Computational studies of high-dose radiation damage in hcp Zirconium

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Abstract

Heavy damage in materials induced by high-dose irradiation is important both for fundamental materials science and nuclear industrial applications. Benefited from recent developments of computational power, resources, and methods, it's possible now to simulate high-dose irradiation damage in metal crystals on the atomic scale. In this talk, I'll introduce our recent computational studies on high-dose radiation damage in hcp Zirconium (Zr), a widely-used material for fuel tubes in nuclear reactors. First, I'll show that a simple simulation of repeated collision cascades in the same box (i.e. cascade overlap) is able to give some novel insights on the formation of basal vacancy loops (<c>-type loops), which is a typical and important defect in heavily-irradiated Zr. Then I'd like to introduce another efficient method to simulate high-dose radiation, i.e., Frenkel pair accumulation (FPA) method, which is able to reach a dose level as high as several dpa. Using this method, I explore the extreme radiation damage in Zr, observing an asymptotic approach to a steady damage level, which features a high point defect content (~3%), nanoscale dislocation lines and loops, and significant anisotropic deformation strains. Finally I'd like to compare the defect accumulation in metals and non-metals from a potential energy landscape perspective.