Alloy plasticity: from the atoms up

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Abstract The optimal performance of advanced materials requires an in-depth understanding of the microstructural defects that control mechanical and functional properties. Modelling these defects directly from the atomic scale has made tremendous progress, in particular with the dissemination of first-principles calculations that can yield quantitative predictions. Such calculations remain however limited in space and time. More approximate potentials are still needed and undergo currently a revolution with the development of machine learning potentials. However, to really change scale, continuum theories based on elasticity remain in high demand to understand generic behaviors.

I will discuss some fundamental issues related to modeling plasticity in metals and ceramics at different length scales, highlighting the successes and limitations of first-principles calculations and interatomic potentials. I will talk about the modeling of dislocation cores and how their structure and mobility is affected by solute atoms, with a special attention for screw dislocations in body-centered cubic alloys [1,2,3]. I will also address transformation-induced plasticity in zirconia-based ceramics, which we address thanks to machine learning potentials allowing to account for stable and metastable phases [4]. In a bottom-up approach, I will finally discuss what we can learn using only elasticity on the plasticity of solid solutions [5,6].

References

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