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The interplay of short-range order and exceptional mechanical properties in fcc VCoNi concentrated solid solutions: A combined molecular simulation study of dislocation defect dynamics and thermal aging effects

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Single-phase, concentrated solid solution (CSS) CrCoNi medium-entropy alloys with face centre cubic (fcc) crystal structure, have been recently found to display excellent mechanical properties. In particular, equiatomic CrCoNi solid solutions show higher yield strengths than the famed Cantor CrMnFeCoNi high entropy alloy at cryogenic and room temperatures [1-2]. The main explanation for the exceptional behavior of CrCoNi solid solutions, is based on the Labusch-Varvenne class of solid solution analytical models, which point to the larger atomistic mismatch that is induced by Cr atoms. To further investigate the extent of the validity of this theory, in this study, we numerically investigate equiatomic VCoNi fcc CSS alloys, given that vanadium has a larger atomic volume than chromium and produces a larger atomic mismatch. Using Molecular dynamics (MD) simulations, we calculate the depinning stress, dislocation roughness, and stacking fault width for edge and screw dislocations for four fcc VCoNi CSS alloys including $V_{0.33}Co_{0.33}Ni_{0.33}$, $V_{0.35}Co_{0.2}Ni_{0.45}$, $V_{0.33}Co_{0.17}Ni_{0.5}$, and $V_{0.17}Co_{0.33}Ni_{0.5}$. With a random distribution of atoms, we find that the alloy composition $V_{0.35}Co_{0.2}Ni_{0.45}$ displays the larger atomic mismatch, and also exhibits the largest depinning stress at 300 K. Furthermore, we use Hybrid Molecular-dynamics/Monte-Carlo simulations to facilitate thermally induced kinetics, and in this way, we investigate possible effects of annealing/aging at various temperatures, and investigate the possible correlation to short-range order effects. We identify the emergence of chemical short-range order that increases with decreasing annealing temperature, a finding that is analogous to the behavior seen both numerically and experimentally in CrCoNi solid solutions. The causal effect of short-range order on the magnitude of the depinning stress is discussed.

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