Hall-Petch Analysis from a Combined Mechanics and Materials Viewpoint

**TOPICS**

1. Outline and historical introduction
2. Hall-Petch and TASRA model descriptions
3. Experimental measurements
   3.1. Stress-strain results:
   3.2. Thermal activation
   3.3. Hardness
4. Nanopolycrystal results
   4.1. Log/Log representations
   4.2. Grain boundary disorder
5. SUMMARY

**CHARTS**

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18th – 20th century crystal microstructures

19\textsuperscript{th} century assessment of $\alpha$-Fe(C) and Cu results

20th century testing of single crystals

20th century single crystal results
Mechanics/materials based H-P equations

1934, G.I. Taylor – deformation of Al

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

1951, E.O. Hall; 1953 N.J. Petch – yielding and cleavage of \( \alpha \)-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. Petch - fcc, bcc and hcp metals

\[ \sigma_\varepsilon = m[\tau_{0\varepsilon} + k_{S\varepsilon} \ell^{-1/2}] \]

1983, R.W. Armstrong - pile-up relation

\[ k_\varepsilon = mk_{S\varepsilon} = m[\pi n^* Gb\tau_C / 2\alpha]^{1/2} \]

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)

\[
\frac{d\varepsilon}{dt} = \left(\frac{1}{m}\right)\rho b v
\]

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

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

Computational (Z-A) equations:

\[
\sigma = \sigma_G + B \exp[-\beta T] + B_0 [\varepsilon_r (1 - \exp\{-\varepsilon/\varepsilon_r\})]^{1/2} \exp[-\alpha T] + k_e t^{-1/2}
\]

in which

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

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.

H-P “m’s” for pure magnesium and AZ-type alloys

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

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

BCC-type Z-A equations for tantalum

Z-A application with EPIC finite element code

Taylor Test conditions: 0.01 < ε < ~1.5; 0 < (dε/dt) < ~10⁵ s⁻¹; 300 < T < ~600 K
H-P results for Cu micro- to nano-hardnesses

An H-P dependence for the hardness of Ni

\[ \sigma_H = \sigma_{0H} + k_H \ell^{-1/2}; \quad k_H \approx k_\varepsilon; \quad \varepsilon \approx 0.08 \]
Log/Log Hall-Petch dependencies for Al, Ni, and Cu

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

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)
The H-P dependence for iron and steel on a log/log basis

SUMMARY

1. The topic of polycrystal grain size influences on the strength of materials has spanned the 18-20th centuries and is now of great engineering interest in the 21st 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.