Mesoscale Modeling of High Burn-up Structure (HBS) Formation and Evolution in UO_2

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A novel phase field model was developed to simulate the High burn up structure (HBS) formation in UO_2. Derived from irreversible thermodynamics, the model makes no prior assumptions on the nucleation rate or recrystallized grain size and shape. The model parameters were evaluated in terms of kinetics and thermodynamic properties. Moreover, this model takes into consideration the interfacial energies of grain boundaries and bubble surfaces, strain energy associated with dislocations, and the chemical energy of gas atoms. This render the model capable of simulating the formation and growth of sub-grains and bubbles concurrently. The model predicted strong influence of dislocation density (its magnitude and distribution), grain boundary energy, and bubble surface energy on the sub-grains formation. For polycrystalline UO_2, the model results for the recrystallized average grain size was performed to be on the order of 0.6-1.3 microns associated with a critical dislocation density range of $\rho = 9x10^{15} - 1.2x10^{16}\ m^{-2}$, which corresponds to burn-up values between $98 - 105\ GWD/TU$, in agreement with the range reported in literature.