



MD Studies of Solute Strengthening in Stainless Steel Alloys

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Accurate dislocation mobility laws are necessary to inform deformation in reduced order models. Molecular dynamics (MD) simulations enable direct observation of dislocation glide mechanisms under applied shear stress. Using a novel embedded atom method (EAM) interatomic potential developed for FeNiCr¹ as a surrogate for 3XX-series stainless steels, we investigate mobility and strengthening as a function of alloy composition, temperature, and stress. The results are compared with literature analytical models and show reasonable agreement with predicted strengthening trends.

Molecular Dynamics Method

A displacement field is applied to the atoms such that the upper and lower halves of the crystal are displaced by $\pm \vec{b}/2$ near the lower boundary of z and such displacements decay to zero near the center of z . This process creates a screw dislocation with both its line direction and Burgers vector $\vec{b} = [\bar{2}20]a/2$ parallel to x . Our simulations employ periodic boundary conditions in x and z , and a free boundary condition in y . Shear stresses parallel to the x are applied, and velocity is determined by tracking atomic displacement in the slip plane.

$\tau = 60\text{MPa}$; $T = 300\text{K}$; $x\text{Ni} = 0.15$; $\sim 2M$ atoms

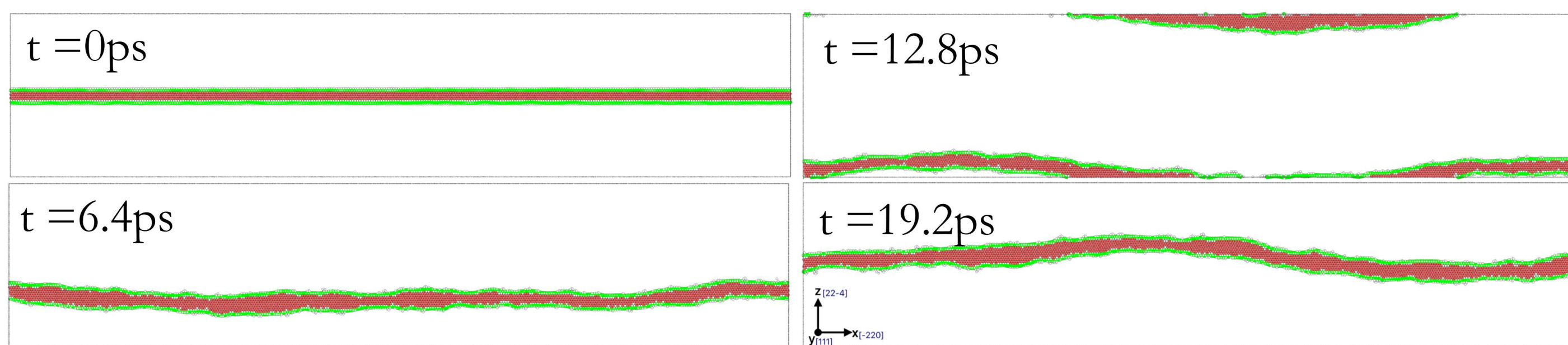


Fig 1: Dislocation adopts wavy configuration in presence of solute field. (200nm x 15nm x 18 nm)

