Chen *et al.* Reply: In their Comment [1] on our earlier Letter [2], Stallinga *et al.* demonstrate that in their proton and deuteron implanted silicon samples the photo-EPR (electron paramagnetic resonance) spectrum is dominated by the excited state of the neutral oxygen-vacancy (OV) complex. Based on the nearly identical spin-Hamiltonian parameters of the spin-triplet excited states between OV and VH_2, they conclude that the VH_2 complex, which we observed by optical detection of magnetic resonance (ODMR) [2], is instead OV. They thereafter speculate that the difference we observed in hyperfine structure between the hydrogen- and deuteron-treated samples [2], which they failed to observe, is due to some saturation effects.

Stallinga *et al.* ignore the fact that the OV and the VH_2 complexes are indeed expected to be very similar. Here one oxygen atom (in the case of OV) or two hydrogen atoms (in the case of VH_2) passivate efficiently two of the four broken bonds of a monovacancy, and the wave function of the unpaired electrons giving rise to the photo-EPR and ODMR signals is highly localized on the molecular orbital formed between the other two unpassivated dangling bonds. In fact, the overlap of the electron wave functions at O or H is nearly negligible, accounting for no more than 5% of the total spin density in both cases, shown previously by EPR [3], electron-nuclear double resonance (ENDOR) [4] and ODMR [2] studies. This means that the unpaired electrons localized at the two dangling bonds will not feel much difference whether it is one O atom or two H atoms which passivate the other two broken bonds, as long as they do passivate. This therefore determines that the electronic structure of the two defects, which is governed by the electrons localized at the unpassivated dangling bonds, should be very similar. It may not be at all surprising if they are nearly identical, unless a weak hyperfine structure from O or H has been monitored. This explains why we have observed the hyperfine structure from H and D [2], which Stallinga *et al.* have failed to do so [1], since VH_2 was detected in one case [2] and OV in the other [1]. It should be pointed out that the ODMR experimental conditions for the hydrogen- and deuteron-treated samples in our work were identical [2]. It should also be noted that saturation effects of a relatively short-lived excited state monitored by ODMR are expected to be much less important as compared with the EPR of a ground state, since it is the electronic decay time to the ground state, rather than the spin relaxation time among the spin sublevels, that determines the saturation. Therefore the argument by Stallinga *et al.* [1] that the ODMR signal in our work was saturated in one case and not in the other case is an unfounded speculation.

Although the electronic structure of the two defects is very similar, their thermal stability may, however, be rather different. In fact, VH_2 and OV show markedly different properties upon thermal annealing. The former can be annealed out at a rather low temperature at about 100–200 °C [5], while the latter has been shown to be thermally stable up to 400–500 °C [6]. This provides evidence for a different origin of the defects studied by us [2] and Stallinga *et al.* [1].

Stallinga *et al.* also ignore the strong difference in sample preparation, which may determine which defects are mainly produced. Their samples were treated by a high-energy proton and deuteron implantation. Our samples were first exposed to a low-energy H_2 or D_2 plasma, and were then irradiated with 2.0 MeV fast electrons. Because of a different formation mechanism for the two defects, this strong difference in sample preparation may lead to the fact that OV is the predominant defect in their samples.

In summary, the similarity in the electronic structure between the OV and VH_2 defects in silicon is not at all surprising. It is, in fact, expected. Clear evidence for their difference is, however, provided by the weak hyperfine interaction from the hydrogen and deuteron atoms and by their distinctly different annealing temperatures. Stallinga *et al.* show that their samples from a particular treatment OV is the predominant defect observed by photo-EPR. They provide no evidence against our earlier conclusion on the VH_2 defect, except some speculations.

W. M. Chen, O. O. Awadelkarim, and B. Monemar
Department of Physics and Measurement Technology
Linköping University
S-581 83 Linköping, Sweden
J. L. Lindström
Swedish Defense Research Establishment
Box 1165, S-581 11 Linköping, Sweden
G. S. Oehrlein
Department of Physics
State University of New York
Albany, New York 12222

Received 16 July 1997 [S0031-9007(97)04936-3]
PACS numbers: 76.30.Lh, 76.70.Hb

[1] P. Stallinga and B. Bech Neilsen, preceding Comment, Phys. Rev. Lett. **80**, 422 (1998).
[2] W. M. Chen *et al.*, Phys. Rev. Lett. **64**, 3042 (1990).
[3] K. L. Brower, Phys. Rev. B **5**, 4274 (1972).
[4] R. van Kemp *et al.*, Phys. Rev. B **40**, 4054 (1989).
[5] W. M. Chen *et al.*, Proceedings of the 20th International Conference on the Physics of Semiconductors, edited by E. M. Anastassakis and J. D. Joannopoulos (World Scientific, Singapore, 1990), p. 2035.
[6] J. W. Corbett *et al.*, Phys. Rev. **121**, 1015 (1961).

