ERRATA

First-Principles Calculations of the Electronic Properties of Silicon Quantum Wires [Phys. Rev. Lett. 69, 1232 (1992)]

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Equation (1) of this paper should read

$$d = a_0(2M)^{1/2}/4\,, \tag{1}$$

i.e., the correct value of d is a factor of $\sqrt{2}$ smaller than stated in our paper. The results of the effective-mass theory (EMT) and the first-principles calculations are all correct, but the latter are plotted in Fig. 2 with values of $1/d$ that are too small. The corrected figure is shown below. Evidently the 9×8 wire is significantly narrower than the thinnest of the wires observed in transmission electron microscopy, contrary to the statement made in our paper. Because of the error in Eq. (1), the band-gap upshift for the 9×8 wire was incorrectly thought to agree with EMT, so that the latter was used for wires wider than 9×8. On the basis of a reasonable interpolation, shown by the dashed curve in the amended figure, we now expect good agreement between the EMT and first-principles band-gap upshifts for wire thicknesses greater than 33 Å. The theoretical band-gap energy, and the width of the crystalline Si core in the "aged" (oxidized) wires, can be calculated as in our original paper, but using this interpolated curve rather than the EMT curve. Such analysis shows that (a) the experimental photoluminescence (PL) energy remains consistent with the theory that the PL arises from quantum confinement of excitons in narrow Si wires; (b) E_B, the sum of the exciton binding and localization energies, is 0.16 eV rather than 0.32 eV; and (c) the aged sample has crystalline Si wires 19 Å wide, rather than 23 Å as stated in our paper.

The agreement between experimental and theoretical lifetimes for the aged sample is likely to be slightly worse than reported in our paper. Although no one has calculated first-principles lifetimes for wires as wide as 19 Å, the theoretical lifetime is expected to be longer for a 19 Å wire than for the slightly narrower 16 Å (9×8) wire that we calculated, because of the reduced effect of quantum confinement in breaking the momentum selection rule. The concluding discussion of our paper, on the reasons for the high quantum efficiency of porous silicon, remains valid, since it depends only on the fact that the measured and calculated lifetimes are long.

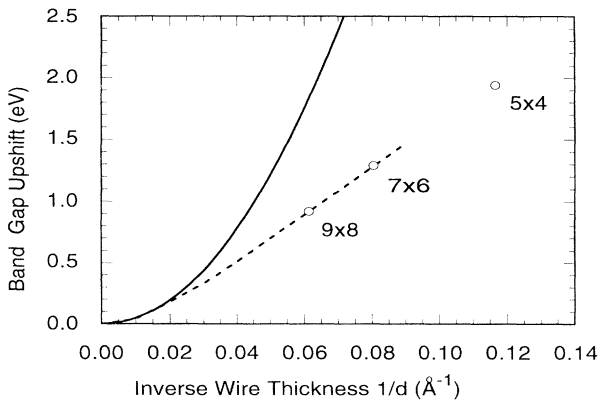

FIG. 2. The band-gap upshift of the wire structures with respect to bulk Si plotted against the inverse of the wire thickness (circles). The EMT upshift of Eq. (2) of the original manuscript with $C=0.900$ is also plotted (continuous line). The wire thickness d is defined by Eq. (1) above. The dashed line is an interpolation coinciding with the EMT curve near the origin and passing through the results of the first-principles calculations for the 9×8 and 7×6 wires.