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Pressure dependence of the band gaps in Si quantum wires

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The pressure coefficients *a* of interband transitions in (001) silicon wires are calculated using a plane-wave basis and carefully fitted empirical pseudopotentials. We find purely red shifts ($a<0$). [redacted]

[redacted]

(i) As the pressure increases above ~25 kbar the PL [redacted] coefficient of $a\sim-3$ meV/kbar. This value is more negative than the value for the indirect gap of crystalline Si (−1.41

[redacted] are described by local pseudopotentials, simultaneously fit[12] [redacted] function. Using this Si potential we then fit the hydrogen potential to reproduce the observed chemisorption-induced

TABLE I. Observed pressure coefficients a of photoluminescence energy in porous Si. Values in square brackets denote experiments in which the pressurizing liquid medium was alcohol.

Authors and Reference	$P=0$ peak (eV)	ΔP (kbar)	a_{wire}(meV/kbar)
Camassel *et al.*[a]	1.8	0–10	−1.1 to −3.2
Zhou *et al.*[b]	1.85	0–20	[+4.0 to +9.0]
Sood *et al.*[c]	1.68–1.80	0–70	−3 to −4
Zhao *et al.*[d]	1.74–1.86	0–26	[+6.2 to +6.5]
Zhao *et al.*[d]	1.74–1.86	≥30	[−2.8 to −4.1]
Ookubo *et al.*[e]	1.77	0–40	−3.0 to −5.0
Ryan *et al.*[f]	1.85	0–25	[+7.0]
Ryan *et al.*[f]	1.85	25–80	[−2.0]

[a] Reference 1.
[b] Reference 2.
[c] Reference 3.
[d] Reference 4.
[e] Reference 5.
[f] Reference 6.

we excite higher energy bands in a given wire size [compare [redacted]

ments on porous Si (Table I) where the pressure coefficient is [redacted] values, our calculated result for the wire falls *within* the range of the calculated bulk values. These observations hold [redacted]

These trends in the calculated wire pressure coefficients [redacted]

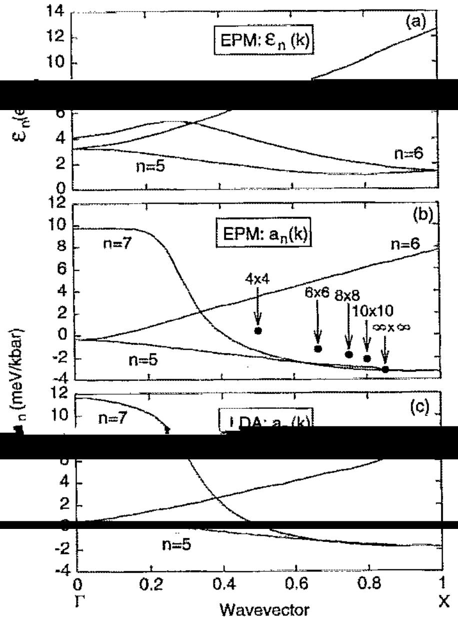
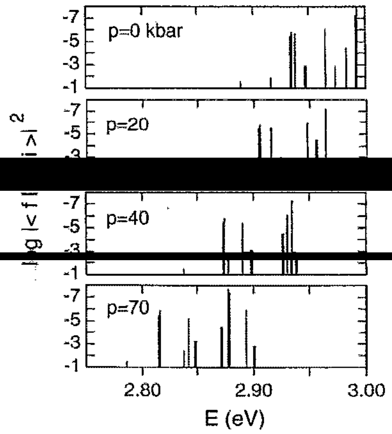


FIG. 1. (a) Calculated dispersions of three lowest bulk Si conduction bands [redacted] three bulk bands; (c) same as (b) but using the LDA. The solid dots in part [redacted]

decomposed into bulk wave functions $\phi_{n,k^*}(\mathbf{r})$ of band index [redacted]

Our previous work showed that the quantization of particle [redacted]

$\langle\psi_i|\phi_{n,k^*}\rangle$ We find that the wire CBM is composed predominantly from bulk states in the first and second conduction bands ($n=5,6$), evaluated at k^*. For example, in a 8×8 wire, [redacted] lence band minimum (VBM) comes from the two highest bulk valence bands at $k^*=2\pi/a_0(0,\frac{1}{4},0)$. Because the projection coefficients are not sensitive to the pressure, Eq. (1)



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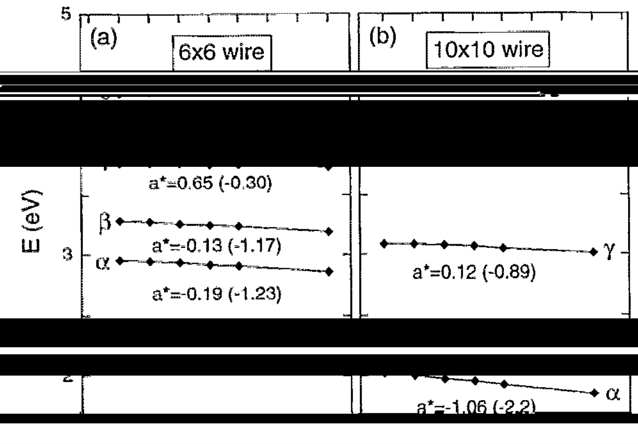

FIG. 3. Pressure dependence of the different groups of transitions (α,β,γ,δ)

[redacted]

$$\frac{\partial \epsilon_i}{\partial P} \cong \sum_n \sum_{k^*} |A^{(i)}_{n,k^*}|^2 \frac{\partial \epsilon_{n,k}}{\partial P}. \tag{3}$$

We thus interpret the calculated red shift of (001)-oriented wires with [110] surfaces as a manifestation of the analogous bulk properties along the $2\pi/a_0(0,1,0)$ direction in the Brillouin zone. The value of k^* having the largest projection will be denoted $k^*_{\max}$. Analyzing our directly calculated wire wave functions, we find that as the wire size in-

[redacted]

cients for the larger wires approach the bulk value $a(\Delta_{1c})$ at

[redacted]

approaches the CBM. (ii) The band edge pressure coefficients of small wires are *less* negative than $a^0(\Delta_{1c})$, since, by Eq. (3), the wire CBM represents a mixture of a few bulk states $|n,k^*\rangle$, most of which have $a_n(k^*)>a(\Delta_{1c})$ [Fig. 1(b)]. (iii) The fact that the *observed* wire pressure coefficients (Table I) are often most negative than the (observed) $a(\Delta_{1c})$ bulk value suggests either nonbulk (i.e., surface) or nonideality effects. (For example, the different compress-

[redacted]

shear that will split the wire VBM, pushing states further into

[redacted]

of our LDA-calculated pressure coefficients of bulk Si for off

[redacted]

caused by intrinsic quantum confinement, we expect a small

[redacted]

its orientation, shape, and size. (v) Since higher energy *wire* bands (β,γ,δ...) are constructed from correspondingly higher energy *bulk* bands, their pressure coefficients are less nega-

[redacted]

Given the predicted off-Γ character of the wire CBM at ambient pressures,[10–13] the analogy[6] draw by Ryan *et al.*[6] between porous Si and the direct gap GaAs under pressure clearly does not hold. The confusion arises, in part, because

[redacted]

that takes place in the pressure cell: Sood *et al.*[3,17] noted that the conventional methanol–ethanol mixture used as a

[redacted]

alcohols as a pressure medium but not in experiments

[redacted]

terms.

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