

## Comment on "Microscopic Identification and Electronic Structure of a Di-Hydrogen-Vacancy Complex in Silicon by Optical Detection of Magnetic Resonance"

In a Letter, Chen *et al.*, [1] reported the observation of a dihydrogen-vacancy complex in silicon ( $\text{VH}_2$ ) by ODMR (optical detection of magnetic resonance). A careful look at the spin-Hamiltonian parameters indicates that they coincide with those of the excited state ( $S = 1$ ) Si-*SL1* spectrum of the monovacancy-oxygen center,  $\text{OV}^*$  [2,3], also known as the *A* center (see Table I, Fig. 1). Clearly, this raises some questions as to the validity of the identification of the spectrum of Chen *et al.* to  $\text{VH}_2$ .

However, the similarity could still be accidental. To check whether the spectra are different or are indeed one and the same, we have recreated the spectrum of Chen *et al.* by proton and deuteron implantation into float-zone and Czochralski (oxygen-rich) silicon. We found that the signal was 2 orders of magnitude more intense in the Czochralski material, and therefore conclude that it is oxygen related, as expected in the model of  $\text{OV}^*$ . In view of this, the choice of Czochralski silicon for the experiments of Chen *et al.* was unfortunate.

The identification of the spectrum to  $\text{VH}_2$  by Chen *et al.* was based on a difference between linewidths of the resonances in proton- and deuteron-implanted silicon. This broadening was assigned to an unresolved hyperfine (HF) interaction with two equivalent hydrogen nuclei. Unfortunately, the linewidth in ODMR is very large ( $\approx 0.3$  mT). In conventional EPR (electron paramagnetic resonance) the resonances have a much smaller linewidth (0.09 mT), and the seemingly 1:2:1 splitting assigned to HF interaction with two hydrogen nuclei is resolved into a 1:6.8:1 splitting (see Fig. 2) caused by the hyperfine interaction with a shell of six equivalent silicon atoms. In the model of  $\text{OV}^*$  these are the six second-shell atoms that are bonded to the two first-shell atoms accommodating the two paramagnetic electrons in dangling bonds. Note that the latter HF interaction with the first-shell silicon atoms is already well resolved by ODMR. The difference of the resonances of the Si:D and Si:H samples as observed

TABLE I. Spin-Hamiltonian parameters according to Chen *et al.* [1] and Brower [2]. The spectra have orthorhombic- $I$  ( $C_{2v}$ ) symmetry and  $S = 1$ .  $H = \mu_B \mathbf{B} \cdot \mathbf{g} \cdot \mathbf{S} \cdot \mathbf{D} \cdot \mathbf{S} + \mathbf{S} \cdot \mathbf{A}_{\text{Si}} \cdot \mathbf{I}$ .

	[100]	[011]	[01 $\bar{1}$ ]	
Chen <i>et al.</i>				
$g$	2.002	2.005	2.002	
$D$	-348	-302	650	MHz
$A_{\text{Si}}$	$A_{\parallel} = 200, A_{\perp} 114$			MHz
Brower				
$g$	2.0076	2.0102	2.00577	
$D$	-350	-307	657	MHz
$A_{\text{Si}}$	$A_{\parallel} = 216, A_{\perp} = 112$			MHz

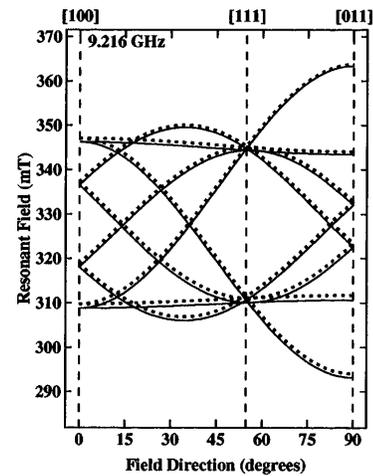


FIG. 1. Comparison of the angular dependences of the spectrum simulated with the Hamiltonian of Table I (without Si-HF) with the parameters given by Chen *et al.* (dashed) and Brower (solid).

by Chen *et al.*, i.e., the apparent enhancement of the hyperfine lines, is possibly due to saturation effects; hyperfine lines can saturate at a later stage. The resonance shown in Fig. 3(b) of Ref. [1] (Si:D) could be less saturated and the line shape more closely reflecting the 4.7% abundance of silicon.

P. Stallinga and B. Bech Nielsen  
Aarhus University, Denmark

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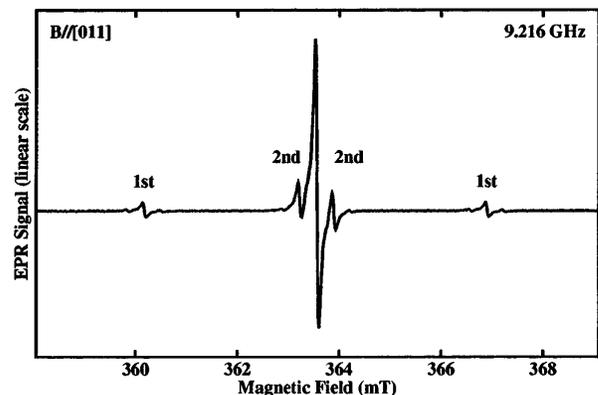


FIG. 2. Details showing a fine structure resonance with the first (1st) and second (2nd) shell  $^{29}\text{Si}$ -HF satellites.