Simulations of primary damage in a High Entropy Alloy: probing enhanced radiation resistance

High Entropy Alloys attract attention as possible radiation resistant materials, a feature observed in some experiments that has been attributed to several unique properties of HEA, in particular to the disorder-induced reduced thermal conductivity and to the peculiar defect properties originating from the chemical complexity. To explore the origin of such behavior we study the early stages (less than 0.1 ns), of radiation damage response of a HEA using molecular dynamics simulations of collision cascades induced by primary knock-on atoms with 10, 20 and 40 keV, at room temperature, on an idealized model equiatomic quinary fcc FeNiCrCoCu alloy, the corresponding “Average Atom” material, and on pure Ni. We include accurate corrections to describe short-range atomic interactions during the cascade. In all cases the average number of defects in the HEA is lower than for pure Ni, which has been previously used to help claiming that HEA is radiation resistant. However, simulated defect evolution during primary damage, including the number of surviving Frenkel Pairs, and the defect cluster size distributions are nearly the same in all cases, within our statistical uncertainty. The number of surviving FP in the alloy is predicted fairly well by analytical models of defect production in pure materials. All of this indicates that the origin of radiation resistance in HEAs as observed in experiments may not be related to a reduction in primary damage due to chemical disorder, but is probably caused by longer-time defect evolution. [Deluigi2021] Deluigi, O., et al. Acta Materialia 213 (2021): 116951. https://doi.org/10.1016/j.actamat.2021.116951.