Comment on "Superdiffusion of 4*T*-Hydrogen in Vanadium"

In a recent Letter[1] Suzuki *et al.* have reported Huang diffuse x-ray measurements on hydrogen in vanadium. They conclude that the displacement field has a tetragonal symmetry with $|A-B| = 0.97$ eV for the $1T$ site. Although the experimental details are very sketchily described it seems to be quite likely that their data evaluation and consequently the above conclusion is wrong.

The change of the diffuse x-ray intensity in $\langle 1\bar{1}0\rangle$ direction is not unambiguously given by the tetragonality $|A-B|$ of the displacement field around hydrogen in vanadium. In fact it can also stem from the hydrogen-induced decrease of the elastic constant c', which determines the main contribution of the thermal diffuse background intensity in this direction. This decrease of c' is particularly large for hydrogen in vanadium.[2] In the case of a nonvanishing $|A-B|$ the expected intensity increase in $\langle 1\bar{1}0\rangle$ direction is given by

$$I_{\mathrm{HDS}}/I_{\mathrm{TDS}} = c(A-B)^2/3V_c kTc', \qquad (1)$$

where the thermal diffuse background I_{TDS} is assumed to be given by the one-phonon scattering formula in the high-temperature limit.[3] V_c is the volume of the unit cell, c the H concentration. Quantitatively ($c = 0.014$ H/V, $A-B = 0.97$ eV, $T = 300$ K, $c' = 55.29\times 10^{10}$ dyn/cm^2) the intensiy increase from equation (1) should be 1.8%. If, however, the intensity increase is due to the change of the elastic constant c' we obtain, using Magerl's[2] value $\Delta c'/c'$ per % H/V $= -0.0183$,

$$\Delta I_{\mathrm{TDS}}/I_{\mathrm{TDS}} = -\Delta c'/c' = +0.026.$$

This rough estimate shows that $I_{\mathrm{HDS}} \approx \Delta I_{\mathrm{TDS}}$ and indicates that Suzuki's conclusion about the tetragonality of the dipole moment tensor is at least doubtful.

Additional doubts are raised by the influence of the H loading procedure on the evaluation of the measured x-ray intensity data. It is well known that oxygen in vanadium cannot be degassed as described by Suzuki. An oxygen concentration of only 0.028% O/V would give rise to the same Huang scattering in $\langle 1\bar{1}0\rangle$ direction as 1.4% H/V. Under the conditions where Suzuki loaded his vanadium crystal (Sievert's apparatus) it is very likely that this amount of oxygen has diffused into the sample.

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