

## High Frequency Vibrations of H-Atoms in Transition Metals and Alloys Measured by Inelastic Neutron Scattering\*

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New hydrides of Ni, Cr, Mo,  $V_{0.9}Ru_{0.1}$ ,  $Nb_{0.75}Ru_{0.25}$  have been synthesized under high  $H_2$  pressure (up to 90 Kbar) with subsequent thermobaric quenching/1,2/. Some of these materials are superconducting.

The procedure to prepare clean initial metal and alloy ingots has been described in detail for Ni, Cr, Mo/3/ and V(Nb)Ru/4,5/. The samples were hydrogenated by being held in an atmosphere of high pressure ( $P_H$ ) molecular hydrogen at fixed  $P_H$  and fixed temperature  $T_1$  followed by quenching under pressure down to about minus 180°C/1,2/. Each sample consisted of many flat pieces of different areas and thicknesses (0.13–0.30 mm), total masses between 0.5 and 4.0 gr. We used the Beryllium filter spectrometer/6/ on the hot source of the High Flux Reactor at the ILL. The monochromator was Cu(220). The scattering angle was kept constant at 90°. Special precautions were taken during the final preparation of the samples to avoid water vapor and nitrogen condensation on the sample.

The measured IINS spectra of the investigated hydrides are shown in Figs. 1 to 4. These spectra were obtained from the measured ones by subtracting a background measured with an empty aluminium container.

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The investigated hydrides have the following metal sublattices : NiH-fcc, CrH and MoH-hcp [1,2]. It is generally accepted that hydrogen occupies the octahedral sites (O-sites) in all transition metal hydrides of the VI-VIII groups which have been studied up to now/7,8/. In the hydrides under investigation the O-sites as well as the tetrahedral sites (T-sites) possess cubic symmetry. It should be noted that for hcp structures this type of symmetry is valid only for the lattices with the ideal ratio of cell parameters ( $c/a = 1.633$ ). Fortunately this value is nearly realized for chromium and molybdenum hydrides/7-9/.

As can be seen in fig. 1 all peaks have a rather complicated structure for every sample. The main peak frequencies of different orders have a regular ratio 1:2:3. A preliminary discussion of possible reasons for the structure around the first peak is written elsewhere/3/.

In Fig. 2 the concentration dependences of the IINS spectra from chromium and nickel hydrides are shown (see Fig. 1 for the compounds NiH<sub>1.01</sub> and CrH<sub>1.0</sub>). In the Cr-H spectra no noticeable changes are seen with varying concentration. This observation may indicate that there is no continuous solid solution series for this system. This would lead to the conclusion that the samples with lower H-concentration show co-existence of two phases. One part of the sample would be pure Cr metal and the other one would have the highest concentration CrH<sub>max</sub> with H<sub>max</sub> > H<sub>1.13</sub>. Unfortunately the T-C phase diagram of Cr-H is not studied in detail.

As concerns the Ni-H, there is a wide set of solid solutions in the concentration region H/Me = 0.7-1.25 in the T-C phase diagram. Therefore the substances with these hydrogen concentrations should be in a single-phase state and the small spectral changes will reflect properly the physical state of the samples. For example the relative height of the first maximum is increasing with increasing H concentration.

The choice of the V(Nb)-Ru alloys hydrides, see Fig. 3, is explained by the fact that these hydrides with the concentration H/Me  $\approx$  1 are superconductors with  $T_c = 3.0K$  and  $T_c = 5.08K$ , respectively/4,5/. It is known/4,5/ that the V<sub>0.9</sub>Ru<sub>0.1</sub>H<sub>1.83</sub> and Nb<sub>0.75</sub>Ru<sub>0.25</sub>H<sub>1.56</sub> samples consist of the coexistence of two phases. The pure high concentration

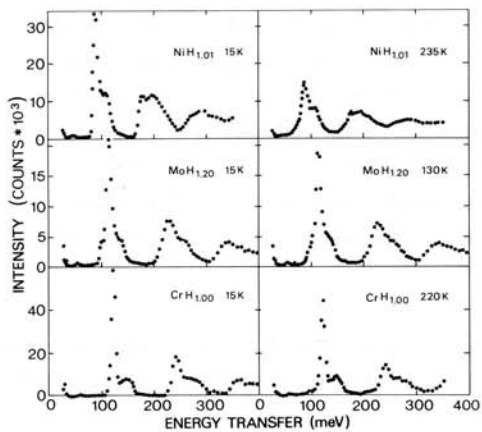


Fig. 1 - Temperature dependence of hydrogen spectra.

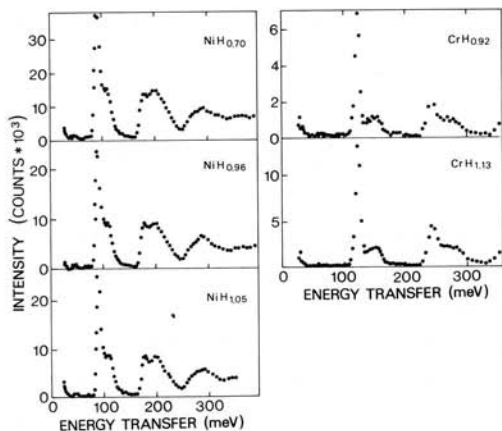


Fig. 2 - Concentration dependence of hydrogen spectra at 15K.

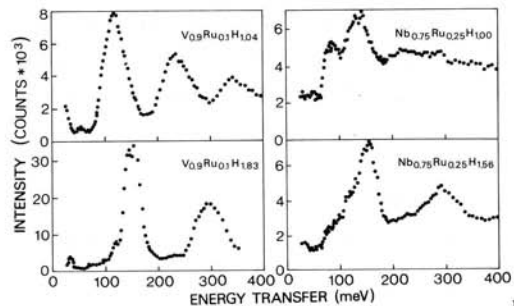


Fig. 3 - Hydrogen spectra at 15K.

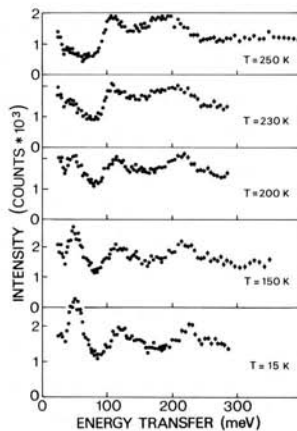


Fig. 4 - Temperature dependence of hydrogen spectra.

phases are estimated to be the highest ones achieved experimentally, i.e.  $V_{0.9}Ru_{0.1}H_{2.0}$  and  $Nb_{0.75}Ru_{0.25}H_{1.72}$ . The examined samples are close to the maximum concentrations. But to convince ourselves that their spectra mainly show the features of H-rich phases, we subtracted 15 % of the  $H_{1.0}$  spectrum in the V case and 20 % in the Nb case. These subtractions did not significantly alter the spectra of the high concentration compounds. Therefore we assume that the H-rich samples are almost monophasic.

Fig. 4 shows the temperature dependent spectra of  $V_{0.9}Ru_{0.1}H_{0.463}$  (body centered tetragonal at  $T = 83K/4/$ ). The drastic change in the spectrum at  $T \approx 230K$  might be connected with a phase transition as known to appear in  $VH_{0.5}$  at about  $440K/10/$ . But a strongly anisotropic Debye-Waller factor may cause as well the disappearance of a peak with increasing temperature. This has been observed in a monodomain single crystal  $VH_{0.5/11/}$ .

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