Chemical disorder and stacking fault width dependence of edge dislocation yielding in face-centered cubic high entropy alloys

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High entropy alloys (HEAs) have attracted much attention within the materials science community owing to an ever-increasing demand, due to their superior mechanical properties [1]. One of the causes of excellent mechanical properties in HEAs is the complexity of dislocation responses to applying stresses, in contrast to traditional alloys. In this study, we investigate the edge dislocation behavior under applying stress in several equimolar face-centered cubic (FCC) single-crystal, single-phase solid solution alloys (i.e., CrCoNi, CrMnCoNi, CrFeCoNi, CrMnFeCoNi, FeNi) using molecular dynamics simulation. In FCC materials, edge dislocations dissociate to two Shockley partial dislocations which are separated by a stacking fault. To describe the complex interaction between stacking faults and chemical disorder during loading, dislocation roughness and stacking fault width as a function of applying stress are tracked. Fig.1 represents two partials separated by a stacking fault at the depinning stress for these configurations. According to our findings, close to depinning stress (σ_c) all these parameters reside at their respective maximum. The velocity of dislocations, as a function of applying stress, is also calculated for these alloys. The alloys with higher dislocation roughness demonstrate overhangs of the two partials, a finding that may require novel theoretical depinning descriptions. Existing analytical yield stress predictions [2] are compared with the identified depinning stresses and the results are discussed. Finally, we find that the ratio of saturation roughness to stacking fault width at depinning stress with (σ_c) is a reliable predictor of strength and possibly, exceptional mechanical properties, in these alloys.

Keywords: Fcc high entropy alloys, dislocation Roughness, depinnining stress, chemical disorder, Stacking fault width.

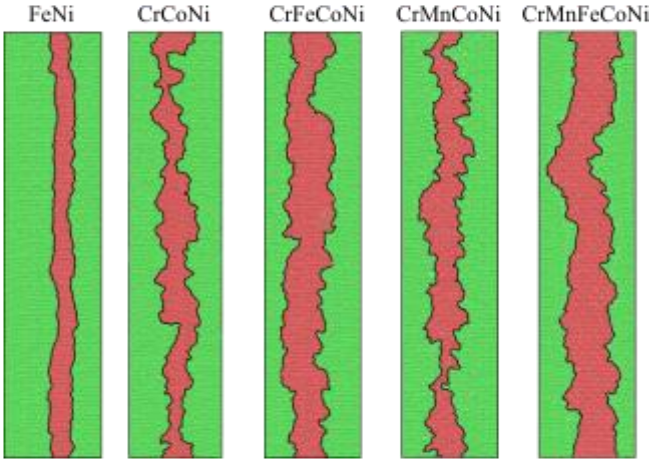

Fig.1 Two partial dislocations separated by stacking fault (red) at depinning stress for equimolar random fcc alloys. Atoms with fcc and hcp structures are colored by green and red, respectively.

References:

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[2] C. Varvenne, A. Luque, W. A. Curtin, Theory of strengthening in fcc high entropy alloys, Acta Materialia,118, 2016, 164-176.