**Molecular Dynamic Simulation of Displacement Cascades in Zr-Nb Layered Composites**

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**Introduction**

The nano-sized multilayer composites have been extensively studied in the past five years. It has been reported that in irradiation cascade simulations the interface of binary layer composites can capture the irradiation produced defects (vacancy and interstitials) drastically. It is believed that certain type of interfaces can adopt several mutable atomic structures with similar degeneration energies, increasing the sink of point defect towards interfaces, and subsequently enhance the recombination/annihilation of the point defects [1]. The experiments also confirmed that nanolayered structures can remain no change in their overall morphology under irradiation, with no mixing or amorphization detected. The defect concentration after irradiation in nanolayered structure is also far below those of pure system at similar dpa levels. With respect to the wide application of zirconium alloy in Canadian nuclear industry, molecular dynamics (MD) simulation has been carried out in this study to investigate the irradiation damage in Zr/Nb nanolayered composites.

**Methods and Results**

MD calculations are carried out in LAMMPS molecular dynamics simulator to simulate irradiation induced cascades in Zr-Nb nano-sized multilayer composite. We design a sandwiches structure of Zr-Nb nano layerered composite as shown in Fig.1 to study the interface effects on irradiation induced defect production. A newly developed Zr-Nb Embedded-Atom Method potential will be applied in the simulation [2]. Various time step and periodical boundary condition are applied during cascade simulations. The Wigner-Seitz method and common neighbour analysis are employed to analyze defects.

An example of our cascade simulation is shown in Fig.2. The irradiation induced defects could be absorbed by the Zr-Nb interface. Based on Wigner-Seitz defects analysis, the number of defects per pka energy unit drops around 50% in Zr/Nb nanolayered composite compared to the simulation results in pure zirconium or niobium system.

**Conclusions**

We unveil the mechanism how interfaces trap and enhance recombination of irradiation induced defects in Zr/Nb nanolayered composite. To recognize the interface effects could help us to identify, design, and manufacture other potential nano-sized multilayer composites for future nuclear application.

**References**