

# 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 FeNiCr<sup>1</sup> 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.

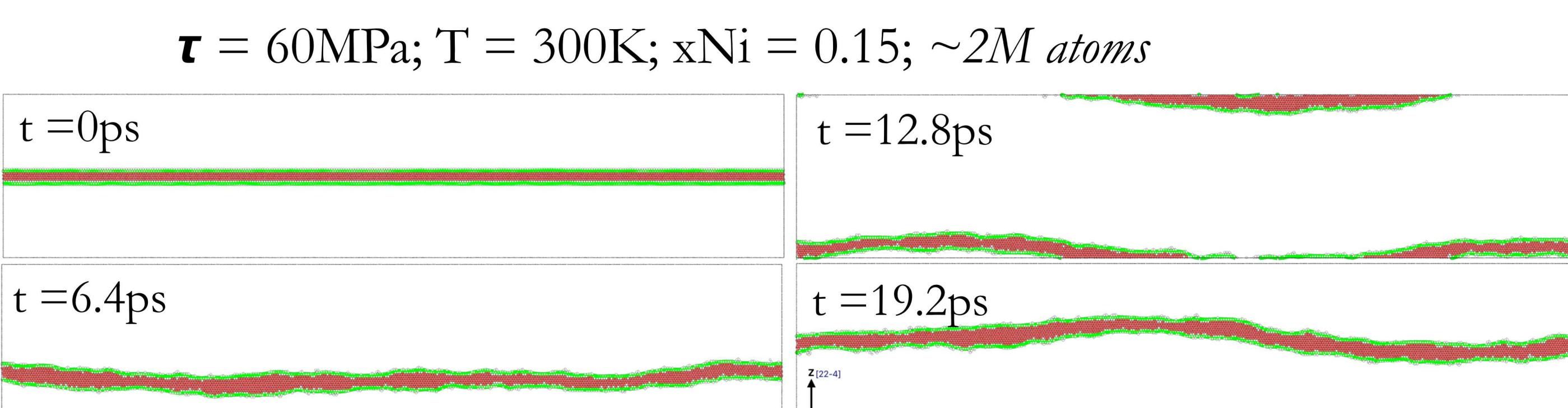


Fig 1: Dislocation adopts wavy configuration in presence of solute field. (200nm x 15nm x 18 nm)