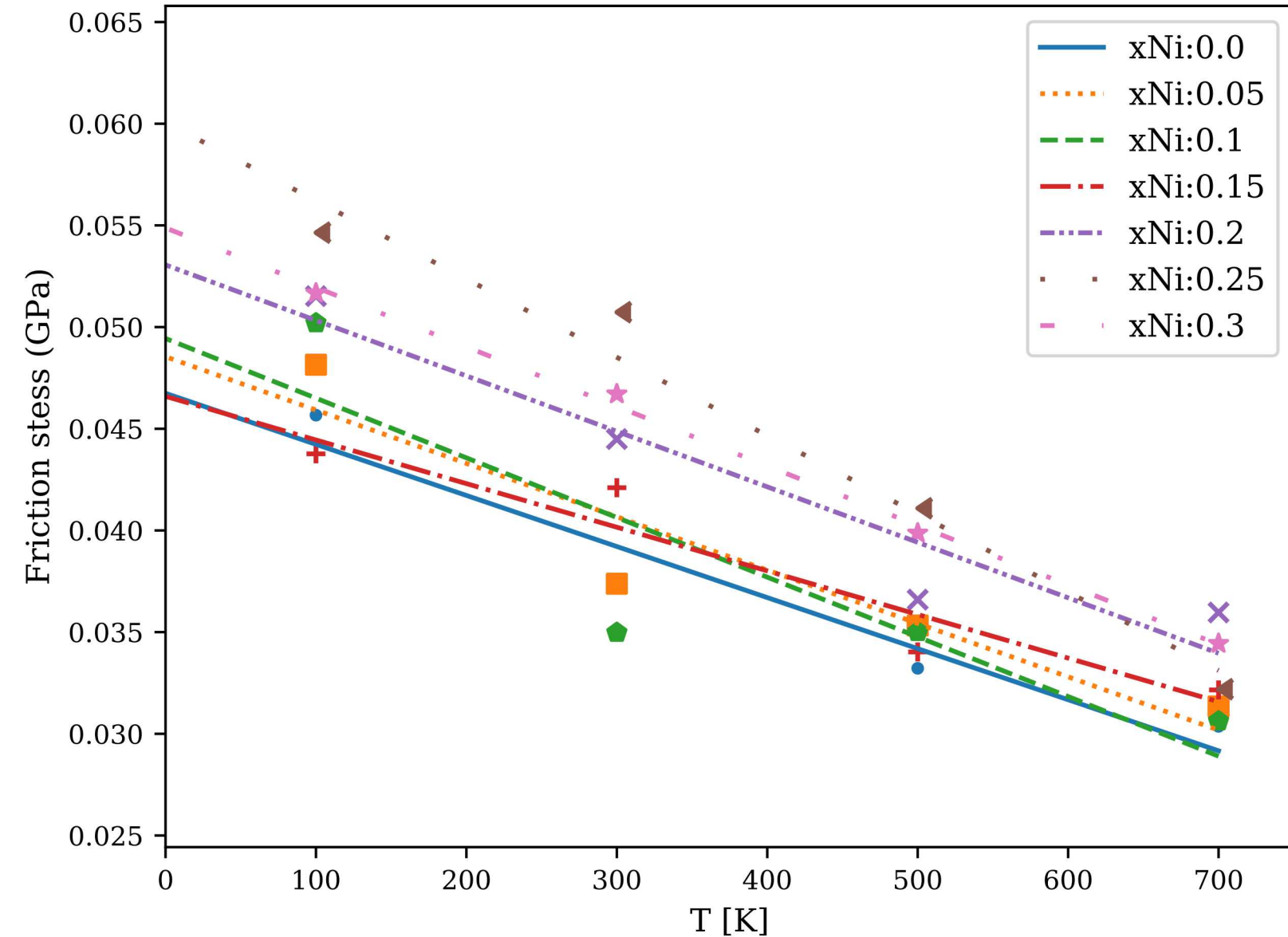


Fig 3: Determination of τ_{y0} by linear fit to MD friction stress

Comparison with Literature Analytical Model²

$$\tau_{y0} = 0.051\alpha^{-\frac{1}{3}}\mu\left(\frac{1+\nu}{1-\nu}\right)^{\frac{4}{3}}f_1(w_c) \times \left[\frac{\sum_n c_n(\Delta V_n^2 + \sigma_{\Delta V_n}^2)}{b^6}\right]^{2/3} \quad (1)$$

$$\Delta E_b = 0.274\alpha^{\frac{1}{3}}\mu b^3\left(\frac{1+\nu}{1-\nu}\right)^{\frac{2}{3}}f_2(w_c) \times \left[\frac{\sum_n c_n(\Delta V_n^2 + \sigma_{\Delta V_n}^2)}{b^6}\right]^{2/3} \quad (2)$$

