

A phase-field approach to predict the formation conditions of the high burn-up structure in U_3Si_2

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Studying the formation conditions of the High Burn-up Structure (HBS) in nuclear fuels is necessary to predict fuel performance under different scenarios. This structure forms at the edge of a fuel pellet below a specific temperature after a relatively long exposure to irradiation. It is characterized by small grains and micro-sized pores. The HBS has been observed in many fuels including U_3Si_2 . U_3Si_2 is a promising accident tolerant fuel for LWR due to its higher thermal conductivity and uranium density compared to UO_2 . The current work investigates the burn-up and temperature thresholds for the HBS in U_3Si_2 using a phase-field grand potential model coupled with a Binary Collision Monte Carlo (BCMC) code. The current work predicts the formation conditions of the HBS by comparing the free energy of an irradiated microstructure to the free energy of the HBS. A radiation damage model has been developed to estimate the free energy of the irradiated microstructure. A collision cascade model is used to calculate point defect generation rates. The interactions between different types of defects and sinks are accounted for. The free energy of the HBS is mainly due to the abundance of grain boundaries. The HBS is more energetically favorable after a certain dose rate, depending on the temperature. The thresholds for the HBS in UO_2 have been determined experimentally and therefore, the current work is first applied on UO_2 . This work was performed using MARMOT and MyTRIM, a mesoscale fuel performance code and a BCMC code, respectively. Results for both fuels will be shown across a range of temperatures.