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Atomistic Investigation of Elementary Dislocation Properties Influencing mechanical behaviour of fcc CrFeMnNi alloy and $FeNi_{10}Cr_{20}$ alloy

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In HEA, some specific features such as high solid solution, strain hardening, unusual combinations of strength and ductility, slowed down phase transformation kinetics and improved irradiation resistance have been largely identified. Crystal defects such as dislocation's structure are obviously at the origin of many observed features. This present work gives a better understanding of the impact of dislocation elementary properties on the plastic behaviour of single phased HEAs thanks to atomistic simulation techniques using an embedded-atom method (EAM) potential developed by Ayobami et al., [1]. This potential has been shown to describe the dislocation properties of fcc single-phase CrFeMnNi systems and their subsystems. Static properties namely: dislocation core structure, stacking fault energy, dissociation distance was evaluated as a function of local chemical environment and temperature. The work shows that structure and mobility of <110>{111} edge dislocation depends on the fluctuation of the local stacking fault energy, therefore, resulting in high critical shear stress required to cause dislocation motion due to the chemical complexity of the HEA. The obtained results were compared to austenitic stainless steel (Cr20Fe70Ni10 at. %). The results are in reasonable agreement with experimental measurements and theoretical explanations.

References:

[1] A. Daramola, G. Bonny, G. Adjanor, C. Domain, G. Monnet, A, Fraczkiewicz, Development of a Plasticity-oriented Interatomic Potential for CrFeMnNi High Entropy Alloys, Computational Materials Science, 203 (2022) 111165. https://doi.org/10.1016/j.commatsci.2021.111165.