Cascades in fcc Ni-Fe Solid Solution and He Interaction with Solutes and Impurities in Nano-structured Ferritic Alloys

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Molecular dynamics is employed to simulate atomic collision cascades in a Ni-30at.%Fe fcc solid solution. Electronic stopping is modeled as a frictional force for atoms with kinetic energy > 10 eV. Cascades are performed at 700 °C, with a primary knock-on atom energy (E_{PKA}) up to 70 keV. Comparison of cascades initiated with Ni versus Fe PKAs shows that the defect production is similar. Both types of PKA also produce a similar fraction of Ni defects, which is approximately the same as the fraction in the alloy. The defect production curve as a function of E_{PKA} exhibits two regimes of power law, where the high-energy regime occurs for E_{PKA} > 10 keV. In the high-energy regime, > 80% of interstitial defects are clustered and the average size (number of interstitials) of the largest clusters is > 10. For small clusters (size < 10), the dominant Burgers vector is <100>, while for larger clusters (>10), it is <110>. Cascades in pure Ni are simulated with E_{PKA} = 20 and 50 keV for comparison. The results show that defect production and clustering in the alloy is smaller than in Ni. In the second part of this presentation, density functional theory is employed to study the interaction between He and transmutation products, alloy solutes, and impurities in 14-YWT nano-structured ferritic alloy. Strong attraction is found between a substitutional He with Y (binding energy = 1.24 eV), Mg (0.52), Ti (0.34), Si (0.34), Al (0.32), Ni (0.26), Ta (0.23), Mn (0.16), Mo (0.10). For an interstitial He, it is strongly attracted to Y (0.46), Mg (0.32), Ti (0.16). These interactions could potentially promote He bubble nucleation and increase the population of small He bubbles that are invisible under an electron microscope; yet contribute to void swelling. Interstitial He is also attracted to impurity O (0.33), C (0.15), and N (0.12). Under fusion neutrons, approximately 3-5 times more H is produced than He. Thus, the interaction with H is also studied. Hydrogen is found to be strongly attracted to substitutional He (0.56), suggesting that hydrogen may exacerbate the He bubble formation in these alloys.