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Solute Strengthening Mechanisms in Concentrated Solid Solutions: Role of Short Range Order

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Tailoring fine-scale compositional order/disorder features in Concentrated Solid Solutions (CSSs) is considered as one of the most effective approaches to enhance alloy strengths at design levels. It has been known for many years now that Short Range Ordering (SRO) and associated microstructural heterogeneities, along with lattice distortion effects, tend to impede motion of dislocations within CSSs, leading to significant hardening features at macro scales. However, atomic-level details of such complex solute-precipitate-dislocation interactions, as the most relevant solution strengthening mechanisms, has yet to be understood. Here in this work, we report on molecular dynamics simulations of model NiCoCr medium-entropy alloys (MEAs) which have been shown to nucleate segregated (Ni-rich) nano-scale phases under special heat treatments (i.e. annealing) [1, 2]. Our focus will be on the structure of (residual) stress fluctuations and local elastic properties across scales as relevant metrics that are closely tied to SRO-induced heterogeneities. Our analysis indicates bi-modal distributions of local elastic constants that resemble the spinodal-type decomposition of phases in MEAs. We show that the presence of SROs introduces a stress noise field that is not quite random but rather correlated over certain lengths that tend to scale with the characteristic size of precipitates. Such correlations may have important implications in terms of solute strengthening theories in multi-component alloys that typically assume random arrangements of solute atoms within the alloy matrix.

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