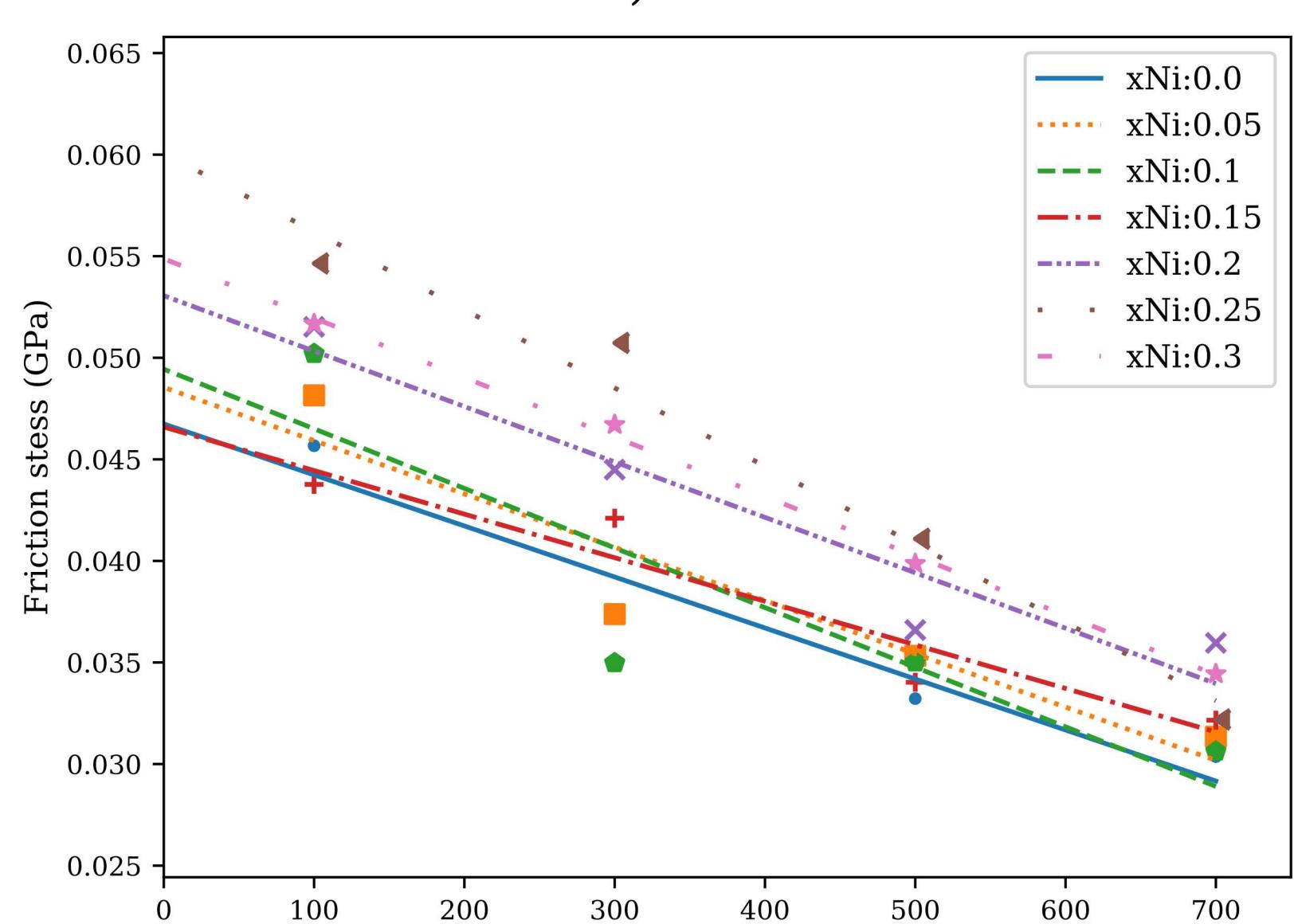


Fig. 3: Determination of  $\tau_0$  by linear fit to MD friction stress

## Comparison with Literature Analytical Model<sup>2</sup>

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

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

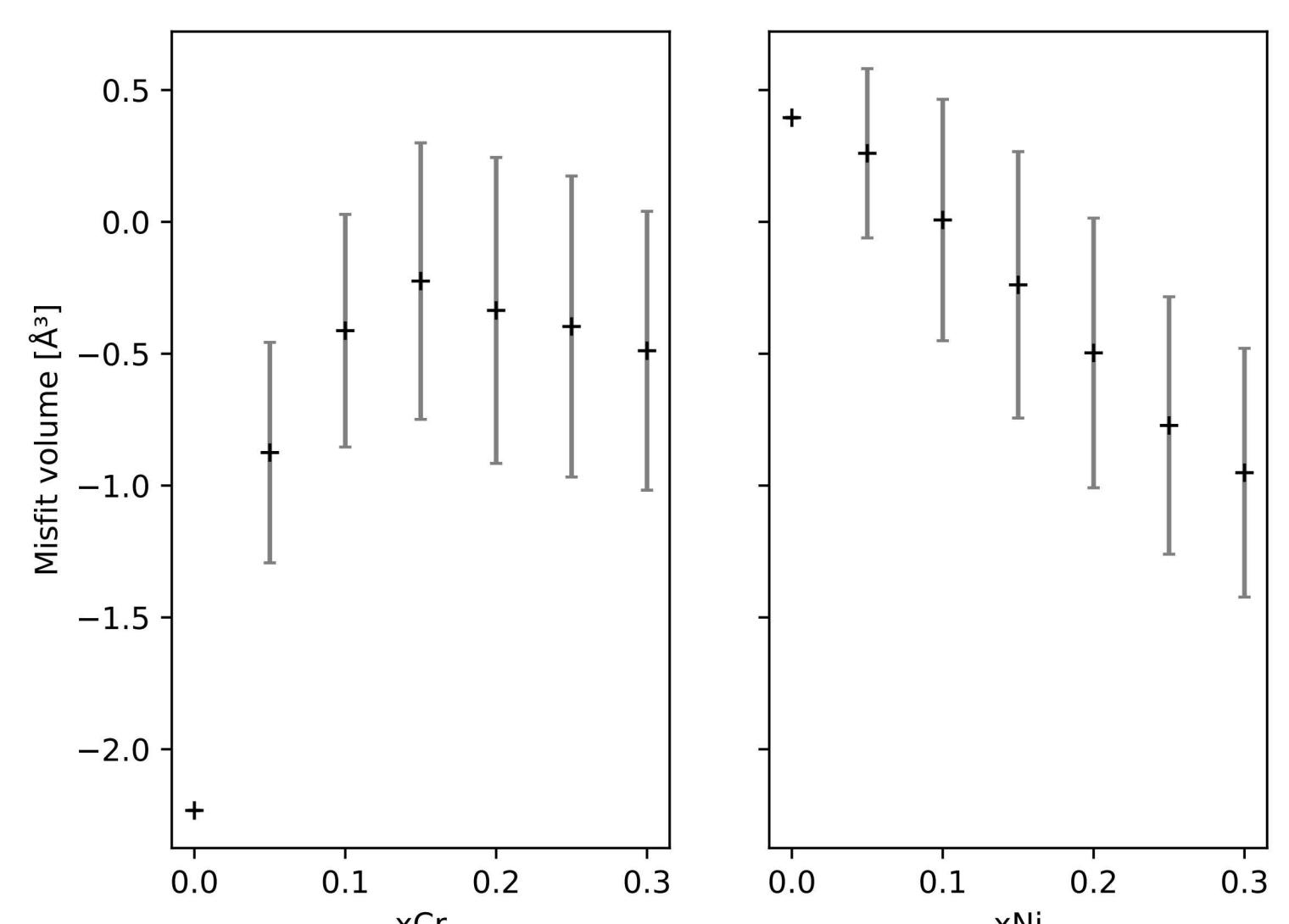


