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ROLE OF HE IN SWELLING OF NEUTRON IRRADIATED BERYLLIUM

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Beryllium is foreseen to be used as a neutron multiplier material for breeder blanket and as plasma facing material for the first wall of future fusion reactors. Helium as well as hydrogen isotopes are produced by neutron induced nuclear reactions and result in formation of gas filled bubbles and volumetric swelling of irradiated beryllium. It is known for a long time that swelling after irradiation in fission reactors at temperatures below 400-500C is directly proportional to the accumulated helium content suggesting importance of helium for this process.

In this paper we investigate the role of helium in low temperature swelling of beryllium using first principles quantum mechanical calculations. It was found that interstitial helium exists in beryllium in the form of a mixed dumbbell, which migrates preferentially along basal planes. Several helium interstitial are bound together and may form clusters. Two interstitial helium atoms can form either planar configuration where both helium atoms are laying in the same basal plane or inter-planar configuration. Both configurations are mobile at 800K and can transform into each other providing a migration path for three dimensional diffusion of the cluster. However if not helium end of dumbbells are met together no cluster formation was observed.

On the other hand being put into a vacancy cluster helium binds vacancies together which are unstable otherwise. In particular, using ab initio molecular dynamics we have observed a helium-three vacancy planar cluster which was stable at 800K during 13 ps while no diffusion jumps were observed. On the contrary helium-divacancy cluster is rather mobile and diffuses by classical ring diffusion mechanism though an intermediate split configuration vacancy-substitutional helium.

These findings are discussed with respect to helium induced gas bubble growth and swelling of neutron irradiated beryllium.