Defects Act in an "Introverted" Manner in FeNiCrCoCu High-Entropy Alloy under Primary Damage

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Threshold displacement energy (E_d) is a critical parameter in radiation damage theory, which is defined as the minimum energy required to displace an atom from its lattice site and create a stable pair of Frenkel defects in the perfect crystal. To search for E_d along a given incident direction, we adopted a binary search algorithm [1] as the following steps: initially, the recoil energy of the upper limit E_{up} was set as 200 eV, which was warranted to sufficiently displace a sited atom; the lower limit E_{lo} was set as 0 eV, then the average energy E_{av} of E_{up} and E_{lo} was assigned to the chosen recoil atom centered the box. After the system recovered from recoil-induced displacement cascades, the Wigner-Seitz method was used to examine whether a Frenkel pair has been created. If yes, then the E_{av} will be set as the new E_{up}, otherwise it will be E_{lo}. This process was iterated until the difference between E_{up} and E_{lo} was less than 1 eV, then the final E_{av} was the searched E_d. We know, E_d is dependent on the primary recoil direction, atom type and local chemical environment [1,2]. The flowchart for calculating threshold displacement energy is shown in Figure S1. In order to reveal the pattern of E_d distribution on magnitude and direction, the recoil events with directions

randomly selected from a 4π solid angle were simulated for 500 times for each recoil element in all crystals studied here.

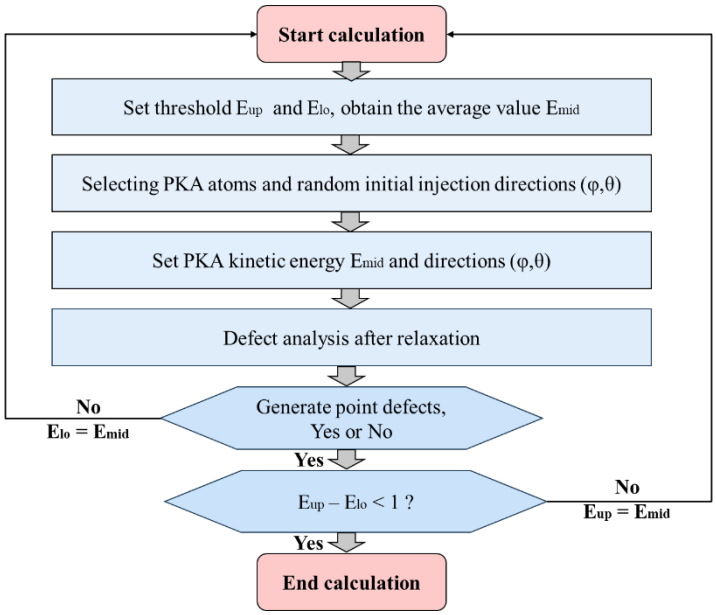

Figure S1. Flowchart for calculating threshold displacement energy.

References

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