Towards a full analytic treatment of the Hall-Petch behavior in multilayers: putting the pieces together

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Abstract

There is much interest in the mechanical properties of multilayer films because of their potential as protective coatings. [1]. In multilayers, yielding is governed by the dislocation punching-through mechanism as predicted by Koehler. [2] Multilayers exhibit a size-effect where the mechanical strength is related to the multilayer's compositional wavelength. A full treatment of the Hall-Petch-like size-effect in multilayers is presented that accounts for the following factors: anomalous stress-concentration of dislocations piled up against a layer interface dislocation source characteristics, such as the stress to operate a dislocation source, and a dislocation stopping stress that can vary with layer thickness.[1] The model is the applied to Cu/Ni multilayers.

Model

A semi-analytic integration of these ideas is presented in [3]. This model gives a formula for the resolved yield stress in terms of the stress to operate a dislocation source (σ_c), the height of the "soft" layer (h), the geometric ratio of the pileup length L to the layer height h (β), the stress pinning a dislocation at the layer interface (σ_p), the burgers vector magnitude of the pileup dislocations (b), the scaling exponent (a), the effective shear modulus (μ^*), and a dimensionless number of order unity (k). See [3] for a full description of these parameters. The model is developed via a *divide and conquer* strategy. There are three regimes to examine: (1) dislocation source dominated, (2) dislocations source independent, (3) discrete or single dislocation controlled. In regime (1), the yield stress is simply the stress to activate a dislocation source,

$$\sigma_y = \sigma_c. \tag{1}$$

In regime (2), there is perfect scaling,

$$\sigma_y = \sigma_y^0 = KL^{-a} = k\,\mu^* \left(\frac{\sigma_p}{\mu^*}\right)^{1-a} \left(\frac{\beta h}{b}\right)^{-a}. \tag{2}$$

In regime (3), the yielding is controlled by only a few or even a single dislocation. For a single dislocation, the yield stress is controlled by either Orowan bowing, or by single dislocation transmission,

$$\sigma_y = \sigma_p \tag{3}$$

Attention here is directed to bridging regimes 1 and 2. Bridging regimes 2 and 3 is an important discussion that will have to await further results. It has been proposed in [3] that regimes (1) and (2) can be bridged by the equation

$$\sigma_y = \sqrt[n]{(\sigma_c)^n + \left(\sigma_y^0\right)^n}, \tag{4}$$

with $n = 2$. Its applicability is demonstrated in Fig. 1.

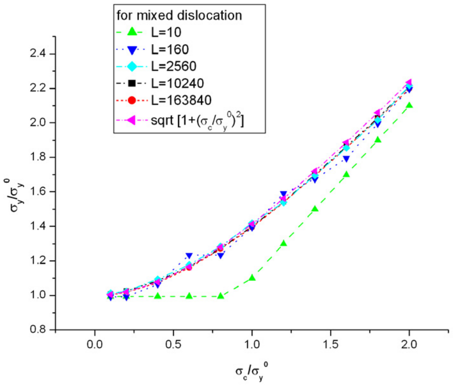
Application to Cu/Ni Multilayers

The assembled semi-analytic model is now directed towards Cu/Ni multilayers as an example. First, the modeling parameters appropriate to Cu/Ni multilayers are discussed. Second, it is demonstrated by way of numerical simulation that Eq. 4 correctly captures the behavior of dislocation pileups in transition between scales 2 and 3. Third, the model is applied to Cu/Ni multilayers using the value of σ_p calculated in[4].

Modeling Parameters

The first step is to calculate the modeling parameters. The scaling exponent a, appearing in Eq. 2 is obtained from knowledge of the elastic moduli of the component layers, the orientation of the pileup, and the pileup character [5]. The elastic moduli for Cu are shear modulus, $\mu = 54.6$ GPa, and Poisson ratio, $\nu = 0.324$. For Ni, $\mu = 94.7$ GPa, and $\nu = 0.276$. Pileups are assumed to form in the softer Cu layers. The growth direction is (001). The glide planes are (111), and the burgers vectors are $< 110 >$ type. Thus, the glide planes form and angle of 54.74° with the layer interfaces, and the dislocations are either of the screw type, parallel to the interface, or mixed, forming a 60° angle with the dislocation line. The appropriate scaling exponent, a, is obtained analytically by solving an eigenvalue problem. [6] It is found to be 0.434 for the screw-type pileup and 0.439 for the mixed-type pileup. Given these exponents, the coefficients k (see Eq. 2) are

[1]The effect of long-range coherency stresses may also need to be incorporated, but that is not addressed here.