Fig 4: FeCr, FeNi binary swelling volumes  $\Delta V_n$  and standard deviation  $\sigma_{\Delta V_n}$  calculated via molecular statics (MS)

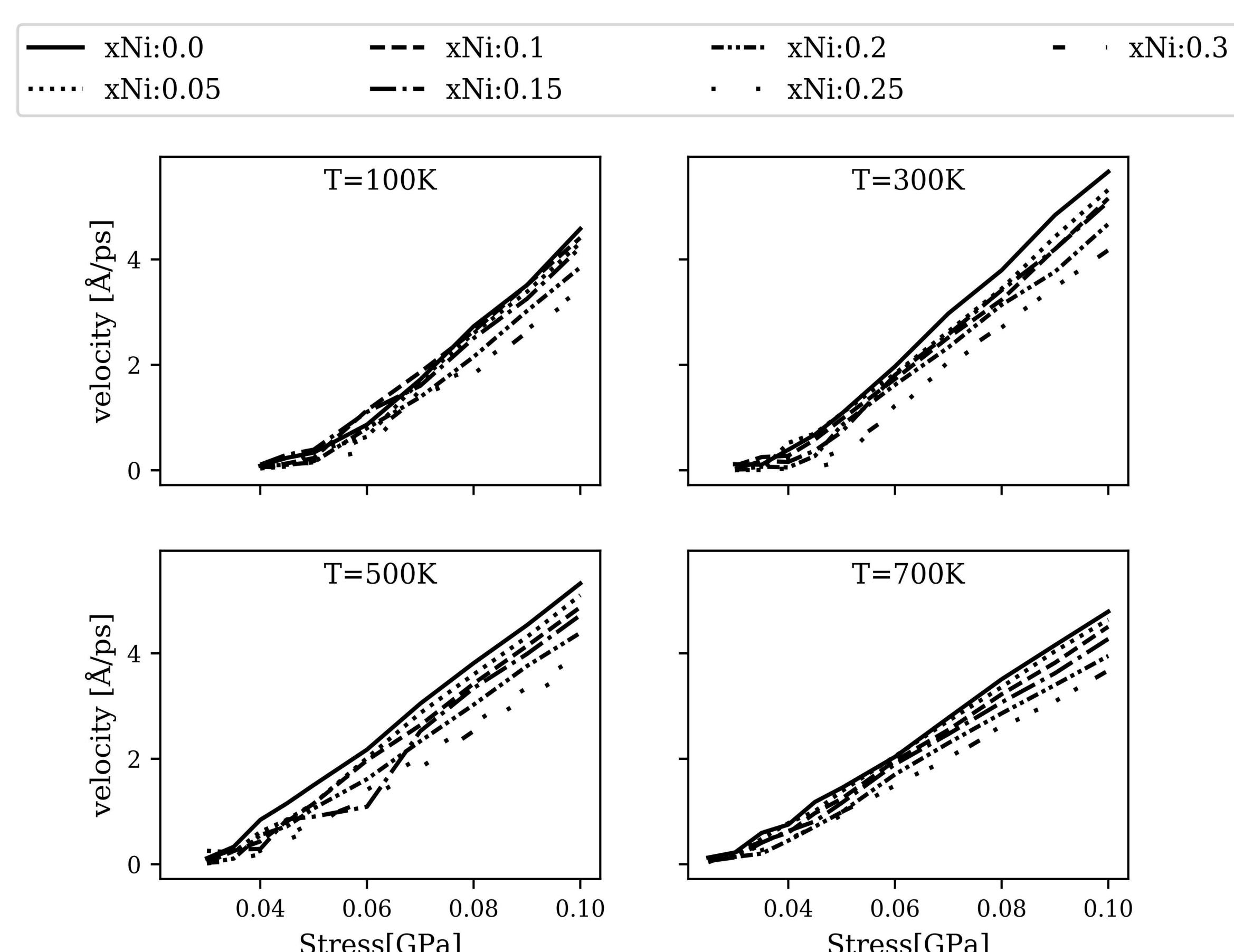


Fig 2: Dislocation mobility vs. applied stress in the  $\text{Fe}_{0.70}\text{Ni}_x\text{Cr}_{0.3-x}$  ternary alloy

