

## Site change of hydrogen owing to lattice distortion in Nb alloys<sup>†</sup>

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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 newly developed.<sup>1)</sup> Hydrogen can be detected by measuring emitted  $\alpha$  particles. This method has been demonstrated to be very useful to locate hydrogen dissolved in metals.<sup>1,2)</sup> The lattice location of hydrogen has hitherto 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 ( $C_{\text{Mo}}$ ) range, maintaining a bcc crystal structure, although the lattice parameter changes.

It has been demonstrated that the lattice location changes very sensitively with  $C_{\text{Mo}}$  and, with the help of measurement of width of X-ray reflection lines (Fig. 1), that such change can be interpreted in terms of lattice distortion induced by alloying.<sup>3)</sup> Broadening of reflection lines serves as a measure of lattice distortion averaged over the whole specimen. At low  $C_{\text{Mo}}$ , lattice is strongly distorted around Mo atoms. Hydrogen is trapped by a Mo atom to be located at a  $T_{\text{tr}}$  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.<sup>4)</sup> With increasing  $C_{\text{Mo}}$ , 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  $C_{\text{Mo}}$  higher than 39 at. %, the lattice distortion gradually increases again with increasing  $C_{\text{Mo}}$  because of the increase in the number of undersized Mo atoms in a unit cell, but not so strongly as that at low  $C_{\text{Mo}}$ , i.e., up to an intermediate level (the range II in Fig. 1). In this case, H atoms are distributed over  $T$  and  $d$ - $T$  sites, which are 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. Hydrogen preferentially occupies  $T$  sites in undistorted or very weakly distorted region, but, as the concentration of available  $T$

sites is limited, excess H atoms occupy  $d$ - $T$  sites in the region distorted at the intermediate level.<sup>3)</sup> Therefore, it is expected that H atoms are located at  $T$  sites in the alloys whose lattice is very weakly distorted.

Then, in the present study, the site occupancy of hydrogen in Nb alloyed with 50 at. % of oversized Ta atoms with a very closer atomic radius to Nb atoms, 1.44 Å,  $\text{Nb}_{0.50}\text{Ta}_{0.50}\text{H}_{0.021}$  and  $\text{Nb}_{0.50}\text{Ta}_{0.50}\text{H}_{0.053}$ , was investigated by the channelling method at room temperature. It was observed that H atoms are located at  $T$  sites, irrespective of hydrogen concentration ( $C_{\text{H}}$ ), in contrast with the results on Nb alloyed with similar concentration of undersized Mo atoms,  $\text{Nb}_{0.52}\text{Mo}_{0.48}$  ( $C_{\text{H}}=0.0097\text{--}0.05$ ). In approximately the same  $C_{\text{H}}$  range as that in the  $\text{Nb}_{0.50}\text{Ta}_{0.50}$  alloys, in the  $\text{Nb}_{0.52}\text{Mo}_{0.48}$  alloys, at low  $C_{\text{H}}$ , most of the H atoms are located at  $T$  sites and excess H atoms are at  $d$ - $T$  sites, while at high  $C_{\text{H}}$ , most of them are at  $d$ - $T$  sites.<sup>3)</sup>

Widths of X-ray diffraction lines in the  $\text{Nb}_{0.50}\text{Ta}_{0.50}$  alloys are much smaller than those in the  $\text{Nb}_{0.52}\text{Mo}_{0.48}$  alloys and are very close to those in pure Nb (Fig. 1), indicating much smaller lattice distortion in the  $\text{Nb}_{0.50}\text{Ta}_{0.50}$  alloys than in the  $\text{Nb}_{0.52}\text{Mo}_{0.48}$  alloys, owing to the smaller size difference between Nb and Ta atoms. The present result on site occupancy of hydrogen in the  $\text{Nb}_{0.50}\text{Ta}_{0.50}$  alloys is in good agreement with the expectation. Therefore, considering also the hitherto obtained results for Nb alloyed with 2–5 at. % Ta atoms, it is concluded that the site occupancy of hydrogen in Nb-Mo and Nb-Ta alloys can be well explained on the basis of the lattice distortion induced by alloying.

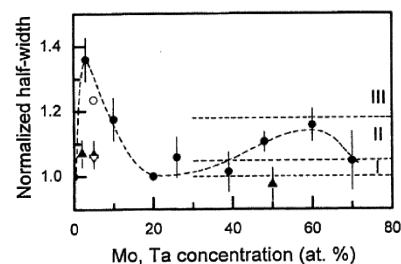


Fig. 1. The half-widths of the  $\{321\}$  X-ray reflection lines of the non-H-doped Nb-Mo (●) and Nb-Ta (▲) alloys. Open symbols, Nb-Mo (○) and Nb-Ta (▽), represent those by Matsumoto et al.<sup>5)</sup>

### References

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