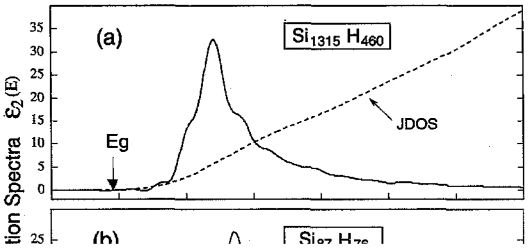
decreases, this must imply a greater role of surface effects on the electronic structure. This is true only if the wavefunction has an amplitude on the surface atoms. We test this next.

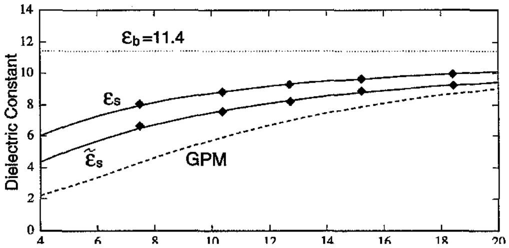
Shown in Fig. 2a,b are the wavefunction square of the CBM and VBM of the rectangular quantum box with $d = 34.1$ Å ($N_{\mathrm{Si}} = 1035$ atoms). The VBM and CBM states are found to be localized in the interior of the quantum dot, with zero amplitude on

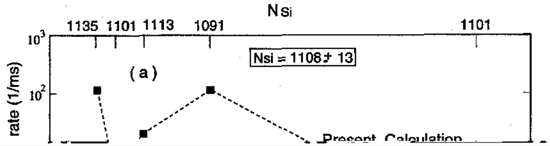
proximation (EMA) of Takagahara and Takeda [6] and the model of Rama Krishna and Friesner (RKF) [7].

2.3.1. Comparison with the effective mass method

As could be seen in Fig. 2, the VBM and CBM states found in our direct calculations are not surface states, hence a comparison with the results of the (surfaceless) EMA is warranted. Our 'exact' calcula-


(a)
Si1315 H460
35
30
25
20
15
10
5
0
tion Spectra ε2(E)
Eg
JDOS
25
(b)
Si87 H76


14
12
10
8
6
4
2
0
εb=11.4
εs
ε̃s
GPM
Dielectric Constant
4
6
8
10
12
14
16
18
20



in the empirical pseudopotential fitting. As a result, our fitted potential $V(\mathbf{r})$ is very close to LDA screened potential, except that our potential gives the correct bulk band gap and band structure, while the