Modeling the microstructure change for irradiated systems within the phase field crystal method

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We study a microstructure change of crystalline systems described in the framework of the phase field crystal approach. We consider the system behavior in three stages following one after another. The first stage is a growth of he crystal (initial pattern). Starting from chaotic configugarion (liquid state) with fixed number density we investigate ordering processes and configuration of point defects with grain boundaries formation. This object we subject to irradiation modeled by ballistic diffusion with stochastic character (athermal mixing of atoms due to interactions of atoms with high energy particles representing influence of irradiation). In this stage we study formation of structural disorder and emergence of amorphous configurations. At final (the third) stage we switch off irradiation flux and consider recrystallization processes studying dynamics and statistics of defects (point defects, dislocations and grain boundaries). Such hybride phase field crystal approach describes defects annealing in the irradiated systems on the level of diffusion time scales and microscopic spatial scales.

It was found that during irradiation a melting processes in the vicinity of defects belonging to grain boundaries are realized. Here action of correlated stochastic component of the ballistic flux sustaining ordered (crystalline) configuration of the system competes with it regular component producing athermal mixing. Considering recrystallization processes it was found that the perturbed system relaxes to the stationary configuration (defects annealing) with low point and linear defect densities. An influence of the stochastic component of the ballistic flux is able to form stripe patterns where atomic density smears along atomic closed packed directions. Such patterns are stationary due to atomic densities of neighbor sites are overlapped. A transition to equilibrium initial configuration in statistical sense is possible only at elevated temperatures.