

Bridging the Atomic Scale and the Mesoscale in the Characterization of Defect Production and Evolution in High Entropy Alloys

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High entropy alloys (HEAs) have recently emerged as a new type of alloying of about five elements in equal or near equal ratios and form random in face centered cubic (f.c.c) or body centered cubic (b.c.c) crystal structure. They feature improved mechanical strength and high resistance to radiation owing to their unique electronic structure [2]. While previous transmission electron microscopy (TEM) and other studies showed that damage accumulation is reduced by increasing chemical disorder, they could not reveal vacancy clusters below 1-2 nm leaving critical gap in understanding defect formation and buildup in these alloys. To bridge this gap, we employ in this work positron annihilation spectroscopy, which has unique capabilities in probing atomic scale defects with remarkable sensitivity [2].

Single phase HEA samples of CrFeMnNi, AlCrFeMnNi and AlCrFeCuNi with different alloying percentage prepared by spark plasma sintering were characterized by X-ray diffraction and TEM, then measured by depth resolved Doppler broadening spectroscopy (DBS) [3] and positron annihilation lifetime spectroscopy (PALS) [4] before and after irradiation by 10 MeV Si ions. High energy ions were selected to avoid introducing foreign atoms in the alloys which may complicate the interpretation of the data. This work represents the first depth resolved PALS measurements on HEAs. They reveal two positron lifetime components in the as-cast samples corresponding to two dominant groups of defects, small vacancy clusters (~ 5 V) and large vacancy clusters (~ 40 V) [5], their size and density distributions are varied by changing the order and nature of chemical disorder. After passing high energy Si ions through the matrix, we observed reduction in the size of the small and large clusters. The magnitude of reduction was strongly dependent on the nature of chemical composition.

The decrease in the size of vacancy clusters in the as-cast samples after irradiation indicates that interstitials created in collision cascades fill some of the original vacancies in the matrix. It is interesting that the size of the original vacancy clusters and its change with irradiation is very dependent on the nature of chemical disorder, and it is strongly affected by replacing even one element or modifying its percentage. The increase in the number of small vacancy clusters after irradiation was also impacted by the nature of chemical disorder.

The work reveals how the nature of chemical disorder impacts cascade void interactions in HEAs [6].

References:

[1] DS AIDHY et al., *Acta Materialia* **99** (2015), p. 69.

[2] FA Selim, *Materials Characterization* **174** (2021), p. 110952.

[3] FA Selim et al., *Radiation Physics and Chemistry* **68** (2005), p. 427.

- [4] L Zhang et al., *Photonics Research* **7**(5) (2019), p. 549.
- [5] S Agarwal et al., *Science advances* **6**(31) (2021), p. eaba8437.
- [6] The authors acknowledge funding from the National Science Foundation (NSF) under Award # DMR-2005064.6 and thank the staff scientists at Helmholtz-Zentrum Dresden-Rossendorf in Dresden, Germany for valuable contributions.