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利用課題名（日本語） ：二体分布関数を利用した $Mg_{1-x}Ti_x$ 薄膜の局所構造の調査

Program Title (English) :Investigating the local structure of $Mg_{1-x}Ti_x$ thin films using the atomic pair distribution function technique

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1. 概要（Summary ）

$Mg_{1-x}Ti_x$ thin film absorbs a large amount of hydrogen at ambient conditions and this makes it very attractive for potential battery materials [1]. Moreover, its optical properties drastically change when it absorbs hydrogen. The lattice parameters of $Mg_{1-x}Ti_x$ thin film gradually decrease with increasing Ti content, x, as if it is a solid solution alloy [2]. However, its optical and electrical properties are not well explained by such a simple solid solution model. Indeed, a more complex model like nanosized clusters embedded in a large structurally coherent matrix is required [2]. For instance, nanosized Ti-clusters are embedded in a Mg-matrix in a $Mg_{0.7}Ti_{0.3}$ thin film [3]. Although this complex model explains the compelling optical and electrical properties of $Mg_{1-x}Ti_x$ thin films, there has been no clear experimental evidence for the presence of nanosized clusters. In this study, we use the atomic pair distribution function (PDF) analysis [4] on X-ray total scattering data to look for nanosized Ti-clusters in a $Mg_{0.7}Ti_{0.3}$ thin film.

2. 実験(目的,方法)（Experimental）

A $Mg_{0.7}Ti_{0.3}$ thin film capped with a thin Pd layer was deposited on a kapton substrate. The film thickness was 400 nm. The thin film was cut into small pieces and loaded in a cell developed for an in-situ hydrogenation study. Synchrotron X-ray total scattering experiment was carried out at BL22XU at SPring-8 using RA-PDF setup [5]. The X-ray energy was 70.430 keV. Data were collected at room temperature at several different stages of hydrogenation.

3. 結果と考察(Results and Discussion)

The X-ray PDF of the $Mg_{0.7}Ti_{0.3}$ thin film is well explained by a hexagonal close packed (hcp) structural model. At the early stage of hydrogen absorption, changes in the PDF only occur at the low-r region (below 30 Å). This indicates that a part of the sample is transformed into a face centered cubic (fcc) structure. On the other hand, the high-r region of the PDF (above 30 Å) stays in an hcp structure. This strongly suggests that Ti-clusters (~30 Å in size) are present in the film and transformed into an fcc structure while the Mg-matrix stays in a hcp structure at the early stage of hydrogenation. Further analysis is currently underway.

4. その他・特記事項（Others）

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