

# Graduate Student Research Seminar

## Fall 2023

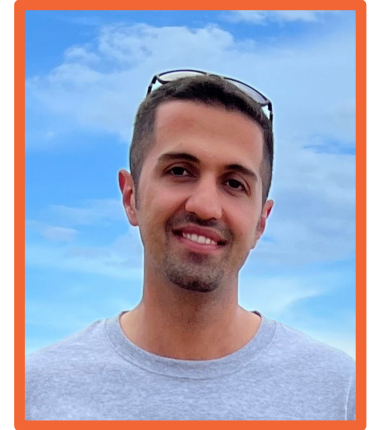
### From anti-Arrhenius to Arrhenius behavior in a dislocation-obstacle bypass

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**Advisor: Dr. Enrique Martinez-Saez**

**Monday, November 6<sup>th</sup>**

**3:00 pm (EST) – 132 Fluor Daniel Building**



### Abstract

Dislocations are the primary carriers of plasticity in metallic material. Understanding the basic mechanisms for dislocation movement is paramount to predicting the material mechanical response. Relying on atomistic simulations, we observe a transition from non-Arrhenius to Arrhenius behavior in the rate for an edge dislocation to overcome the elastic interaction with a prismatic loop in tungsten. Beyond the critical resolved shear stress, the process shows a non-Arrhenius behavior at low temperatures. However, as the temperature increases, the activation entropy starts to dominate, leading to a traditional Arrhenius behavior. We have computed the activation entropy analytically along the minimum energy path following Schoeck's methods, which capture the cross-over between anti-Arrhenius and Arrhenius domains. Also, the Projected Average Force Integrator, another simulation method to compute free energies along an initial transition path, exhibits considerable concurrence with Schoeck's formalism. We conclude that entropic effects need to be considered to understand processes involving dislocations bypassing elastic barriers close to the critical resolved shear stress. More work needs to be performed to fully understand the discrepancies between Schoeck's and PAFI results compared to molecular dynamics.



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