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Theoretical Analysis of Hydrogen-Dislocation Interactions

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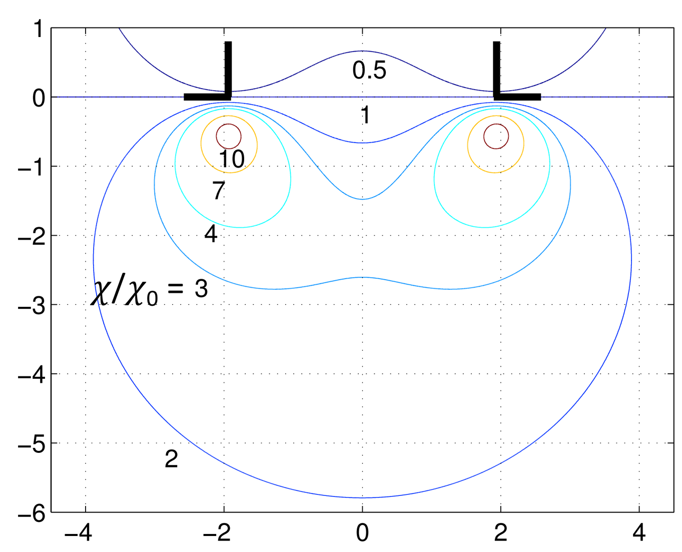
Introduction

A primary contributor to hydrogen effects on plasticity is interstitial hydrogen atoms interacting with dislocations. Our objective is to understand and quantify each of the potential interaction modes between hydrogen solutes and dislocations. Through these efforts we elucidate the dominant interaction modes, and enable dislocation dynamics (DD) studies of hydrogen-affected plasticity.

Model



We use a continuum, elasticity-based model where hydrogen atoms are treated as Eshelby inclusions each producing a volume change ΔV. The chemical potential is

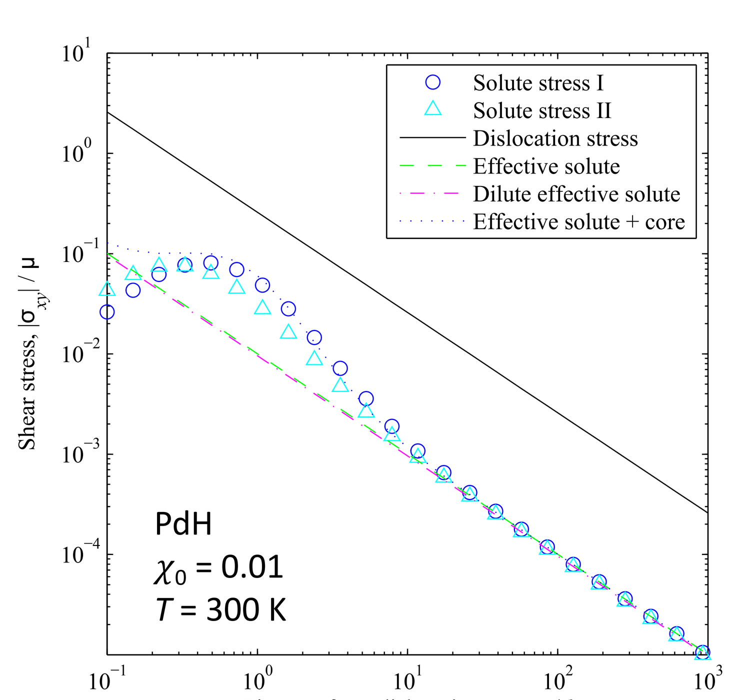
$$\mu(\mathbf{x}) = E_f + p(\mathbf{x})\Delta V - \xi\bar{\chi} + k_B T \ln\left(\frac{\chi(\mathbf{x})}{1-\chi(\mathbf{x})}\right)$$

