12-4 Development of Steel Impurity Behavior Simulation Technology
–Estimation of Impurities in Materials Based on Thermal Desorption Gas–

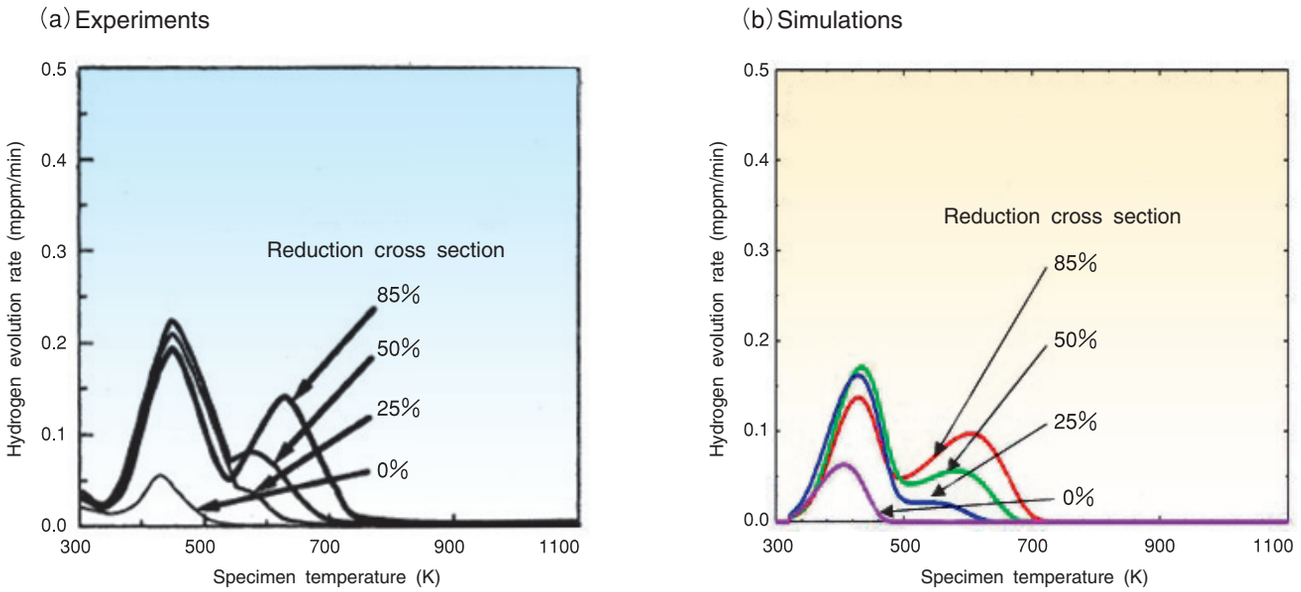

Fig.12-7 Comparison of the hydrogen desorption profile of deformed eutectoid steel: (a) Experiment results (b) Simulation results
The numerical model simulates one peak at the low temperature side, which may relate to hydrogen desorption from defects of vacancy or dislocation, and the other peak at the high temperature side, which may be due to an increase in phase interfaces caused by the cold drawing.

Steel is a basic structural material which is used for various constructions. Steel material inevitably includes impurities and defects disrupting the crystal structure. which are vacancies, dislocations, grain boundaries, phase interfaces, and inclusions. Hydrogen, the smallest and lightest element, also enters into materials from the environment as impurities. Furthermore hydrogen seriously changes the mechanical properties of materials by migrating and combining with defects. The change of mechanical properties causes the degradation of material strength. Therefore, the estimation of the hydrogen and defects within materials is an important issue.

Defects in the steel lattice structure are called trapping sites because they capture hydrogen migrating from the defect-free crystalline regions. Type of defects can be distinguished by their differing energy for capture of hydrogen. Defects with deep energy valleys trap hydrogen strongly and defects with shallow energy valleys trap hydrogen weakly. Thus, the former defects release hydrogen at higher temperature, and the latter defects release at lower temperature. Inferring from this property, if there is a peak of desorbed hydrogen from a specimen heated at a constant rate, one can regard the hydrogen of the peak as being released from the defects with a specific trapping energy. Therefore, we can determine the type and amount of defect in the specimen, the trapping energy of the types of defects, and the amount of trapped hydrogen by analyzing the profile representing the relation between specimen temperatures and desorbed hydrogen. This analysis is called thermal desorption analysis. In order to estimate these quantities and the relation between them, we developed a numerical model of the hydrogen desorption process and tried to simulate the hydrogen desorption profile obtained by the thermal desorption analysis. Our model computes the equilibrium state between the hydrogen in trapping sites and the hydrogen in surrounding regions at each temperature, and regards hydrogen in the surrounding regions as desorbed hydrogen that produces the profile, though in practice hydrogen in the surrounding regions diffuses within materials. This model of the hydrogen desorption process is based the assumption that hydrogen migration is very fast in the defect-free crystalline regions.

As shown in Fig.12-7, our numerical model simulates very well the actual hydrogen desorption profile of eutectoid steel, which indicates several types of defects distinguished by different trapping energy. This successfully simulated profile has two peaks, which was difficult for previous models to reproduce, and allow us to estimate the amount of defects and trapped hydrogen and the trapping energy of the defects of each peak. This simulation also may suggest experimental conditions which will isolate the peak of a specific defect.

This idea and technique can also be applied to the estimation of helium in steel materials. The estimation of the amount of defects and trapped impurities, and the trapping energy of defects should be of use for research into the mechanical property change that causes embrittlement or hardening of nuclear steel materials.

Reference

Ebihara, K. et al., Modeling of Hydrogen Thermal Desorption Profile of Pure Iron and Eutectoid Steel, ISIJ International, vol.47, no.8, 2007, p.1131-1140.