Appendix A

Algorithm developed for validating the mesoscopic GBS controlled flow model for inverse Hall-Petch effect.

Equations used in the algorithm:

1. $\dot{\varepsilon} = \dfrac{2cw\gamma_0 v}{d}\sinh\left(\dfrac{(\sigma - \sigma_0)c\gamma_0 V_0}{2kT}\right)\exp\left(-\dfrac{\Delta F_0}{kT}\right)$

2. $\Delta F_0 = \dfrac{1}{2}(\beta_1\gamma_0{}^2 + \beta_2\varepsilon_0{}^2)GV_0$

3. $A = \dfrac{1}{n}\Sigma\,\dfrac{\dot{\varepsilon}}{\sinh\left(\dfrac{(\sigma - \sigma_0)c\gamma_0 V_0}{2kT}\right)}$

4. $B = \dfrac{2cw\gamma_0 v}{L}$

5. $\Delta F_0 = kT(\ln B - \ln A)$

Flowchart:

- Start
- Digitize Data
- Initial assignment: $\sigma_0 = \delta\,(>0)$ to $\sigma_{\min}-\delta$, $\gamma_0 = 0.1$
- Use equation 1, 3, 4 & 5 to compute values of ΔF_0 and σ_0 at each temperature
- Use the computed values of ΔF_0 and σ_0 to predict $\dot{\varepsilon}$ at each temperature
- Compute the error as the ratio between $\dot{\varepsilon}_{\text{predicted}}$ and $\dot{\varepsilon}_{\text{experimental}}$ with the larger quantity in the numerator
- Define Permissible errors
- Choose those combinations of ΔF_0 and σ_0 where $\dot{\varepsilon}$ is predicted within defined limits at each temperature
- Compare the values of ΔF_0 at each temperature and choose the closest combination and the corresponding σ_0
- Substitute ΔF_0 in equation 2 and refine the value of γ_0
- Is γ_0 converging?
  - No → Update γ_0 → (back to Use equation 1, 3, 4 & 5 ...)
  - Yes → Stop