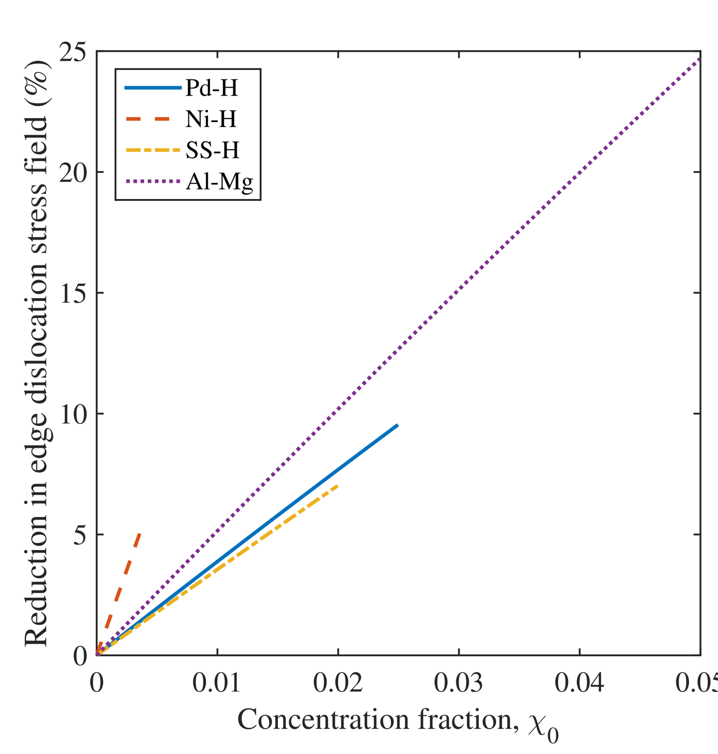
Stress Field Screening

The Cottrell atmosphere formed by the H atoms acts to cancel a dislocation's shear stress field. This effect can be computed analytically in terms of a modified bulk modulus[1]:

$$\frac{1}{K_{eff}} = \frac{1}{K} + \frac{\chi_0(1-\chi_0)c_{max}\frac{\Delta V^2}{k_B T}}{1-\chi_0(1-\chi_0)\frac{\xi}{k_B T}}$$

This screening effect is typically small (<10%), however, for hydrogen solid solutions, as shown below.



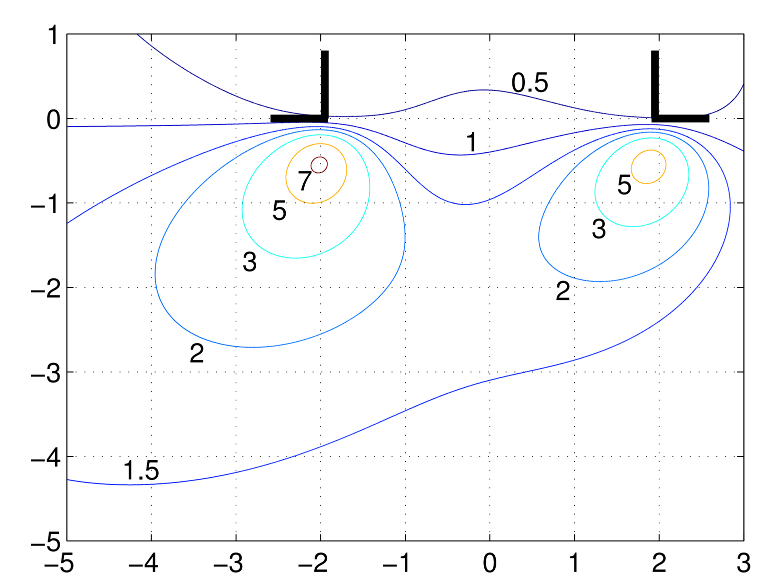


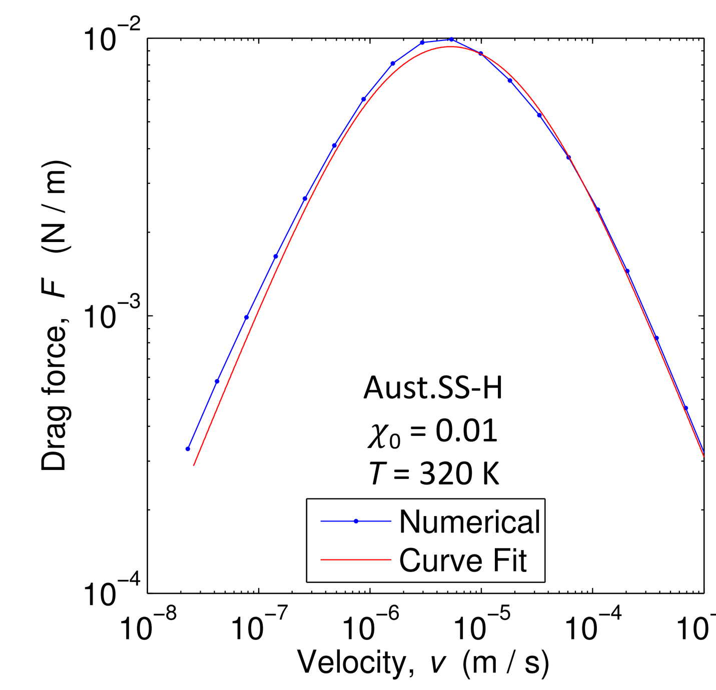
References

[1]W. Cai, R. B. Sills, D. M. Barnett, and W. D. Nix. JMPS 66 (2014).
[2]R. B. Sills and W. Cai. Phil. Mag. 96 (2016).
[3]J. von Pezold, L. Lymperakis, and J. Neugebauer. Acta Mater. 59 (2011).

