Errata

Erratum: Computer simulation of local order in condensed phases of silicon [Phys. Rev. B 31, 5262 (1985)]

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The sentence on page 5263 including Eq. (2.2) should end with the phrase ". . . and σ is chosen to make $f_2'(2^{1/6})$ vanish."

The numerical value given in Eq. (4.4) for the change in mean potential energy at melting is too large by a factor of 2. Correcting that error restores consistency with Fig. 3. The proper versions of Eq. (4.4) and the similarly affected Eq. (4.5) are

$$\langle \varphi \rangle_l - \langle \varphi \rangle_c = 0.15 \ , \quad (4.4)$$

$$\Delta S / N k_B \cong 1.19 \ . \quad (4.5)$$

We are indebted to Dr. Jeremy Q. Broughton for bringing this discrepancy to our attention.

Erratum: Indirect band gap of coherently strained Ge_xSi_{1-x} bulk alloys on $\langle 001 \rangle$ silicon substrates [Phys. Rev. B 32, 1405 (1985)]

R. People

It has been recently brought to my attention that the assumed values of $+3.8$ and -2.9 eV for the respective hydrostatic deformations of Si and Ge are not the accepted values. The experiments from whence these values were derived were not performed under purely hydrostatic conditions.[1] Pure hydrostatic pressure measurements of the hydrostatic deformation potential for bulk Ge_xSi_{1-x} alloys have been performed by Paul and Warschauer.[2] They found that the hydrostatic deformation potential for bulk (Ge,Si) alloys exhibits an almost step-function-like behavior; changing abruptly from $+1.5$ eV for alloys having a Si-like conduction-band structure (i.e., $x \lesssim 0.85$) to -4.5 eV for alloys having a Ge-like conduction-band structure. If, in fact, one assumes a constant hydrostatic deformation potential of $+1.5$ eV over the composition range $0 \leq x \lesssim 0.75$, then the calculated strained alloy band gap is essentially unchanged from the results obtained by assuming a linear interpolation between 3.8 and -2.9 eV.[3] The revised results are identical to the linear interpolation results for $x \lesssim 0.5$ and are lower by $\lesssim 50$ meV at $x = 0.75$. Although it is seen that the use of the correct hydrostatic deformation potential does not dramatically alter the previous results, it is crucial for an understanding of the underlying physics. In particular, the linear interpolation assumption implies a continuous mixing of the Δ_1 and L valleys of the alloy, which is contrary to observation.[2] Indeed, the conduction-band minima of the bulk alloy are either Δ_1 or L in character, rather than a continuous admixture of the two.

[1] G. L. Bir and G. E. Pikus, *Symmetry and Strain-Induced Effects in Semiconductors* (Wiley, New York, 1974), p. 469.
[2] W. Paul and D. M. Warschauer, J. Phys. Chem. Solids **6**, 6 (1958).
[3] R. People, Phys. Rev. B **32**, 1405 (1985).