Comment on "Interstitial Hydrogen and Neutralization of Shallow-Donor Impurities in Single-Crystal Silicon"

It has been well established that shallow acceptor impurities in single-crystal silicon can be neutralized by exposure to monoatomic hydrogen. On the other hand, several studies have concluded that shallow donor impurities in silicon cannot be passivated. Contrary to these previous conclusions, Johnson, Herring, and Chadi[1] have recently reported neutralization of phosphorus by hydrogenation. Here we show that a detailed analysis of the electrical measurements in Ref. 1 indicates that P neutralization is not necessarily implied. The results can also be explained as a combined effect of generation of H-associated acceptors in the n^+ layer and neutralization of substrate boron in the p region. The former reduces the effective free-electron concentration and also the effective mobility as discussed by Johnson, Herring, and Chadi.[1] The effect of the latter is to increase the effective mobility. Since this latter effect was not taken into account in Ref. 1, donor neutralization was considered as the only possibility.

To illustrate this alternative viewpoint, for simplicity, we have chosen a Gaussian distribution for P, close to the P distribution measured by secondary-ion mass spectrometry by Johnson.[2] $Y\%$ of P concentration is taken to be the H-associated acceptor concentration in n^+ layer. $Z\%$ of B in the p layer is considered to be neutralized after hydrogenation. Following Johnson,[2] B neutralization in the n^+ layer is not allowed. The B concentration is taken to be 7×10^{16} cm^{-3}. The secondary-ion mass-spectrometry profiles for H given in Ref. 2 for various conditions of hydrogenation would indicate that these assumptions are appropriate for the sample under consideration.

The effective areal density of free electrons ($n_{\rm eff}$) and the effective mobility ($\mu_{\rm eff}$) are calculated for various values of Y and Z following Petritz's expressions for inhomogeneous samples. The results are tabulated in Table I. Since the mobility is ionized-impurity-scattering limited for most of the layers, the measured effective Hall mobility would be higher than the effective conductivity mobility computed here.

It should be pointed out that the early works by Sah, Sun, and Tzou[3,4] do indicate the possibility of B neutralization by hydrogen in the depletion layer of a metal-oxide-semiconductor capacitor. In fact, neutralization of B, which is used for counterdoping of n-Si, has also been reported.[4] Hence the results in Ref. 2 need further evidence. This is also indicated in the recent analysis by Pantelides.[5] We have already examined this possibility of allowing B neutralization *within* the n^+ layer. Interestingly, for small values of Y, there is an appreciable increase in effective mobility with a decrease in effective carrier concentration. (For the same starting material, with $Y=15\%$ and $Z=99\%$, $n_{\rm eff}=8.8\times10^{13}$ cm^{-2} and $\mu_{\rm eff}=192$ cm^2/V-sec.)

The results of our calculations as given in Table I clearly indicate that the experimental results of Johnson, Herring, and Chadi[1] can be well explained by the assumption of H-associated acceptors in the n^+ layer and neutralization of B due to hydrogen in the p layer. Hence the neutralization of P by hydrogenation cannot be inferred conclusively from these measurements because of the presence of B in the substrate. It is necessary to use a P-doped epilayer without B as reported in the following Reply.[6] Our experiment with only a P-doped polysilicon layer gives a similar result.[7]

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TABLE I. Calculated $n_{\rm eff}$ and $\mu_{\rm eff}$. I, B neutralization in p region. II, H-associated acceptors in n^+ region.

	Y	Z	Junction depth (10^{-5} cm)	$n_{\rm eff}$ (10^{13} cm^{-2})	$\mu_{\rm eff}$ (cm^2/V-sec)
Starting material	0	0	5.2	14.0	173.9
Hydrogenated					
I	0	99	7.4	13.3	185.1
II	30	0	5.2	5.09	146.2
I+II	30	99	7.4	4.00	205.6