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THE STRUCTURE OF THE λ-PHASES OF NIOBIUM-DEUTERIUM

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ABSTRACT

Lambda phases of NbD_x ($0.78 \leq x \leq 0.84$), which exist below 220 K, have been studied by neutron and electron diffraction. The observed modulated structure can be described as a deuteron concentration wave in a slightly distorted bcc Nb matrix. The wave-vector is parallel to <001>, and the wavelength varies from 16.0 Å to 21.4 Å, increasing with increasing concentration.

INTRODUCTION

The phase diagram for NbD_x is very similar to the phase diagram for NbH_x,[1] shown in Fig. 1. The λ-phase structures are based on the β-phase structure at $NbH_x(D_x)$. The β-phase is an orthorhombic structure with dimensions $\sqrt{2}$ a x $\sqrt{2}$ a x a, where a (= 3.43 Å) is the lattice constant of the bcc structure formed by Nb in $NbH_x(D_x)$. In the remainder of this paper, the atomic position as well as the reciprocal lattice will be in reference to the bcc structure. The Nb atoms in the orthorhombic β-phase cell form a f.c.o. lattice with 4 Nb in the f.c.o. basis positions, (000), ($\frac{1}{2}\frac{1}{2}\frac{1}{2}$), ($-\frac{1}{2}\frac{1}{2}\frac{1}{2}$), (010). The arrangement of the 4D atoms in the orthorhombic cell is shown in Fig. 2. For β_1, the D atoms are ($0,\frac{1}{2},\frac{1}{4}$), ($-\frac{1}{2},1,\frac{1}{4}$), ($\frac{1}{2},1,3/4$) and ($0,3/2,3/4$), and for β_2, ($0,\frac{1}{2},3/4$), ($-\frac{1}{2},1,3/4$), ($\frac{1}{2},1,\frac{1}{4}$) and ($0,3/2,\frac{1}{4}$). For the β-phase, the two sets of positions, β_1 and β_2, correspond to a different origin of the orthorhombic lattice. In other words, β_1 and β_2 are related by a ($\frac{1}{2}\frac{1}{2}0$) translation.

RESULTS AND DISCUSSION

The discussion presented here is based on single crystal neutron diffraction,[2] electron diffraction[2] and recent polycrystalline neutron diffraction measurements. In Fig. 3, top half, the results of a neutron diffraction scan are shown for a polycrystalline sample of $NbD_{0.834}$ at room temperature. The (110) and ($\frac{1}{2}\frac{1}{2}1$) reflections are shown, the latter being the characteristic β-reflection. When the sample is cooled below the β-λ transition, the β reflection disappears and two satellites are formed at ($\frac{1}{2}\frac{1}{2}1-\delta$) and ($\frac{1}{2}\frac{1}{2}1-\delta$) (see bottom half of Fig. 3). This characteristic of the λ phases can be interpreted by stacking β_1 and β_2 unit cells as building blocks in the <001> direction as shown schematically in Fig. 2. The β_1-β_2 boundary layer is denoted by ζ_1 in Fig. 2, and the detailed analysis of the D positions in this

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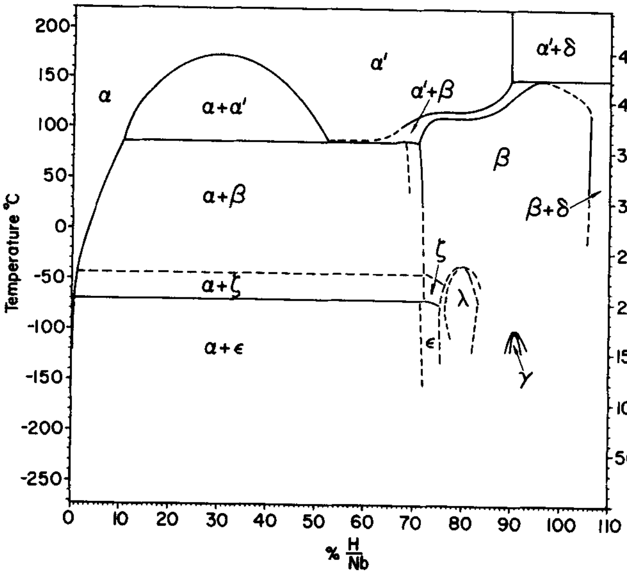

Fig. 1. Phase Diagram for NbH_x.

