学 位 論 文 内 容 の 要 旨

DISSERTATION ABSTRACT

博士の専攻分野の名称　博士（工学）　氏名　王　帥

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Hydrogen effect on dislocation motion in Fe and Ferritic alloys

(鉄およびフェライト鋼中の転位運動に及ぼす水素の影響)

This dissertation contains research work attempting to solve many unknown problems in hydrogen embrittlement phenomenon of BCC iron. Experimental and computational methods have been employed and the dislocation motion under hydrogen environment are investigated.

To evaluate the hydrogen effect on coupled evolution of dislocation velocity and mobile dislocation density in Fe-based alloys, thermal activation parameters and dislocations structures were obtained using repeated stress relaxation tests on pure iron, Fe-8Cr alloy and F82H (IEA heat) steel. For all of the samples, the rates of stress relaxation are increased by hydrogen. Referring to constant strain, hydrogen charging decreases the thermal activation volume, internal stress ratio, and exhausting rate of mobile dislocation density.

In pure iron, The effective activation volume and the thermal stress were determined at different hydrogen concentrations. The effective activation volume decreases immediately with cathodic charging. At high hydrogen concentrations, the activation volume decreases to lower level and the thermal stress increases rapidly. The density of mobile dislocations in the hydrogen-charged iron has lower exhausting rate than the hydrogen-free one. The average dislocation velocity increases as a function of hydrogen concentration. By using transmission electron microscopy (TEM), hydrogen-induced tangled dislocations are found, which indicates that the repulsive stress field between dislocations becomes weak. Hydrogen has two aspect effect in these metals: shielding the dislocation-barrier interaction due to hydrogen concentration difference; impeding dislocation motion in low concentration due to solute-solution effect and the produced tangled dislocation. Normally the softening will be

observed in well annealed steel. However, the two-aspect effect may invoke increase of flow stress in some case, which is depending on the deformation history, surface condition and internal structure of metals.

In Fe-8Cr alloy and F82H steel, due to the existing of precipitates, the hydrogen concentration is 10 times and 100 times more than in pure iron respectively. hydrogen enhanced softening leads to tangled and polygonized dislocation structures along precipitates. A general expression of hydrogen-induced thermal activation energy is derived. The activation energies is reduced in pure iron, while in Fe-8Cr and F82H steel, the activation energies are almost stable on account of the pinning effect of precipitates. The short-range interaction of dislocation and energy barrier is the key factor dominating the hydrogen-dislocation motion in BCC metals. This interaction varies the thermal activation energy in a narrow range, but makes the dislocations be tangled or network or even cell structures. The mechanical property changes mainly due to the organised dislocation structures in local area.

By using the density functional theory, hydrogen atoms are found to increase the density of free electrons in the simulation cell and have bonding interaction with Fe atom. The increased electron density improves metallic character of iron and enhances softening phenomenon observed by stress relaxation tests. Caused by anisotropic strain components of hydrogen atoms in the tetrahedral sites, elastic interaction for hydrogen with screw dislocation has been found.

Employing a density function theory based embedded-atom method potentials, the evolution of edge and screw dislocation core structures are calculated at different hydrogen concentrations. The hydrogen-screw interaction predicted by the density functional theory has been proved. The core energy and Peierls potential of the dislocations are reduced by hydrogen. A broaden-core and a quasi-split core structure are observed for edge and screw dislocation respectively. The screw dislocation and hydrogen interaction in body-centred cubic iron is not due to the change of elastic modulus, but the variation of dislocation core structure. The short-range interaction predict by simulation coincides with our experimental work.