Helium Induces Grain Boundary Fracture of Iron – Finding a Universal Law of Grain Boundary Strength Loss Using a Supercomputer

Reduced activation ferritic steels are being considered as structural materials of future nuclear fusion reactors. However, it is expected that these steels will become brittle after long-term exposure to a fusion reactor’s environment. This may be caused by a decrease in the strength of the grain boundaries (GBs), which are surfaces between two adjacent grains. We suspect that loss of the strength may be caused by helium (He) accumulation at the GBs, which is generated by nuclear transmutation reactions under fast neutron irradiation. He is accumulated either in the form of bubbles or in an atomic form without forming bubbles. The former occurs under high temperatures and can be observed by electron microscopes. The latter is supposed to occur at low temperatures, but it is difficult to determine the locations or the amount of He involved using experimental means; therefore, the relationship between the GB cohesive energy and the amount of accumulated He is not easily known. For this reason, we particularly focused on the application of computational methodology to He embrittlement without bubble formation under low temperatures.

In the present study, we defined GB cohesive energy as the total system energy increase due to ideal fracture (Fig.10-2) at the GB divided by its area. If this total energy increases, the cohesive energy is positive and a fracture is not expected; otherwise, the fracture is more likely to occur. We evaluated this energy using an atomistic modeling method.

Fig.10-2 Calculation method for GB cohesive energy
GB cohesive energy is defined as the total energy increase per unit area after separating the system at the GB, as shown in (a). The GB used for the present study is symmetrical at the boundary, as seen in (b), being called the symmetrical tilt GB.

Fig.10-3 The universal relationship between GB cohesive energy and He concentration
GB cohesive energy decreases as He is accumulated. The above value is normalized to the cohesive energy without He accumulation.

Reference