Hall-Petch Analysis from a Combined Mechanics and Materials Viewpoint

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## 18<sup>th</sup> – 20<sup>th</sup> century crystal microstructures



R.W. Armstrong, "Metallurgical basis for the Strength of Materials" in Centenary of Metallurgy Teaching at the University of Strathclyde, edited by H.B. Bell and D.B. Downie (Metallurgy Department, University of Strathclyde, U.K., 1984) pp. J1-J12; "Dislocation Mechanics Description of Polycrystal Plastic Flow and Fracturing Behaviors", in Mechanics and Materials: Fundamentals and Linkages, edited by M.A. Meyers, R.W. Armstrong and H. Kirchner (John Wiley & Sons, Inc., N.Y., 1999) pp. 363-398.

#### 19<sup>th</sup> century assessment of $\alpha$ -Fe(C) and Cu results



W.C. Unwin, "On the yield point of iron and steel and the effect of repeated straining and annealing", Proc. Roy. Soc. Lond., 57, 178-187 (1894).

## 20<sup>th</sup> century testing of single crystals



Shear strain

20<sup>th</sup> century single crystal results

#### Mechanics/materials based H-P equations

1934, G.I. Taylor – *deformation of AI*  

$$\sigma_T = m \tau_{CRSS} - - - \sum_{i=1}^{5} (d\gamma_i / \gamma_T)$$

1951, E.O. Hall; 1953 N.J. Petch – *yielding and cleavage of α-Fe* 

$$\sigma_{lyp} = [\sigma_{lyp} + k_{lyp}\ell^{-1/2}] \rightarrow \sigma_C$$

1962, R.W. Armstrong, I. Codd, R.M. Douthwaite and N.J. Petchfcc, bcc and hcp metals  $\sigma_{\varepsilon} = m[\tau_{0\varepsilon} + k_{S\varepsilon}\ell^{-1/2}]$ 

1983, R.W. Armstrong pile-up relation  $k_{\varepsilon} = mk_{S\varepsilon} = m[\pi m^* Gb\tau_C / 2\alpha]^{1/2}$ 

1978, 1983, G.W. Weng – Cu

$$\tau_{\varepsilon} = (\tau_{y} + k_{y}\ell^{-1/2}) + (h + a\ell^{-1/2}) \sum_{j} [\alpha + (1 - \alpha)\cos\theta^{i,j}\cos\phi^{i,j}](\gamma^{p})^{n}$$

#### **Thermal Activation Strain Rate Analysis (TASRA)**

 $(d\epsilon/dt) = (1/m)\rho bv$ 

dislocation velocity:  $v = v_0 exp[-(G_0 - \int A^*b d\tau_{Th})/kT]$  in which  $\tau_{Th} = \tau - \tau_G$ 

activation area:  $A^* = (kT/b)[\partial ln(d\epsilon/dt)/\partial T_{Th}]_T$  and  $A^*b = W_0/T_{Th}$ 

Computational (Z-A) equations:

 $\sigma = \sigma_{\rm G} + \mathsf{B}\mathbf{exp}[-\beta\mathsf{T}] +$ 

 $B_0[\epsilon_r(1 - exp\{-\epsilon/\epsilon_r\})]^{1/2}exp[-\alpha T] + k_{\epsilon}\ell^{-1/2}$ 

in which

 $(\beta, \alpha) = (\beta_0, \alpha_0) - (\beta_1, \alpha_1) \ln(d\epsilon/dt)$ 

*bcc case*:  $\alpha = \alpha_0 = \alpha_1 = 0$  *fcc case*: B = 0;  $\beta = \beta_0 = \beta_1 = 0$ 

## Thus on a TASRA basis, thermal activation is in the yield stress for bcc metals and alloys and is in the strain hardening for fcc metals and alloys.

F.J. Zerilli and R.W. Armstrong, *J. Appl. Phys.* 61, 1816-1825 (1987)
F.J. Zerilli and R.W. Armstrong, *J. Appl. Phys.* 68, 1580-1591 (1990)
F.J. Zerilli, *Metall. Mater. Trans. A*, 35A, 2547-2555 (2004)

H-P "m's" for pure magnesium and AZ-type alloys



Addition to Fig. 4 of R.W. Armstrong, in *Proc. 33<sup>rd</sup> Risoe Int. Symp. on Mater. Sci.*: *Nanometals – Status and Perspective*, S. Faester et al., eds. (Tech. Univ. Denmark, Roskilde Campus, 2012) pp. 181-199.

