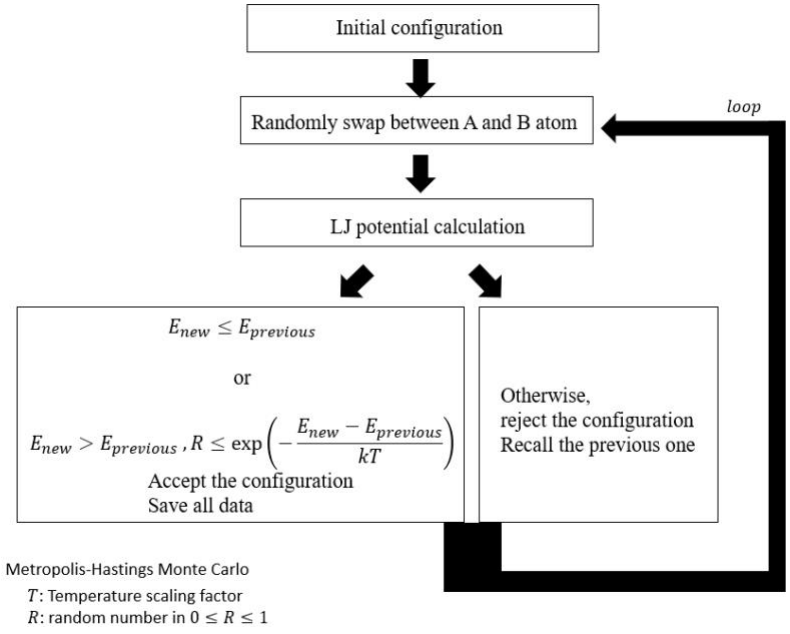
MSE 485 Final Project Proposal – Fall 2023

Gavin DeBrun, Youfu Qian, Daegun You

Abstract
Hydrogen diffusion into various materials is an important area of study for many disciplines. Metals exposed to hydrogen gas can lead to hydrogen embrittlement and result in hydrogen induced cracking, making the long-term storage of hydrogen fuel challenging. Furthermore, the introduction of ionic hydrogen into metals results in corrosion. The ability to predict the rate and depth of hydrogen penetration into metals is therefore of great interest. In this study, we will use Monte Carlo (MC) or molecular dynamics (MD) simulations to investigate the effect of hydrogen gas temperature and the short-range order (SRO) of metallic alloys on hydrogen penetration. Through this, we aim to provide a more comprehensive understanding of hydrogen-alloy interactions, particularly focusing on the nuanced changes in diffusion dynamics driven by the SRO variations.

Implementation
To compare the proton (or hydrogen) velocity in consideration of SRO effect of materials, we set the following procedures:

1. We initialize the alloy by selecting the constituent and solute atomic species
2. Alloy configurations are obtained by using Metropolis MC (MMC) swapping of constituent and solute atoms, i.e., changing one atomic species to another.



3. The selected atomic structures from the MMC swapping are equilibrated within MC or MD using the Lennard-Jones potential.
4. The protons are placed on top of supercell with varying initial velocities and temperatures.

Based on the procedure above, we can compare MC or MD results to those found in the literature where applicable. Also, the SRO effect with different variables is comprehensively characterized, which is the novelty of the project (See the next section). To simplify the problem, the following assumptions are made:

1. The protons are assumed to be a hydrogen molecule without electron interactions.
2. The periodic boundary condition is assumed to reflect well the real SRO from the macroscopic scale.

Since the assumptions above are made, the direct comparison with literature may show discrepancies. We aim to show the tendency of the SRO and variable effects on hydrogen penetration.

Novelty

In this study, we innovatively combine two approaches using MD/MC simulation: firstly, we explore the impact of SRO variations in alloys on the diffusion behavior of hydrogen atoms; secondly, we manipulate the initial velocity of hydrogen and temperature of the system. This dual-faceted approach allows for an unprecedented, detailed investigation into both the structural and dynamic aspects of hydrogen-alloy interactions, marking a significant advancement in our understanding of these complex systems.

Timeline

1. Weeks 1-2: Extensive literature review
2. Weeks 3-4: Algorithm development and simulation
3. Weeks 5-6: Parameter optimization and data analysis, final results.

Related Literature

Ren, X. L., Shi, P. H., Zhang, W. W., Wu, X. Y., Xu, Q., & Wang, Y. X. (2019). Swamps of hydrogen in equiatomic FeCuCrMnMo alloys: First-principles calculations. *Acta Materialia*, *180*, 189–198. doi:10.1016/j.actamat.2019.09.014

You, D., Ganorkar, S., Joo, M., Park, D., Kim, S., Kang, K., & Lee, D. (2019). Ab initio study of H, B, C, N, O, and self-interstitial atoms in hcp-Zr. *Journal of Alloys and Compounds*, *787*, 631–637. doi:10.1016/j.jallcom.2019.02.144

Lynch, S. P. (2011-01-01), Raja, V. S.; Shoji, Tetsuo (eds.), "2 - Hydrogen embrittlement (HE) phenomena and mechanisms", Stress Corrosion Cracking, Woodhead Publishing Series in Metals and Surface Engineering, Woodhead Publishing, pp. 90–130, ISBN 978-1-84569-673-3, retrieved 2022-06-10

You, D., Ganorkar, S., Kim, S., Kang, K., Shin, W.-Y., & Lee, D. (2020). Machine learning-based prediction models for formation energies of interstitial atoms in HCP crystals. *Scripta Materialia*, *183*, 1–5. doi:10.1016/j.scriptamat.2020.02.042