[localized vibrations, $NbH_{0.3}$]

The second example is an experiment conducted by S. Ikeda and coworkers on polycrystalline $NbH_{0.3}$ using a chopper spectrometer. Figure 1 shows the tetrahedral and octahedral hydrogen sites in the Nb bcc lattice (left) and a contour plot of the potential centered at the T_1 tetrahedral site (right). The saddle points correspond to a region shared with the neighboring T_2 and T_3 sites.

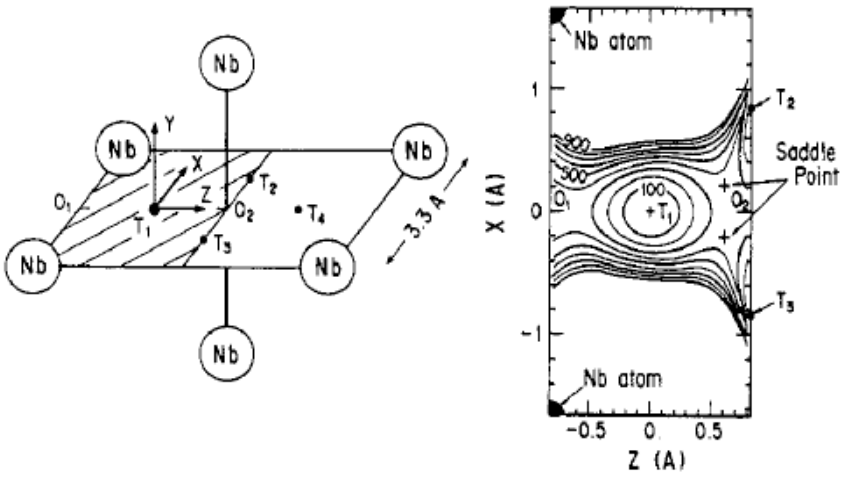

Figure 1 (left) The octahedral and tetrahedral sites of hydrogen in $NbH_{0.3}$. (right) A contour plot of the hydrogen potential of T1 site (from Ikeda et al. 1990).

Three localized vibrational modes were observed at 115, 161, and 220 meV, which correspond to the transitions of $0 \rightarrow 1$ along z, $0 \rightarrow 1$ in the x-y plane, and $0 \rightarrow 2$ along z, respectively. Figure 2 shows the observed intensities of the three transitions as a function of Q. Fitting the data using **Error! Reference source not found.** based on a harmonic potential (solid curves) describes well the Q-dependent intensities of the 115-meV excitation but not so for the 161- and 220-meV excitations. A consideration of the proximity of the T_1 site with the T_2 and T_3 sites on the xy-plane led to a trial wave function for the 161-meV excitation along the T_1-T_2 (or T_1-T_3) line that consists of a linear combination of a major and minor component of the T_1 and T_2 harmonic wave functions, respectively. The fit to the 161-meV excitation (dashed curve in Figure 2), shows a considerable improvement in the fit. Likewise, it was argued that the wavefunction of the second excitation along z-direction at 220 meV contains significant density at the saddle points. Figure 3 depicts the results.

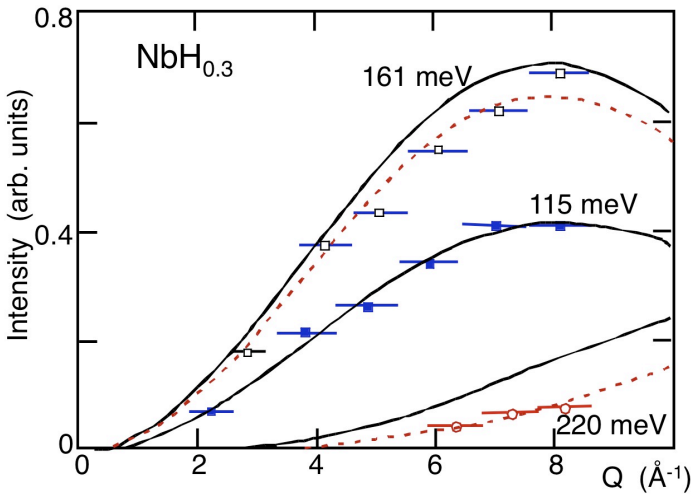

Figure 2 The observed Q-dependent intensities of the three excitations in $NbH_{0.3}$. The solid curves are fits to the data using a harmonic potential. The dashed curves are obtained from using a linear combination of one-dimensional harmonic wavefunctions (see text) (after Ikeda et al. 1990).

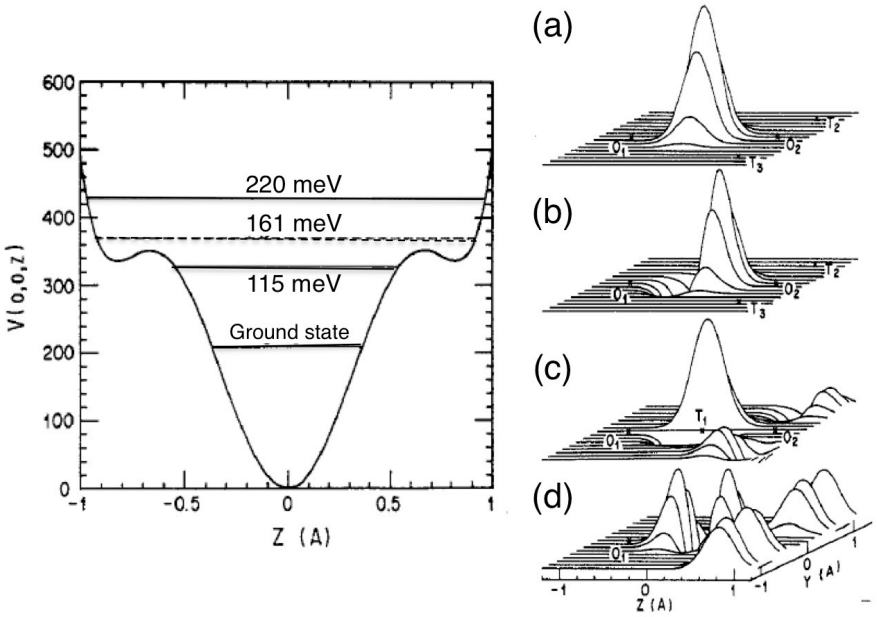

Figure 3 (left) The hydrogen potential and the energy level structure of $NbH_{0.3}$. (right) Hydrogen wavefunctions for (a) the ground state, (b) $0 \rightarrow 1$ along z at 115 meV, (c) $0 \rightarrow 1$ in the x-y plane at 161 meV, and $0 \rightarrow 2$ along z at 220 meV (from Ikeda et al. 1990).

Reference:

Ikeda, S. and J. M. Carpenter (1985), "Wide energy-range, high-resolution measurements of neutron pulse shapes of polyethylene moderators", *Nucl. Instrum. Meth*. **A 239**, 536.