning-transition pressure as a function of grain-size (micro to nanometer regime) was also calculated. The strain-hardening exponent was varied between n=0.5 in the micrometer regime and n=0 in the nanometer regime. The result is shown in Fig. 3. It clearly shows the much higher transition pressure in Ni as compared to NiW as well as the effect of grain size on the slip-twinning transition.

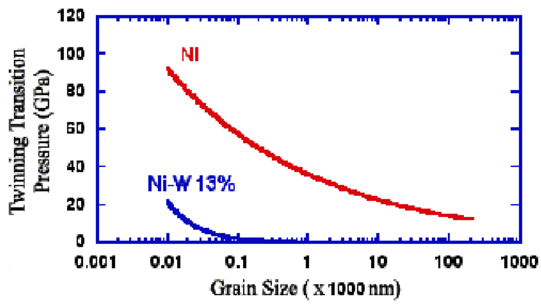

Figure 3: Twinning-transition pressure vs. grain size for Ni and Ni-W, 13 at %.

COMPARISON WITH EXPERIMENTAL RESULTS

Nanocrystalline nickel and nickel-tungsten (13 at. %) samples, prepared by electrodeposition, were shock compressed via a laser technique [1, 2]. The Ni and Ni-W samples had a grain size of 30-50nm and 10-15nm, respectively. The nc Ni samples were subjected to pressures between 20 and 70 GPa, and TEM was carried out as described by Wang et al. [1, 2]. Heavy dislocation activity ($\rho \sim 10^{16}$ m^2) was prevalent in all the samples, indicating that dislocations are a carrier of plasticity. Deformation twins were not present in any of the samples, even at pressures and grain sizes up to 70 GPa and 70 nm, respectively. Fig. 4(a) is a TEM image of a 30-50 nm nickel sample shocked at 40 GPa, showing no evidence of twinning.

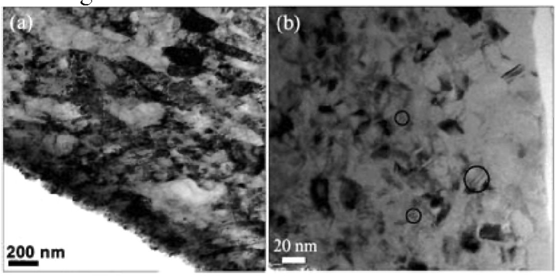

Figure 4: (a) TEM of Ni with G. S. of 30-50 nm shocked at 40 GPa showing dislocations; (b) TEM of Ni-W with G. S. of 10-15 nm shocked at ~40 GPa; deformation twins are evident (circles).

The Ni-W samples, on the other hand, were loaded to ~38 GPa, and a shift in deformation mechanisms was observed. TEM revealed that deformation twins were the predominant defect structures, indicated by circles in Fig. 4(b). A very low density of pre-existing annealing twins was observed in the as-prepared samples. The twin density of shock loaded samples increased dramatically after shock loading.

CONCLUSIONS

An analytical model of the slip-twinning transition in nanocrystalline nickel (GS ~30 nm) under shock compression predicts a critical twinning pressure of 78 GPa, consistent with TEM observations at the same grain size which show no evidence of twinning at shock pressures up to 70 GPa. Instead, dislocations were the main carriers of plasticity. In contrast, conventional polycrystalline Ni (G. S. ~ 100μm) exhibits twinning upon being shock compressed at ~ 30 GPa [14]. On the other hand, the same model applied to nanocrystalline nickel-tungsten (G. S. ~10 nm) under shock compression predicts a critical twinning pressure of 16 GPa. This is consistent with TEM observations showing twin formation in nc Ni-W (G. S. 10-15nm) at a shock pressure of 38 GPa.

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