GRADUATE STUDENT RESEARCH SEMINAR SERIES (2019)

THE EFFECT OF GRAIN BOUNDARY INTERFACE IN HIGH ENTROPY ALLOY (HEA) DEFORMATION

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HEA is gradually gathering more attention from material science field. Through Dr. Brian Cantor's research, it has been found that creating an alloy that has a desirable property by mixing multiple elements is an achievable goal. Despite the research field is highly active right now, studies about the effect of its interface is relatively scarce. Therefore, the aim of this research is to study the effect of interface. It has been suggested that Interfacial defects, such as grain boundaries, affect twin nucleation during deformation process. Hence, the effect of grain boundary types to twin nucleation and propagation is studied in this research. To achieve the stated goal, Molecular Dynamics (MD) simulation approach is adopted. Using the research software LAMMPS, bi-crystal structures are generated to isolate the effect of grain boundaries on a deformation mode. In the bi-crystals, each crystal structure contains an equimolar High entropy alloy (HEA), which have Co, Ni, Cr, Fe, and Mn. Pure tensile stress is applied to each bi-crystal structure to the point of fracture. The current research contains the study of grain boundaries that have (110) and (111) plane normal orientation. Simulation results of defects free single crystal deformation are added for the purpose of comparison.

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