Multiscale modelling of defect evolution in equiatomic multicomponent alloys

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High entropy alloys, and a sub category of them, equiatomic multicomponent alloys, have shown both good mechanical and corrosion resistant properties, desired in future nuclear power plant concepts. The alloys have good mechanical properties both at cryogenic temperatures as well as at high temperatures. But to use them in environments where radiation is present, it is crucial to know their radiation response. In recent studies it have been found, both computationally and experimentally, that they also show a reduction in accumulated defects, compared to their elemental materials [1,3]. It was found that one key mechanisms of this reduction was the mobility of dislocations [1,2,3]. The results show that the binary NiFe and the ternary NiCoCr and NiCoFe all show better response to irradiation damage, compared to pure Ni and binary NiCo. Simulations of dislocation mobility show that the dislocations can easily move in Ni and NiCo, whereas the other alloys show a lower mobility and a higher onset stress. One of the key questions regarding especially nuclear power plants is the long time evolution of the materials, when the expected lifetime of modern power plant are over 50 years. To answer this question, we have started to use a multiscale approach to the problem, to assess the defect annealing and evolution over longer timescales. The defect production is simulated with Molecular Dynamics (MD), which can capture the picosecond primary damage production, and then use a Self Evolving Atomistic Kinetic Monte Carlo (SEAKMC) method to assess the long time evolution. These two methods will be used consecutively after each other, first to produce the correct damage (with MD) and then anneal it at timescales proportional to experimental ones (with SEAKMC).

[1] Granberg et. al, *Physical Review Letters* **116**, 135504 (2016).
[2] Granberg et al., *Nuclear Instruments and Methods in Physics Research Section B* , Accepted for publication (2016).
[3] Levo et al., *In preparation* , (2016).