Evidence for α'-β Transition in Thin Nb Films Upon Electrochemical Charging with Hydrogen

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Abstract No. Jisr1465
Beamline(s): **X22A**

Introduction: The H-Nb phase diagram in thin films has been studied extensively with evidence that it is grossly modified from that of the bulk.[1] The grain size, film microstructure and grain boundaries each play a crucial role in the way hydrogen is absorbed and in which phases are formed. There has been an active debate on which phases are formed during hydrogen charging in thin metal films like Nb. The debate usually centering on whether is it possible to form the Nb β-hydride in thin films or a gas-like α-phase is possible only in thin films. We show here using in situ x-ray diffraction during electrochemical charging that both phases might form. We also show using high quality spectra that the phase transformation between the α' and β phases can be properly studied.

Methods and Materials: Thin Nb films, deposited on Si were electrochemically charged with hydrogen in a specially designed cell that allowed simultaneous x-ray diffraction patterns to be obtained.[2] The large intensity available in the synchrotron x-rays makes it possible to observe the phases as they form even though a layer of electrolyte as thick as 1mm remains on the film surface.

Results: Figure 1 shows a series of x-ray patterns produced in the reflection geometry. The scans are obtained as more hydrogen is charged in the Nb film and illustrate the process of creation of the different phases. The initial position for the Nb[110] reflection is marked in the figure at a 2θ position of about 30 degrees. As more hydrogen goes into the film a peak appears below 2θ ~ 29 degrees which is identified with the dense gas-like phase called the α'. With more charging another phase appears around 2θ ~ 28.5 degrees which is interpreted to be the hydride phase β. Subsequently, it is possible to transform the samples between the two phases in a lever rule fashion by increasing or decreasing the charging current.

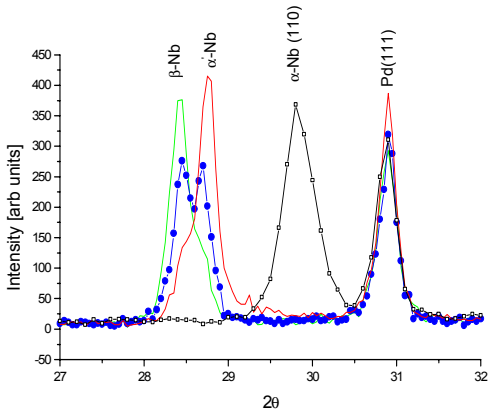

Figure 1. A series of x-ray diffraction patterns showing the conversion between the α' and β phases in epitaxial Nb films.

Conclusions: Evidence exists for the formation of both α' and β phases in epitaxial Nb films. The α'-β phase transformation can be carefully studied by in situ x-ray diffraction during electrochemical charging.

References: 1) G. Reisfeld et. al., PRB 53, 4974(1996). 2) N. Jisrawi et.al., J. Mater. Res. 8, 2091 (1997).