

Site occupancies of hydrogen in Nb alloyed with oversized Ta atoms or undersized Mo atoms†

H. Matsuba,^{*1,*2} E. Yagi,^{*1,*2} C. Sugi,^{*2} Y. Okada,^{*2} K. Hirabayashi,^{*2} T. Iida,^{*2} S. Koike,^{*3} T. Hayashi,^{*2} N. Higami,^{*2}
Y. Murakami,^{*2} A. Takebayashi,^{*2} T. Yoshida,^{*2}, T. Sugawara,^{*4} T. Shishido,^{*4} and K. Ogiwara^{*1}

An interaction of hydrogen with solute atoms is one of the fundamental problems on hydrogen in metals, because various hydrogen-related properties are strongly affected by alloying. In order to understand the interaction, the knowledge of the atomistic state of hydrogen in alloys is highly required. However, such information has been extremely limited, because of experimental difficulties. Therefore, the channelling method utilizing a nuclear reaction of $^1\text{H}(^{11}\text{B},\alpha)\alpha\alpha$ with a $^{11}\text{B}^+$ beam of about 2 MeV had been developed.¹⁾ This method has been demonstrated to be very useful to locate hydrogen dissolved in metals.^{1,2)} In previous studies, the lattice location of hydrogen has been investigated systematically in detail in Nb alloyed with undersized Mo atoms up to 60 at. % by the channelling method at room temperature with a tandem accelerator. Their atomic radii are 1.43 Å for Nb and 1.36 Å for Mo atoms. This alloy system forms a solid solution over the entire Mo concentration (C_{Mo}) range, maintaining a bcc crystal structure, although the lattice parameter changes.

It has been demonstrated that the lattice location changes very sensitively with Mo concentration and, with the help of the measurement of width of X-ray reflection lines, that such change can be explained in terms of lattice distortion introduced by alloying with Mo atoms.³⁾ At low C_{Mo} , lattice is strongly distorted around Mo atoms. Hydrogen is trapped by a Mo atom to be located at a T_{tr} site, which is displaced from an original tetrahedral (T) site by about 0.6 Å towards the Mo atom, so as to reduce the distortion around Mo atom. There exists a strong attractive interaction between hydrogen and Mo atoms.⁴⁾ With increasing C_{Mo} , the lattice distortion is reduced owing to interference between strain fields around individual Mo atoms, and most of the H atoms occupy T sites as in Nb. For C_{Mo} higher than 39 at. %, the lattice distortion gradually increases again with increasing C_{Mo} because of the increase in the number of undersized Mo atoms in a unit cell, but not so strongly as that at low C_{Mo} , i.e., up to an intermediate level. In this case, H atoms are distributed over T and d - T sites, which is displaced from T sites to their nearest neighbour octahedral (O) sites by about 0.25 Å. The T -site occupancy is energetically more favourable than the d - T -site occupancy.

In the present study, the site occupancy of hydrogen in Nb alloyed with 2 or 5 at. % of oversized Ta atoms (atomic

radius: 1.44 Å), $\text{Nb}_{0.98}\text{Ta}_{0.02}\text{H}_{0.01}$, $\text{Nb}_{0.98}\text{Ta}_{0.02}\text{H}_{0.029}$ and $\text{Nb}_{0.95}\text{Ta}_{0.05}\text{H}_{0.01}$, was investigated by the channelling method at room temperature. The objectives of the present study are to investigate a difference in an interaction of hydrogen with solute atoms between oversized Ta and undersized Mo atoms and to examine the above-described interpretation on the basis of the lattice distortion.

The following results were obtained. Taking account of the previously reported results on $\text{Nb}_{0.95}\text{Ta}_{0.05}\text{H}_{0.018}$ and $\text{Nb}_{0.95}\text{Ta}_{0.05}\text{H}_{0.025}$,⁵⁾ in both $\text{Nb}_{0.98}\text{Ta}_{0.02}$ and $\text{Nb}_{0.95}\text{Ta}_{0.05}$ alloys, at low hydrogen concentration C_{H} , most of the H atoms are located at T sites, while at high C_{H} , most of them are at d - T sites displaced by 0.25 Å from T sites towards their nearest neighbour O sites, and the remains are at T sites. This result is different from that in Nb alloyed with similar concentration of undersized Mo atoms, where hydrogen preferentially occupies T_{tr} sites. It was deduced that, in both $\text{Nb}_{0.98}\text{Ta}_{0.02}$ and $\text{Nb}_{0.95}\text{Ta}_{0.05}$ alloys, the T site occupancy is energetically more favourable than the d - T -site occupancy, but the concentration of available T sites is limited. In these alloys, the lattice distortion is small and at an intermediate level, because of the smaller size difference between Nb and Ta atoms than between Nb and Mo atoms. This difference in lattice distortion is reflected in the X-ray line widths. Therefore, hydrogen preferentially occupies T sites in the undistorted or very weakly distorted tetrahedra some distance away from Ta solutes and excess H atoms enter d - T sites in the tetrahedra distorted at an intermediate level near Ta solutes. Therefore, the interaction between hydrogen and an oversized Ta atom is not attractive in Nb, in contrast to the attractive interaction between an undersized Mo atom and hydrogen in Nb.

With the help of measurements of the half-widths of X-ray reflection lines in Nb-Mo and Nb-Ta alloys, the site occupancy of hydrogen in the Nb-Ta alloys is explained in terms of an effect of lattice distortion induced by alloying, as in the case of the site occupancy in Nb-Mo alloys with Mo concentration higher than about 39 at. %. The d - T site is a stable site for hydrogen in a slightly distorted bcc lattice.

References

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*1 RIKEN Nishina Center

*2 School of Science and Engineering, Waseda University

*3 Department of Physics II, Tokyo University of Science

*4 Institute for Materials Research, Tohoku University