

Assali and Leite Respond: The most important issue raised by DeLeo and Fowler (DF)¹ is that the computed H vibrational frequency is in agreement with recent infrared experiments for the model of Pankove and co-workers, but not for our (AL) model. Here we show that the H-B complex configuration, suggested by us as responsible by the passivation effect, is fully consistent with the experiments mentioned by DF. According to our *MS-X α* calculations the passivation effect is originated from a covalent mechanism which involves, besides H and B, also the Si neighbors. Therefore we claim that the measured infrared frequencies are associated with the vibrations of a complex rather than be primarily related to the vibrations of H on a Si—H bond as suggested by Pankove and co-workers and by DF in their Ref. 3. In order to prove our point we build a model, schematically shown in Fig. 1, and perform the analysis of the computed vibrational frequencies of the H-B and D-B complexes according to the atomic configuration proposed by AL.

As depicted in Fig. 1, H at an antibonding interstitial position is tied to B by the spring constant f' and to its three Si neighbors by f'' . The $B_5H_7Si_3$ unit is then embedded in a rigid lattice. The bulk-cluster coupling is simulated by connection of the B and the three Si atoms to their four "rigid" neighbors by f . Here we follow the procedure of Feenstra, Hauenstein, and McGill² and describe the vibrational modes by adopting sets of two independent parameters which can be interpreted as "bond-stretching" (f_1, f'_1, f''_1) and "bond-bending" (f_2, f'_2, f''_2) spring constants.

The values $f_1 = 9.33 \text{ eV/\AA}^2$ and $f_2 = 0.54 \text{ eV/\AA}^2$ have been chosen to reproduce the phonon energies of the Si perfect lattice by matching of the TO_Γ and TA_χ energies, 518.6 and 145.2 cm^{-1} , respectively.³ The energies of the complex vibrational modes have been determined as functions of the scaling parameters $\alpha = f'/f$ and $\beta = f''/f$. These modes transform as the $4A_1 \oplus A_2 \oplus 5E$ irreducible representations of the C_{3v} point group and both A_1 and E are infrared active. We found that the measured values of the frequencies for H and D are reproduced by the A_1 mode, which involves the motions of H (D) and B in the (111) direction, and by a unique choice of the scale factors, $\alpha = 0.84$ and $\beta = 0.90$.

Therefore, the set of spring constants $f'_1 = 7.84 \text{ eV/\AA}^2$, $f'_2 = 0.46 \text{ eV/\AA}^2$ and $f''_1 = 8.40 \text{ eV/\AA}^2$, $f''_2 = 0.49 \text{ eV/\AA}^2$ yield the wave numbers 1870 cm^{-1} for the H-B complex and 1360 cm^{-1} for the D-B complex, an exact reproduction of the experimental results (see Refs. 3 and 8 in DF). Since the energies of the A_1 mode lie far above the TO_Γ energy, it is expected to be a sharp localized mode, in agreement with experiment. Moreover the AL model is also consistent with Raman-scattering measurements which imply a lack of inversion symmetry (see Ref. 7 in DF). In all cases

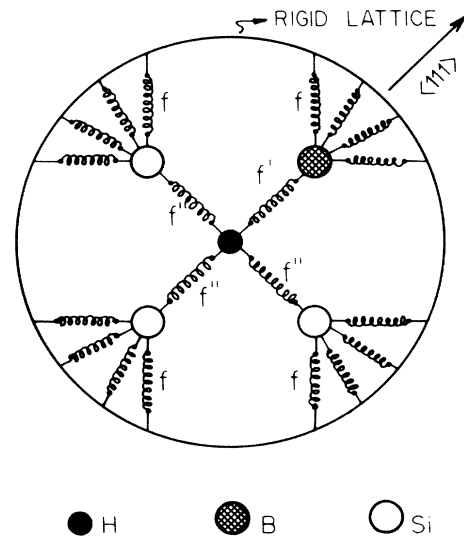


FIG. 1. Schematic representation of a $B_5H_7Si_3$ cluster imbedded in an immovable Si lattice. Each spring constant indicated corresponds to the "bond-stretching" and "bond-bending" parameters defined according to Ref. 2.

the B vibrations as well as the Si vibrations play a relevant role in determining the frequencies.

What we have shown is that the AL model fulfills the ultimate test of the theory, that is, it accounts for the passivation of the shallow acceptor activity of the complex and is consistent with the infrared experiments. Therefore, it seems to us that the model suggested by Pankove and co-workers is not definitive. In particular, we have verified from our *MS-X α* calculations that the T_d interstitial site for H is lower in energy than the minimum of the configuration suggested by Pankove and co-workers.

Thus, we conclude that further theoretical and experimental works are required to establish a consolidated microscopic model for the H-passivation mechanism of acceptor shallow levels in silicon.

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