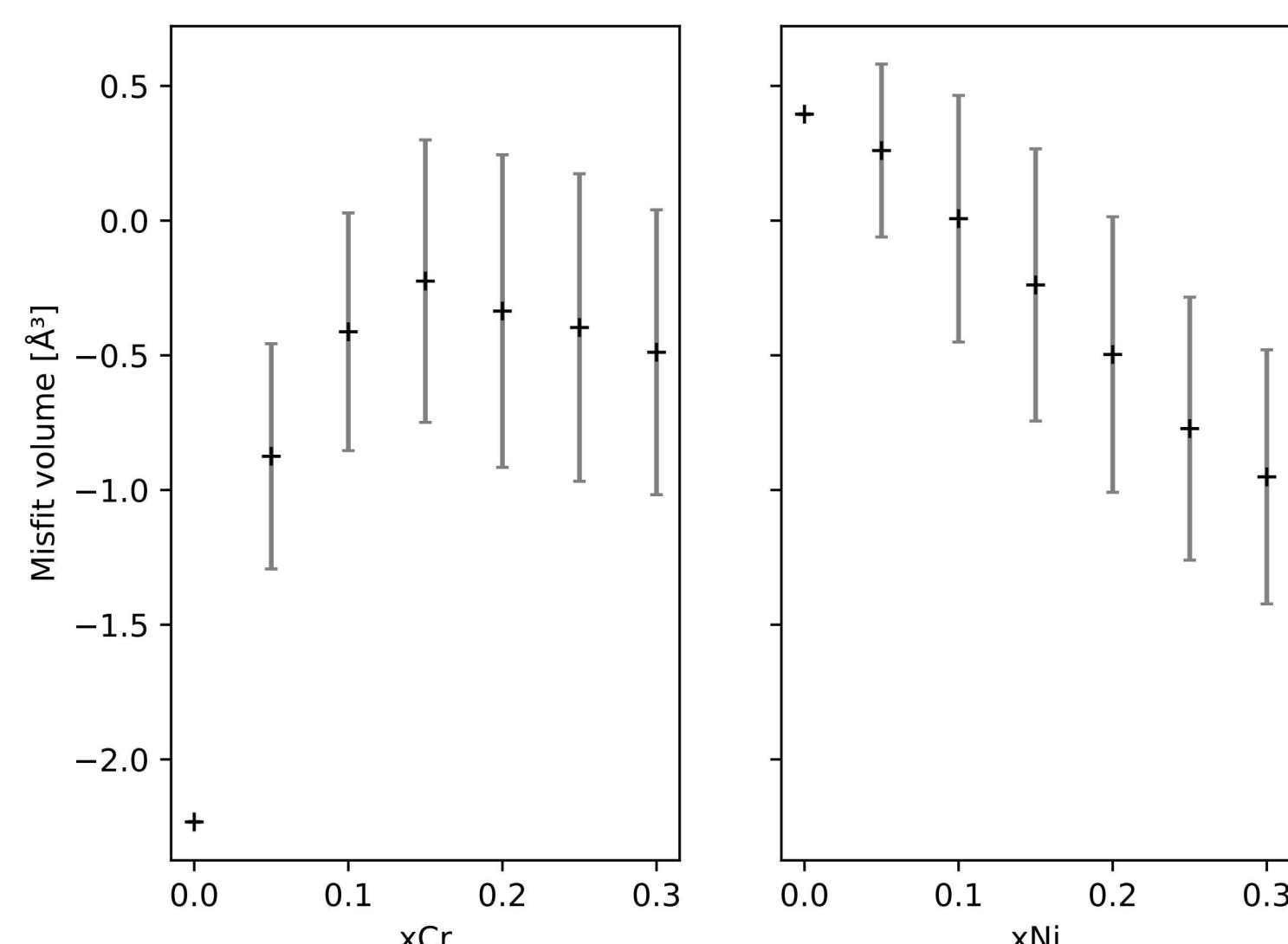


Fig 4: FeCr, FeNi binary swelling volumes ΔV_n and standard deviation $\sigma_{\Delta V_n}$ calculated via molecular statics (MS)



Fig 2: Dislocation mobility vs. applied stress in the Fe_{0.70}Ni_xCr_{0.3-x} ternary alloy