Solute Drag

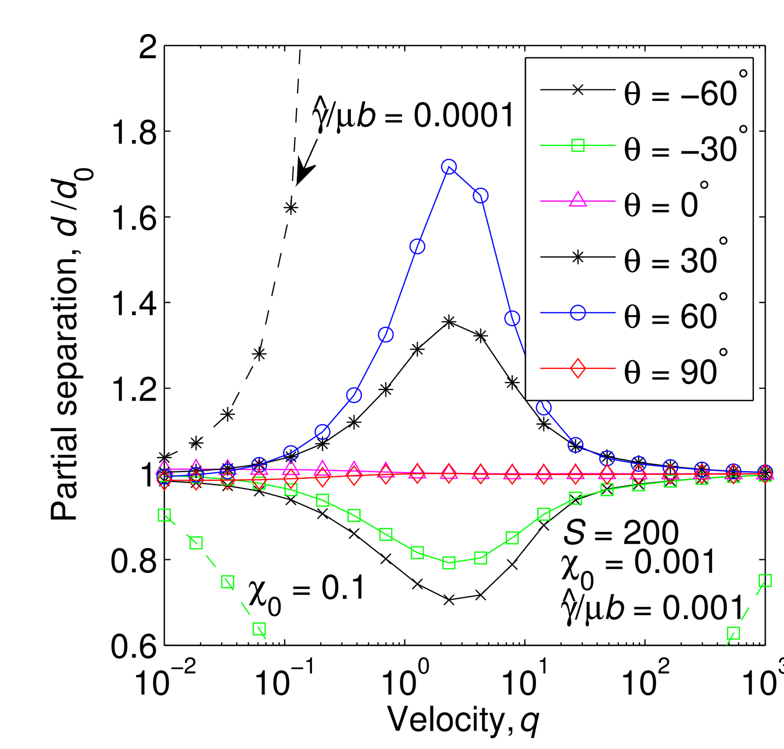
Cottrell atmospheres reorganize as a dislocation moves, leading to a drag force on the dislocation.





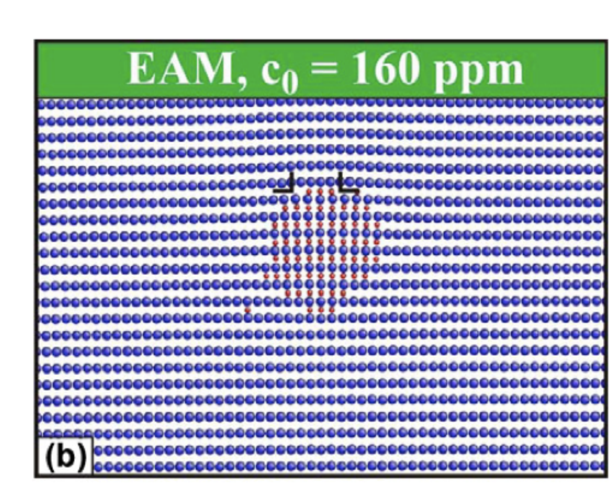
We have numerically studied solute drag and generated a closed-form drag force expression[2], enabling incorporation of solute drag in DD simulations.

We find that solute drag on extended dislocations can change the separation distance between partial dislocations, in some cases forming unbounded stacking faults[2]. This provides a mechanism for deformation twinning and deformation-induced phase transformations in the presence of hydrogen.

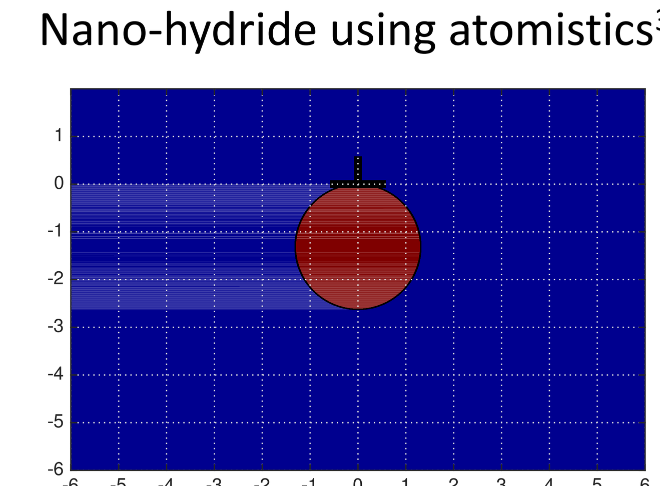


Nano-hydrides

It has been shown that H-H interactions can lead to hydride formation on dislocations in NiH[3]. Our continuum model is capable of capturing this behavior without needing to include nonlocal solute interactions.



Nano-hydride using atomistics[3]



Nano-hydride with continuum model

Future Work

- *DD simulations with solute drag*
- *Solute drag simulations with nano-hydrides*