ICSMA19 Metz, France, June 26 - July 1, 2022
International Conference on Strength of Materials

Deformation behaviour of $(CoCrFeMn)_{1-x}Ni_x$ cantor alloy

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Equimolar CoCrFeMnNi, commonly known as Cantor alloy, has been the most widely studied among high-entropy alloys (HEAs) because of its excellent mechanical properties. Recently, the strength of these alloys has been studied as a function of concentration of individual constituents in pseudo-binary subsystems, like $(CoCrFeMn)_{1-x}Ni_x$, with the help of diffusion couple and nanoindentation *[1]*. This helps in isolating the effect of individual elements on the concentration. $(CoCrFeMn)_{1-x}Ni_x$ is an important series since its candidates remain single-phase fcc throughout the composition range from Cantor alloy to pure Ni. And the nanoidentation tests reveal that the alloy hardness remains constant for $0.2 < x < 0.7$ and then steadily decreases with $x>0.7$ upto pure Ni. However the strengthening and work hardening mechanism(s) in these alloys has not been completely explored. These alloys are known to be metastable with negative stacking fault energies (SFEs) , making them prone to deformation twinning or deformation induced hcp transformation via extended faults; and the preferred deformation mechanism strongly depends on the SFE *[2]*. In our study, we use MD simulations to perform uniaxial strain-controlled tensile tests at different test conditions on nanocrystalline cantor alloy, $(CoCrFeMn)_{40}Ni_{60}$ and pure Ni described by MEAM empirical potential, where grain boundaries provide nucleation sites for twins and extended stacking faults. We use the same initial microstructure for all our simulations to isolate the effect of composition and compositional fluctuations on the different deformation mechanisms. Our aim is to study the deformation mechanisms in these alloys and correlate them to SFE, which varies widely from negative SFE for cantor alloy to positive medium-high SFE for Ni. We study the influence of composition and compositional fluctuations on yield strength, which is controlled by grain boundary nucleation of partials in our specimens. We also anneal our nanocrystalline specimens of different alloys and pure Ni at different temperatures without loading, to see the effect of chemical fluctuations on grain growth.

Keywords: cantor alloy, low stacking fault energy, deformation twins, deformation induced hcp transformation.

References:

[1] T. Keil et.al, JMS 36, 2558-2570 (2021).

[2] X. Sun et.al, Materials and Design 199, 109396 (2021).