Suzuki and Koike Respond: According to Dederichs,[1] the diffuse scattering intensity of x rays due to lattice distortion in the surrounding volume of point defects of concentration c can be written for the $(hh0)$ reflection as

$$S(\vec{s}) = cN|f_h|^2(h/q)^2(1/V_c)^2Q,$$

where $\vec{s}$ is the scattering wave vector, f_h the atom form factor, V_c the volume of the unit cell, and $\vec{q}$ the deviation vector from the Bragg peak which is given by $\vec{s}=\vec{h}+\vec{q}$. The contribution from the thermal diffuse scattering is $\Delta Q_{\mathrm{TDS}} = [Q_{\mathrm{TDS}}(c) - Q_{\mathrm{TDS}}(0)]$, i.e., the difference of the contributions of thermal diffuse scattering between a matrix with defects of concentration c and the same matrix with no defects. Metzger[2] suggested that when $\vec{q}$ is parallel to $[1\bar{1}0]$, ΔQ_{TDS} in the case of the V-H system gives rise to a positive contribution to Q as large as Q_{HDS}, which is the contribution of the Huang scattering due to hydrogen atoms. Then it gives $Q = Q_{\mathrm{HDS}} + \Delta Q_{\mathrm{TDS}}$. Using the high-temperature approximation to the Debye model for the mean square dispacement of lattice atoms as Metzger did, we can express ΔQ_{TDS} for $\vec{q} \parallel [1\bar{1}0]$ as $\Delta Q_{\mathrm{TDS}} = -100\Delta c' V_c kT/c'^2$, where $c' = (c_{11} - c_{12})/2$ and $\Delta c'$ is the change of c' per percent H/V, in which H/V is the concentration c as expressed by atom numbers ratio. Taking values such as $c' = 55.29\times10^{10}$ dyn/cm^2, $\Delta c' = -1.10\times10^{10}$ dyn/cm^2 per percent H/V (Ref. 3), $V_c = 2.77\times10^{-23}$ cm^3 and $kT = 1/40$ eV, it gives $c'^2\Delta Q_{\mathrm{TDS}} = 0.476$ eV^2. While, c'^2Q measured by the present experiment is given as $c'^2Q_{\mathrm{obs}} = 0.118 \pm 0.008$ eV^2, which is only one fourth of the calculated value. Since the Debye temperature of vanadium is reported[4] to be 350 to 370 K, the calculation surely overestimates ΔQ_{TDS}.

On the other hand, the application of compressive stress of 7 kg/mm^2 in the direction [001] gives rise to a large increase of Q_{obs}, which is given by $c'^2Q_{\mathrm{obs}} = 0.421$ eV^2. Since this increase of Q_{obs} should be independent of ΔQ_{TDS}, it led us to conclude that the increase was caused by a change in the state of hydrogen, i.e., the transition from $1T$ to $4T$ state.[5] In the present experiment, the obtained value of $(A+2B)_{1T}$ is not influenced by ΔQ_{TDS}. (In our calculation of Q_{HDS}, we took account of the correlation between the displacement fields due to different configurations of hydrogen, i.e., $1T_x$, $1T_y$, $1T_z$, and also the ones in the case of coexisting $1T$ and $4T$ hydrogen atoms. While, most theories treated such defects as independent defects, neglecting the correlations Thus our expression of Q_{HDS} differs from others.) We found ΔQ_{TDS} to be consistent with the value derived from the volume change due to hydrogenation obtained by measurements of lattice parameters. The contribution of ΔQ_{TDS} mainly appears in the estimate of $|A - B|_{1T}$. If $Q_{\mathrm{HDS}} \simeq \Delta Q_{\mathrm{TDS}}$ as Metzger assumed, $|A - B|_{1T}$ will be reduced by 30%, which becomes 0.69 eV, as compared to 0.97 eV tabulated in our paper. The values of $|A - B|_{4T}$ will be reduced at most by 6%, which is within experimental error ± 8%. We are now measuring ΔQ_{TDS} as a function of temperature (to be reported later).

TABLE I. Changes in weight after hydrogenation and dehydrogenation of two samples.

Sample	Before hydrogenation (g)	After hydrogenation (g)	After dehydrogenation (g)	c, H/V (%)
No. 8-2	0.364 610	0.364 704	0.364 613	1.29
No. 2-3	0.144 746	0.144 786	0.144 748	1.34

Next, we would reply to the question about oxidation of samples during hydrogenation. Weights of all the samples were measured before and after hydrogenation and also after dehydrogenation which was carried out in vacuum at 450 °C. The following Table I shows only two examples. The ratio of the change of weight between the initial state of a sample and the one after dehydrogenation to the increase of weight after hydrogenation is 0.061 and 0.032, respectively. Since the desorption of oxygen once introduced during hydrogenation into vanadium can hardly occur by such a heat treatment,[6] the present data show that the atom numbers ratio O/H should be at most 3.9×10^{-3} and 2.0×10^{-3}, respectively. The ratios of other samples are similar.

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Received 4 October 1983
PACS numbers: 66.30.Jt

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