Reply to "Comment on volume relaxation around defects in silicon upon electron emission"

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(Received 7 March 1988)

The proposed method of Nolte, Walukiewicz, and Haller for evaluating the conduction-band deformation potential for Si may be a step in the right direction; however, some cautions are emphasized.

As indicated by Nolte, Walukiewicz, and Haller[1] our method for calculating the volume lattice relaxation (ΔV) accompanying carrier emission from deep levels requires knowledge of the value of the conduction-band-edge hydrostatic deformation potential. Since this value was not available, we made the assumption that the experimentally-observed hydrostatic pressure shift of the Si band gap is taken up equally by displacements of the valence- and conduction-band edges.[2,3] We have argued that this assumption leads to a maximum uncertainty in ΔV of ± 1.2 Å^3 per emitted carrier.

In their Comment, Nolte, Walukiewicz, and Haller use a deduced (not measured as stated) conduction-band deformation potential to reevaluate ΔV of the Au acceptor and oxygen-vacancy in Si. An accurate method of evaluating this deformation potential is definitely needed, and the approach of Nolte, Walukiewicz, and Haller may be a step in that direction. However, some cautions need to be emphasized.

The approach of Nolte, Walukiewicz, and Haller is based on the notion that a universal reference energy level for transition-metal impurities in III-V semiconductors exists, and that this "reference level translates naturally to Si,"[4] and, furthermore, that "by measuring the universal pressure derivative of transition-metal defects, one is in fact measuring the band-edge deformation potential."[1] It is clear that a lot of presumptions are made, and, as discussed by the authors in another paper,[4] there are a number of difficulties with Si (including the small pressure dependence of its band gap) which suggest to us that the "translation" from the III-V to Si may be fraught with considerable uncertainties. Additionally, there is disagreement in the literature concerning the existence and nature of such a reference state.[5] Considering all of these factors along with the estimate of Nolte, Walukiewicz, and Haller that the error in determining the reference level is ± 1 eV, it seems to us prudent to exercise a great deal of caution in using the approach to deduce small pressure effects on the order of 1 meV/kbar.

Finally, we note that, using their approach, Nolte, Walukiewicz, and Haller[1] estimate ΔV for the Au acceptor in Si to be 0.3 ± 1.5 Å^3/emitted electron. Our approach yields $\Delta V = -2.0$ Å^3/emitted electron (with possible uncertainty up to ± 1.2 Å^3) for this acceptor. The negative sign of ΔV implies *inward* relaxation upon emission, and this is what is expected on the basis of the best available model (due to Watkins[6]) for this acceptor. Specifically, Watkins proposed that the Au acceptor level (and also the Pt^- and Pd^- acceptor levels) has antibonding character and is determined by vacancylike Si dangling bond states. The model is supported by results of cluster model calculations of the electronic structure of Au^0 and Pt^- in Si.[7] As these acceptor levels are antibonding in character, we expect pressure to force them higher in the gap (i.e., closer to the conduction-band edge) and that there will be *outward* (*inward*) relaxation on electron capture (emission), as we have found. Capturing an electron by such levels weakens the bonding between the impurity and its nearest Si neighbors causing the latter to relax outward to strengthen their bonds with the next shell of Si atoms. Emission has the opposite effect, i.e., inward relaxation of the impurity's Si neighbors.

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[2] G. A. Samara and C. E. Barnes, Phys. Rev. B **35**, 7575 (1987).
[3] G. A. Samara, Phys. Rev. B **36**, 4841 (1987).
[4] D. D. Nolte, W. Walukiewicz, and E. E. Haller, Phys. Rev. B **36** (1987).
[5] J. Tersoff and W. A. Harrison, *Abstracts Book of the Boston Meeting of the Materials Research Society, December, 1987* (Materials Research Society, Pittsburgh, 1987), and references therein.
[6] G. D. Watkins, Physica B + C **117B** and **118B**, 9 (1983).
[7] J. L. A. Alves and J. R. Leite, Phys. Rev. B **30**, 7284 (1984); see also J. Phys. C **17**, L771 (1984).