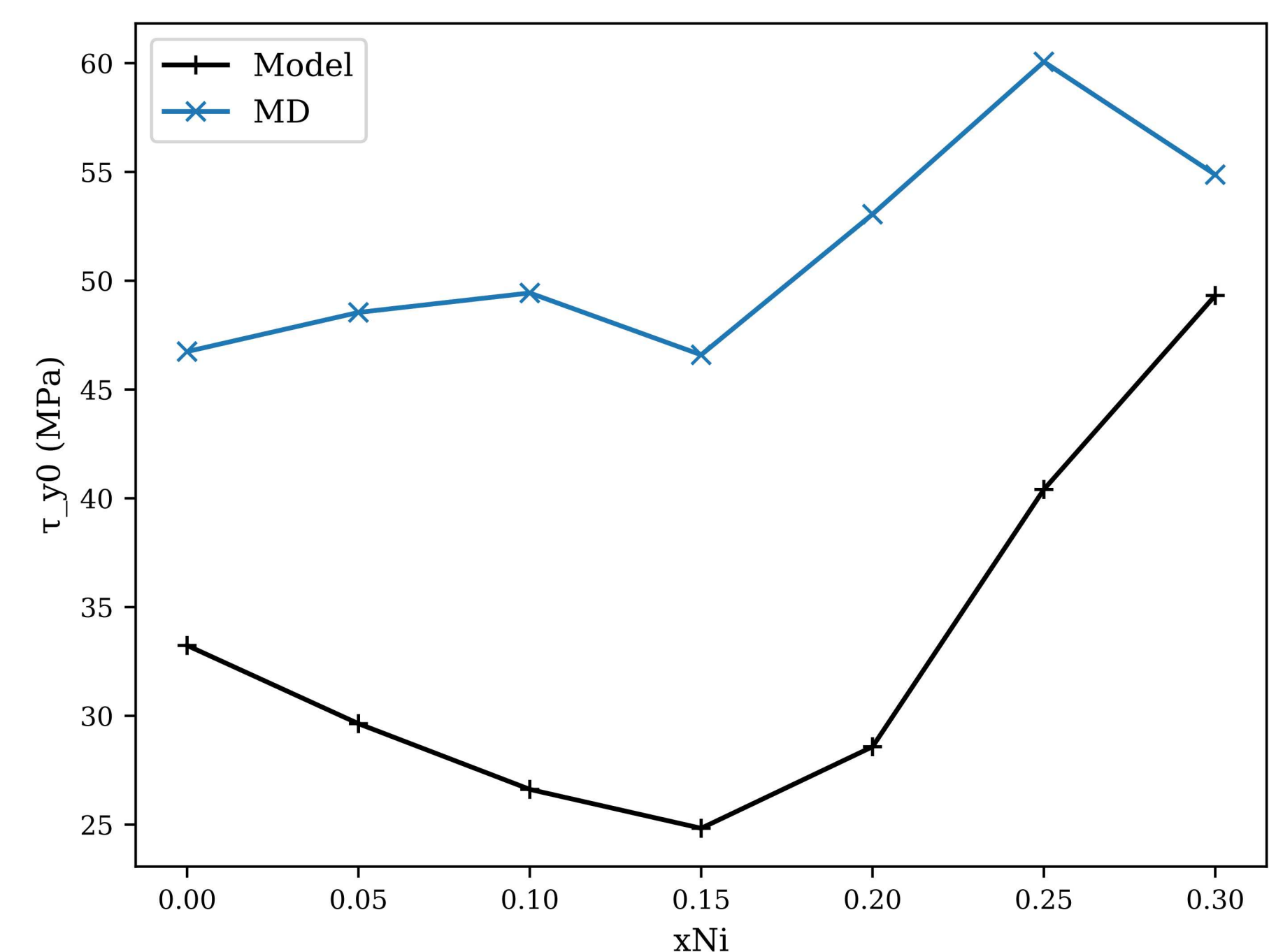


Fig 5: Comparison of MD and model predictions of τ_{y0} as a function of alloy composition

Conclusions:

- We have determined screw dislocation mobility relations for Fe_{0.70}Ni_xCr_{0.3-x} alloys as a function of stress, temperature, and composition.
- τ_{y0} for this alloy generally increases with increasing nickel composition and increases with decreasing temperature.
- A minimum in τ_{y0} is observed in both MD and model predictions due to the non-Vegard's behavior of FeCr swelling volume.
- Analytical model predictions based solely on swelling volume alloys may underestimate τ_{y0} .