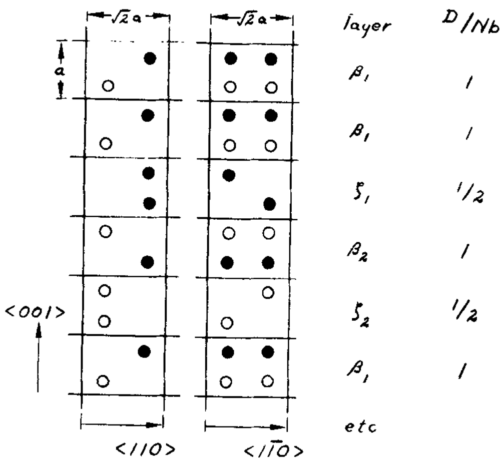

Fig. 2. Schematic model of λ-phase structure. o and ● : D Atoms. Nb not shown.

layer is beyond the scope of this paper. However, in Fig. 2 we have assumed that only 2 of the 4 positions (½,1,¼), (½,1,3/4), (0,3/2,½), (0,3/2,3/4) are occupied in the boundary layer.If 3 or 4 positions were occupied, the D-D distances would become unreasonably small.[3] The ratio, D/Nb, is also shown in Fig. 2 for the different layers. If one assumes for the moment that the ζ layer contains 4 D atoms, then the interpretation of the λ-phase diffraction pattern is simplified; for example a structure consisting of $n\beta_1$ layers followed by $n\beta_2$ would not have a (½½1) β-reflection but instead have satellites at (½½1 ± 1/2n).

The results of our investigations are presented in Table I. We have observed four λ-phases in NbD_x by neutron diffraction, 3 of these have been observed in NbH_x by electron diffraction. The values of δ show that the structures have long range modulation. For an idealized λ-structure, consisting of $n\beta_1$, $n\beta_2$, $m\zeta_1$ and $m\zeta_2$ layers, it is easy to show that the concentration x is equal to 1 - δ, in agreement with the results in Table I. Due to the ζ layers in the λ-structure, the structure can also be described as a deuteron concentration wave. In another paper presented at this conference a model is discussed that predicts the existence of the concentration waves.

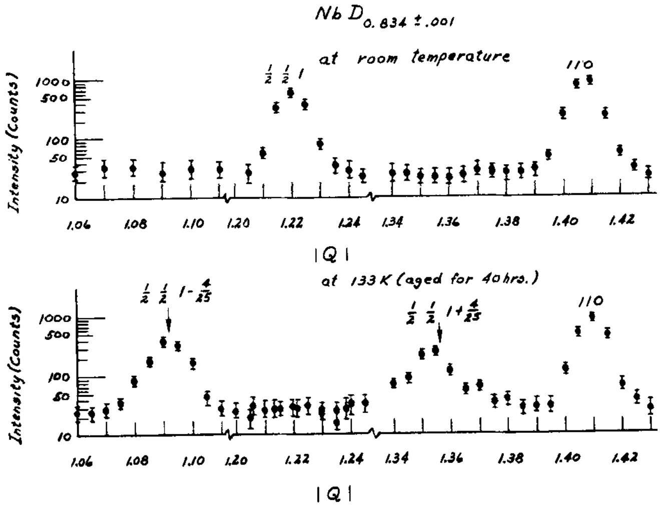

Fig. 3.

Neutron powder diffraction scan. |Q| in 2π/a.

TABLE I

System	x	δ	1 - δ	Comments
NbD_x single crystal	0.77	0.214	0.786	Mix λ-ε, lower λ-phase boundary
" " "	0.85			No λ, upper λ phase boundary
NbD_x polycrystal	0.792	0.200	0.800	
" "	0.815	0.180	0.820	
" "	0.834	0.160	0.840	
NbH_x thin foil		0.21 0.18 0.16		Electron diffraction

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