Abstract

Advancements in fusion reactor technology has led to the construction of ITER and the realisation of fusion energy is closer than ever before. However, realisation of fusion energy critically depends upon breakthrough in the design of structural materials that can withstand large amounts of radiation damage. Most important of the structural materials are the blanket module which is exposed to harsh environment such as high radiation flux, thermal flux and mechanical stresses. These severe conditions restrict the choice of candidate materials for the construction of blanket modules. Among the candidate materials proposed for the construction of blanket modules in fusion reactor, Vanadium alloys are of great interest due to their suitability for the application in terms of its open crystal structure (BCC), low swelling, high melting temperature, and resistance to radioactive transmutation.

Blanket modules directly face the plasma and hence it is exposed to fast moving neutrons that escape the plasma confinement. Most of the damage occurs mainly in the form of generation of point defects viz vacancies and self-interstitials. These points defects evolve over time and agglomerate into clusters, voids and dislocation loops causing further damage to the microstructure leading to embrittlement, void swelling, and radiation induced segregation. Hence controlling radiation damage is of prime importance in enhancing the life of blanket modules which involves annihilation of point defects as they produce.

Annihilation of point defects and consequently controlling radiation damage is possible via interface engineering and grain boundary engineering. Especially, grain boundaries are shown to be effective in reducing the damage in nuclear reactors by acting as sinks to generated point defects. Efficacy of a grain boundary to annihilate the point defects is closely related to its character. However, the nature of grain boundary character and point defect interaction is not well understood. This understanding would inform the designing of radiation damage resistant materials via grain boundary engineering.

So, in this work, we studied the effect of GB character on damage accumulation in Vanadium <001> Symmetrical tilt GBs. For the present work molecular dynamics is used as it is most suitable to study the phenomenon of radiation damage. Grain boundaries are constructed, and cascade damage is simulated by MD software, LAMMPS. Then, grain boundary character was analysed by various parameters like GB energy, GB structure, free volume, vacancy and self-interstitial formation energies.

Cascade damage is conducted on some of the selected boundaries and the damage accumulation is quantified in terms of potential energy increase before and after the damage. Effectiveness of grain boundary in controlling the radiation damage is defined in terms of grain boundary efficacy for comparison purpose. Grain boundary efficacy is correlated with grain boundary character to establish design criteria which would inform the design of radiation damage resistant materials.

It was found out that grain boundaries reduce the damage accumulation at two stages one at the production stage by physically obstructing the primary knock on atom and two by absorbing the point defects thus generated. The effect of GB as impeding the PKA is predominant at early stages of radiation damage and sink behaviour of GB is important at later stages of radiation damage.