#### H-P dependencies for the full $\sigma - \epsilon$ behavior of mild steel



R.W. Armstrong, "The influence of polycrystal grain size on several mechanical properties of materials", *Metall. Trans.* **1**, 1169 -1174 (1970).

H-P yield-point-related  $\sigma$  -  $\epsilon$  results for 70-30 brass



W.L. Phillips and R.W. Armstrong, *Metall. Trans.*, **3**, 2571-2579 (1972)

## BCC-type Z-A equations for tantalum



K.G. Hoge and A.K. Mukherjee, *J. Mater. Sci.*, **12**, 1666 (1977); F.J. Zerilli and R.W. Armstrong, *J. Appl. Phys.*, **68**, [4], 1580 (1990).

#### Z-A application with EPIC finite element code



**Taylor Test conditions: 0.01 < ε < ~1.5; 0< (dε/dt) < ~10<sup>5</sup> s<sup>-1</sup>; 300 < T < ~600 K** F.J. Zerilli and R.W. Armstrong, *J. Appl. Phys.*, **61**, 1816-1825 (1987)

#### H-P results for Cu micro- to nano-hardnesses



S.J. Bull, L. Sanderson and N. Moharrami and A. Oila, Mater. Sci. Tech., 28, [9-10], 1177.

#### An H-P dependence for the hardness of Ni



Log/Log Hall-Petch dependencies for Al, Ni, and Cu



R.W. Armstrong, in *Nanometals – Status and Perspective*, 33<sup>rd</sup> Risoe Int. Symp. on Mater. Sci. (Technical Univ. Denmark, Roskilde Campus, 2012) pp. 181-199.

# Cu transition to a single loop expanding against the grain boundary obstacle



R.W. Armstrong, in *Proc. 33rd Risoe Int. Symp. on Mater. Sci.:* **Nanometals – Status and Perspective**, S. Faester et al., eds. (Tech. Univ. Denmark, Roskilde Campus, 2012) pp. 181-199.

Cu grain/twin size strengthening and weakening



R.W. Armstrong, "Hall-Petch analysis for nanopolycrystals", in *Nanometals – Status and Perspective*, 33rd Risoe International Symposium on Materials Sciences, edited by S. Faester *et al.* (Technical University of Denmark, Roskilde Campus, DK, 2012) pp. 181-199; see Fig. 8. L. Lu, X. Chen, X. Huang, K. Lu, "Revealing the maximum strength in nanotwinned copper", *Science*, **323**, 607-610 (2009), see Fig. 3.

## MD modeling of grain/grain boundaries in Ni



J.R. Weertman *et al.*, MRS Bull., **24**, [2], 44 1999) R.W. Armstrong, Emerg. Mater. Res., **1**, [S1], 31 (2012) The H-P dependence for iron and steel on a log/log basis



R.W. Armstrong, "Hall-Petch analysis: Past to present nano-scale connections", *Strength of Fine Grained Materials – 60 years of Hall-Petch*, Tokyo, July, 2013

## SUMMARY

- The topic of polycrystal grain size influences on the strength of materials has spanned the 18-20<sup>th</sup> centuries and is now of great engineering interest in the 21<sup>st</sup> century for additional development of nanocrystalline materials with order of magnitude greater strength levels than exhibited by conventional materials.
- 2. Combined continuum and dislocation mechanics analyses have provided a reasonably quantitative explanation of the grain size dependent strength properties spanning, at effective low temperatures, the role of temperature and applied material deformation rates.
- 3. More work has to be done, for example, on:
- 3.1. Additional quantification of the material strength properties, including assessment of the material nano-scale strain hardening as determining ductility;
- 3.2. Development of improved production methods for obtaining nanopolycrystalline materials; and
- 3.3. Merging of low temperature and higher (creep) temperature model analyses for fully analyzing the solid-state material properties.