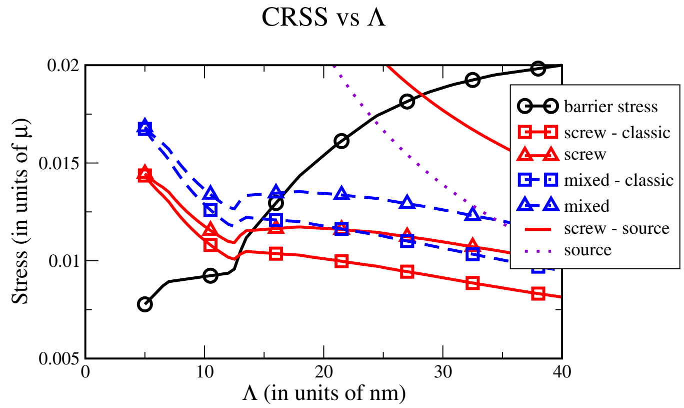


Figure 1: Plot of σ_y/σ_y^0 vs. σ_c/σ_y^0 for single-sided mixed pileups in Cu/Ni for various pileup lengths, L. σ_y is calculated from a numerical model of discrete dislocation pileups. σ_y^0 is obtained from Eq. 2.By Eq. 4, all plots should fall on the theoretical curve, $\sqrt{1+(\sigma_c/\sigma_y^0)^2}$. The shortest pileup with $L = 10b$ shows significant deviation.

Figure 2: Resolved yield stress vs Λ from Eq. 2. Curves labeled "classic", use $a = 1/2$ and $k = 1/\sqrt{\pi}$. "source" indicates the estimated σ_c value, and "screw - source" shows the effect of using Eq. 4 for the screw pileup.

found for each type of pileup by fitting to numerical simulations of discrete dislocation pileups.[2]. For screw-type pileups, $k = 0.664$. For mixed-type pileups, $k = 0.668$. The effective shear moduli, μ^*, are found for each type of pileup (Screw: 54.6 GPa, Mixed: $\mu^* = 74.2$ GPa).

numerical verification

Next, it is demonstrated that the theory bridging the large L, source dominated regime and the mezoscale L scaling regime is correct (at least anecdotally) for Cu/Ni multilayers. Fig. 1 show a test of Eq. 4.

Yield Stress Prediction

Using theoretical predictions of σ_p, it is possible to apply the theory quantitatively to Cu/Ni multilayers.

σ_p as a function of multilayer wavelength, Λ is given for Cu/Ni multilayers grown in the (001) orientation in [4] This function is shown in Fig. 2. The authors caution that this function is only "schematic", but it will sill serve here for the purposes of demonstration. This function and the above mentioned modeling parameters are used in Eq. 2 to obtain yield stress predictions. The pileup length (βh) in Eq. 2 is found from geometric arguments to be $\Lambda/(2\sin 54.74°) = 0.612\Lambda$. Plugging all relevant parameters into Eq. 2, the resulting yield stress, is predicted and plotted in Fig. 2.

In Fig. 2, the predicted yield stresses are plotted along with the classic Hall-Petch predictions that use $a = 1/2$ and $k = 1/\sqrt{\pi}$ in units of μ_{Cu}. In the plotted range, the classic Hall-Petch Relation and the proposed formula can differ by as much as %20. In the range of 12-17 nm, the various curves are seen to intersect with the curve for σ_p. The pileup prediction is meaningless when it's strength predictions exceed σ_p, but the intercept is a possibly an estimator of the peak yield stress location.

Next, the effect of sources, $\sigma_p \neq 0$ are considered. In the absence of a theory for the stress to activate a dislocation source, a conservative value of $\mu b/(0.612\Lambda)$ is chosen. This value of σ_c is plugged into Eq. 4. Because of the 1Λ scaling, the source contribution is quite significant, even for this conservative estimate (see Fig. 2).

Finally, to the authors' knowledge, there is no truly reliable way to obtain yield stress - hardness conversions for multilayers. However, one can use the appropriate geometric factors and the Tabor factor of 3. This procedure is somewhat suspect, but the resulting conversion is $H \approx 7.35\sigma_y$.

[2] These results are only exact in the continuum limit

References

[1] A. Misra, H. Kung, and J. D. Embury. *Scripta Mat*, 50(6):707–10, 2004.

[2] J S Koehler. *Phys. Rev. B*, 2(2):547, 1970.

[3] Lawrence H. Friedman. *Scripta Mat.*, 50(6):763–7, 2004.

[4] S I Rao and P M Hazzeldine. *Phil. Mag. A*, 80(9):2011, 2000.

[5] L H Friedman and D C Chrzan. *Phil. Mag. A*, 77(5):1185, 1998.

[6] L H Friedman. unpublished.