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## THE CRYSTAL STRUCTURE OF NICKEL HYDRIDE

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**Résumé.** — L'hydrure de nickel est cubique à faces centrées. H occupe les sites octaédriques avec un rapport H/Ni égal à  $0,6 \pm 0,1$ .

**Abstract.** — Nickel hydride is face centered cubic. H occupies the octahedral sites with a H/Ni ratio equal to  $0,6 \pm 0,1$ .

Coherent neutron scattering measurements were made on electrolytically hydrogenated nickel foils to determine the crystal structure and hydrogen content of nickel hydride. Since the hydride is unstable, decomposing into nickel and hydrogen gas, both the nickel and nickel hydride phases were present in continuously varying proportions during the course of the measurements. Intensities of the four innermost reflections were measured at room temperature as a function of time and pressure of the evolved hydrogen gas. (Seen fig. 1 and 2). The hydride was found to be face centered cubic with a lattice spacing of  $3.717 \text{ \AA}$  in agreement with previous x-ray results [1, 2]. In such a lattice there are two types of sites available to the hydrogen atoms: the tetrahedral sites at  $\pm (1/4 \ 1/4 \ 1/4)$  f. c. c. and the octahedral sites at  $(1/2 \ 0 \ 0)$  f. c. c. The observed intensities show that the hydrogen atoms occupy the octahedral

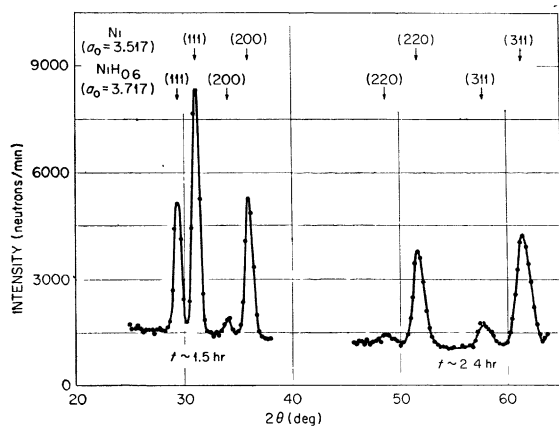


FIG. 1. — Room temperature neutron diffraction. Patterns of the Ni-NiH system.

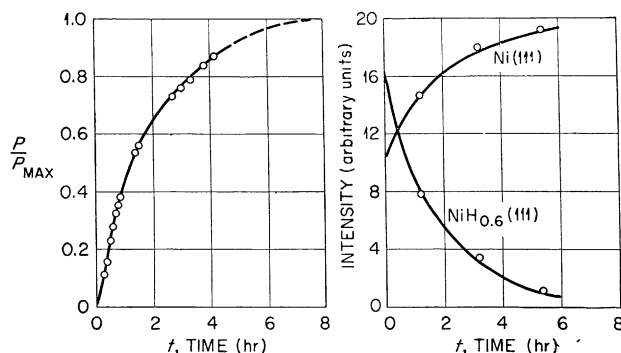


FIG. 2. — Time dependence of the reduced hydrogen pressure and of the (111) Ni and NiH<sub>0.6</sub> reflections. These data yield a H/Ni ratio in the hydride phase of  $0,6 \pm 0,1$ .

sites and that the H/Ni ratio is  $0.6 \pm 0.1$ . In these respects nickel hydride is quite similar to palladium hydride. Since the magnetic behavior of nickel and palladium suggests a difference in their d-band structures, it appears that the hydrogen uptake behavior of these metals is an insensitive probe of that d-band structure except as an indicator of the number of holes in the d band. A full report of this work will soon appear in the *Journal of the Physics and Chemistry of Solids* [3].

## Discussion

Pr BERTAUT. — Dr Cohen (Université de Grenoble) a prouvé que le système Pd-H est biphasé, c'est-à-dire que Pd coexiste avec du Pd-H<sub>0.6</sub>. Est-ce que le système Ni-H est analogue ?

Dr CABLE. — Les observations par diffraction neutronique sur le système Ni-H montrent la présence de deux phases, Ni et Ni-H.

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