Comments

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Comment on volume relaxation around defects in silicon upon electron emission

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The calculation of volume relaxation requires knowledge of the value of the conduction-band-edge hydrostatic deformation potential. The purpose of this Comment is to calculate the volume relaxation of the Au acceptor and the oxygen-vacancy pair (A center) in silicon based on the recently determined conduction-band deformation potential.

In several recent papers, Samara and Barnes[1-3] have proposed that volume relaxation upon carrier emission from deep-level defects in silicon can be calculated from hydrostatic-pressure experiments. The calculation of the volume relaxation requires knowledge of the value of the conduction-band-edge hydrostatic deformation potential. These authors did not have this value for silicon, and therefore set limits on the magnitudes of the relaxations. The purpose of this Comment is to calculate the volume relaxation of the Au acceptor and the oxygen-vacancy pair (A center) in silicon based on the recently determined conduction-band deformation potential.

The band-edge deformation potentials in GaAs and InP have recently been determined by us[4] using the universal pressure derivative of substitutional transition-metal defects as a reference level from which to measure the change in band-edge energy under pressure. Transition-metal impurities have recently been shown to be locked to an internal reference level.[5] Therefore, by measuring the universal pressure derivative of transition-metal defects, one is in fact measuring the band-edge deformation potential. We extended this principle to the case of silicon,[6] using published data on Pt and Pd acceptors.[7] The band deformation potentials in silicon were found to be $a_c = +2.4$ eV and $a_v = +0.9$ eV, in good agreement with theoretical calculations and transport measurements. The error on determining the reference level is ± 1 eV, estimated from the scatter in transition-metal pressure derivatives and from the deviation from the theoretical value.

The volume relaxation of a deep level upon carrier emission is given by[1]

$$\Delta V = d\Delta H/dp - T\, d\Delta S/dp \ , \tag{1}$$

where ΔV is the change in defect volume, $d\Delta H/dp$ is the pressure derivative of the change in enthalpy of the defect, and $d\Delta S/dp$ is the pressure derivative of the change in entropy. The values of $d\Delta H/dp$ provided in Refs. 2 and 3 for the Au acceptor and the oxygen vacancy are relative to the conduction band. These are $+26$ meV/GPa and $+39$ meV/GPa, respectively, by which the defect levels move towards the conduction band under compression. By subtracting the conduction-band energy shift of -23 meV/GPa from these values, the absolute energy change of the defects are found to be $+3$ meV/GPa and $+16$ meV/GPa, respectively. Using these values in Eq. (1) with the values of $d\Delta S/dp$ provided in Refs. 2 and 3 yields the following volume relaxations: $\Delta V_n = +0.3$ Å^3, Au acceptor at 190 K; $\Delta V_n = -2.3$ Å^3, A center at 77 K. A positive volume change denotes an outward relaxation upon electron emission. The uncertainty in the exact position of the reference level introduces an uncertainty of ± 1.5 Å^3 in these volume relaxations.

The relaxation for the Au acceptor is small. In fact, the Au acceptor has a pressure derivative very similar to those of the Pt and Pd levels which define the reference level and which therefore do not couple strongly to the lattice. On the other hand the oxygen-vacancy complex measured by Samara does couple significantly to the lattice, and the sign of the relaxation is consistent with the Watkins's model for this defect.

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