Ab initio calculations shedding light on atypical plastic behaviors

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The goal of this seminar is to show how atomic scale calculations have helped improve our understanding of materials plasticity and how these methods can provide fruitful input for larger-scale simulations. The presentation will mainly be focused on body-centered cubic (BCC) metals, which are known to display an atypical plastic behavior at low temperatures. I will show how *ab initio* calculations have enabled evidence a strong link between dislocation core energies and BCC metals electronic structure [1], as well as how we used these techniques to predict macroscopic Schmid law deviations in good qualitative agreement with experiments [2] (see figure). I will also introduce new research projects I would like to start at Université de Lorraine, within the scope of the Labex DAMAS.

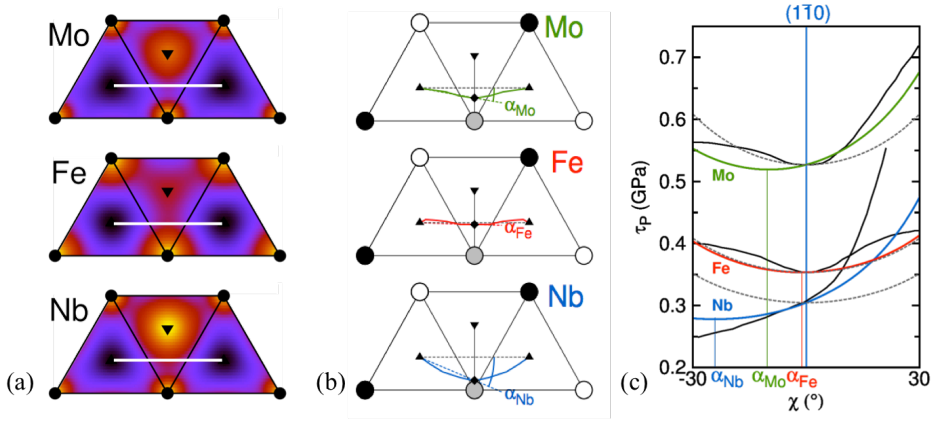

Illustration of link between atomic-scale dislocation core properties and macroscopic BCC metals plasticity in Fe, Mo and Nb. (a) Energy landscape that describes the interactions between dislocation and crystal lattice calculated with *ab initio* methods [1]. The landscape is asymmetric with respect to the glide plane (white horizontal line). (b) In consequence of the asymmetric landscape, the trajectory followed by the dislocations when they glide (colored lines) deviates from the horizontal glide plane. The deviation is quantified by an angle α that depends on the metal [2]. (c) Predictions of plastic anisotropy obtained from *ab initio* calculations (colored lines) compared to experimental measurements (black line). Accounting for the deviation α explains why the anisotropy is the largest in Nb, intermediate in Mo and the smallest in Fe. The Schmid law (dotted lines) that has been used since 1930 to describe plastic deformation fails to reproduce BCC metals' plastic anisotropy and the fact that it is metal dependent.

[1] L. Dezerald et al. *Phys. Rev. B* **89,** 024104 (2014)
[2] L. Dezerald et al., *Nature Commun.* **7**, 11695 (2016)