学 位 論 文 内 容 の 要 旨

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学 位 論 文 題 名

The effect of point defects on irradiation damage of Fe-based composite materials for fusion reactor

(核融合炉用 Fe 基複合材料の照射損傷に及ぼす点欠陥の影響)

Global warming is one of the most serious problem to humanity. It is considered to be predominantly influenced by the greenhouse gases generated by human activities emitting (GHG) into the atmosphere, so one solution is the reduction of these emissions. As a considerable GHG emissions comes from the production of electricity, a major changing of the electrical energy supply system is needed. Nuclear energy, which is considered as a GHG emissions-free energy source, could replace fossil fuel energy sources in the given time scale, safely, economically, reliably and in a sustainable way. Structural materials represent the key for containment of nuclear fuel and fission products as well as reliable and thermodynamically efficient production of electrical energy from nuclear reactors. Similarly, high-performance structural materials will be critical for the future success of proposed fusion energy reactors, which will subject the structures to unprecedented fluxes of high-energy neutrons along with intense thermomechanical stresses. Advanced materials can enable improved reactor performance via increased safety margins and design flexibility, in particular by providing increased strength, thermal creep resistance and superior corrosion and neutron radiation damage resistance.

In fission and fusion reactor environments structural materials generate significant amounts of hydrogen (H) and helium (He) by transmutation. The primary sources of helium are boron and nickel, interacting with both fast and especially thermal neutrons. Hydrogen arises primarily from fast neutron reactions, but is also introduced at often much higher levels by other environmental processes. Although essentially all of the helium is retained in the structural materials, it is commonly assumed that most of the hydrogen is not retained. Both H and He have a strong impact on the microstructure evolution of irradiated materials. To have a deep understanding of the H and He in irradiated materials, it is necessary to study H and He from viewpoint of physical. There are many theorical researches reported the behavior of H and He in metals, while just few focused on synergistic effect of hydrogen and helium.

In this work, synergistic effect of hydrogen and helium in α-Fe has been investigated using density functional theory calculation method. In perfect crystal of Fe, the presence of helium

atom would decrease the dissolution energy of hydrogen atom near helium atom. This implies the existence of an attractive interaction between hydrogen and helium atoms. It is also revealed that the most stable places for both hydrogen and helium atoms are two tetrahedral sites (T-site) with a distance of 2.16 Å. Furthermore, a vacancy-helium complex (Va-He) would be an effective trapping site for hydrogen atom compared with mono-vacancy, a Va-He would be able to trap 8 hydrogen atoms.

Beyond pure Fe, this work also focused on the interface between Fe and W. The dissolution behavior of hydrogen (H) at Fe/W interface and the effect of H on the strength of Fe/W interface are investigated. The dissolution of H atom at Fe/W interface would be easier than that in bulk of Fe or W due to the low charge density at Fe/W interface by the distortion of lattice. Hydrogen atom is expected to diffuse to Fe side of Fe/W interface due to its lower dissolution energy at Fe lattice at interface. While H atom could be trapped by vacancy at Fe/W interface. In addition, H and vacancy reduce the strength of interface, however, H atom at a special site seems to slightly increase the strength of interface. Furthermore, the electronic structures of interface are analyzed to give a physical understanding on the effect of H on Fe/W interface.

Last, Incoherent Fe/W interface, which is the structure close to the real Fe/W interface was focused. The cohesion properties of three incoherent Fe/W interfaces, Fe(100)/W(100), Fe(110)/W(110) and Fe(100)/W(110) interfaces. It is found that Fe(100)/W(110) interface has the lowest interface energy, followed by Fe(100)/W(100) and Fe(110)/W(110) interfaces. For all three Fe/W interfaces, obvious lattice disorder only can be found in Fe lattice. And the lattice disorder in Fe(100)/W(100) interface is most severe, even a pseudomorphic structure formed at the Fe layer in Fe(100)/W(100) interface. While lattice disorder in Fe(100)/W(110) interface is the weakest. Fe(110)/W(110) interface shows the strongest strength, it may be mainly due to the number of Fe-W bonds in Fe(110)/W(110) interface is more than other planes with same area. DOS also shows that compared with other two interfaces, a stronger chemical bond formed in Fe(110)/W(110) interface. Fe at Fe(100)/W(100) interface shows a very abnormal magnetism. In Fe/W interfaces, the formation of monovacancy could be easy than it in bulk Fe or W, and the results also suggest that Fe atom could migrate into W lattice if there is vacancy exist in W lattice. And the dissolution behavior of H and He at this Fe/W interface was investigated. A trapping effect of Fe(100)/W(110) interface are found, both H and He could be easily trapped at Fe(100)/W(110) interface.