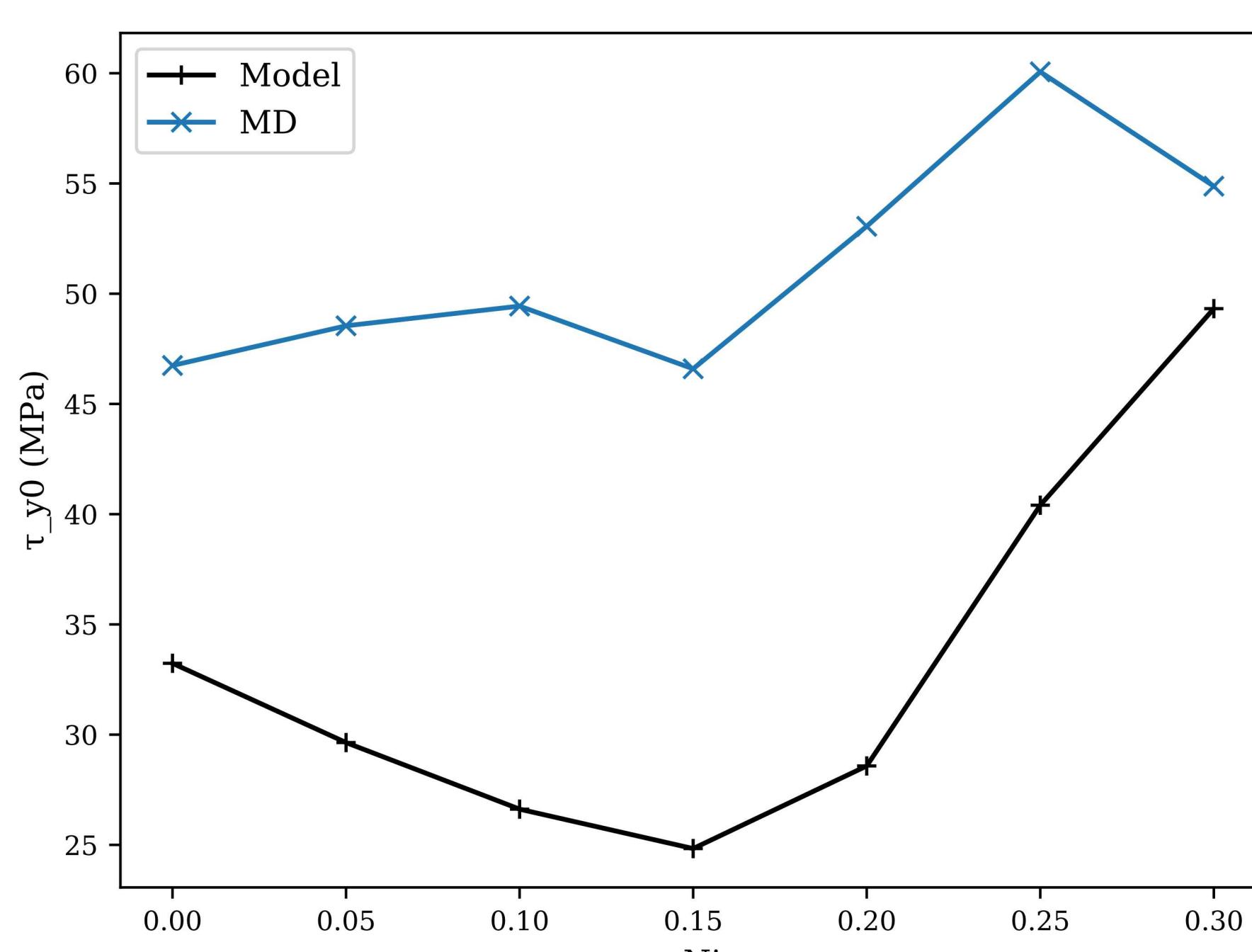


Fig 5: Comparison of MD and model predictions of  $\tau_{y0}$  as a function of alloy composition

## Conclusions:

- We have determined screw dislocation mobility relations for  $\text{Fe}_{0.70}\text{Ni}_x\text{Cr}_{0.3-x}$  alloys as a function of stress, temperature, and composition.
- $\tau_{y0}$  for this alloy generally increases with increasing nickel composition and increases with decreasing temperature.
- A minimum in  $\tau_{y0}$  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  $\tau_{y0}$ .