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On the numerical atomistic characterization of interfacial plasticity

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Interfaces such as grain boundaries and phase boundaries play a crucial role in the plastic deformation of materials. While the interaction between dislocations and grain boundaries has been studied for decades in ideal cases, like for low angle grain boundary or with 2D approaches, realistic features of interfaces have been largely ignored. High angle non-symmetric grain boundaries, phase boundaries with complex intermetallic, interfaces with segregated solute, etc., are few of the parameters that can alter drastically known models and mechanisms of the plasticity at interfaces.

This poster will showcase peculiar plasticity mechanisms at interfaces as revealed by atomistic simulations based on semi-empirical potentials. From superalloy [1], to Mg-base composites [2,3] and MAX phases [4], this endeavor will encounter complex intermetallics, nano-twist phases and zonal dislocations.

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[2] J Guénolé, F-Z Mouhib, L Huber, B Grabowski, S Korte-Kerzel, Basal slip in Laves phases: The synchroshear dislocation, Scripta Materialia 166 (2019).
[3] J Guénolé, M Zubair, S Roy, Z Xie, M Lipińska-Chwałek, S Sandlöbes-Haut, S Korte-Kerzel, Exploring the transfer of plasticity across Laves phase interface in magnesium alloy, Materials & Design 202 (2021).
[4] J Guénolé, V Taupin, M Vallet, W Yu, A Guitton, Features of a nano-twist phase in the nanolayered Ti3AlC2 MAX phase, Scripta Materialia 210 (2022)