

# Strained Silicon, Electronic Band Structure and Related Issues.

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# OUTLOOK (1/4)

INPUT

Strain matrix  
Ansys ...

?

What to do?

DESIRED VALUES

Current & Capacitances

## OUTLOOK (2/4)

Electronic Structure upon Strain

Dispersion relation and Gaps

Abinitio: LDA RPA GW  
Empirical: TB KP EPM

# OUTLOOK (3/4)

**Electronic Structure upon Strain**

**Dispersion relation and Gaps**  
Abinitio: LDA RPA GW  
Empirical: TB KP EPM

**Integration over Brillouin Zone**

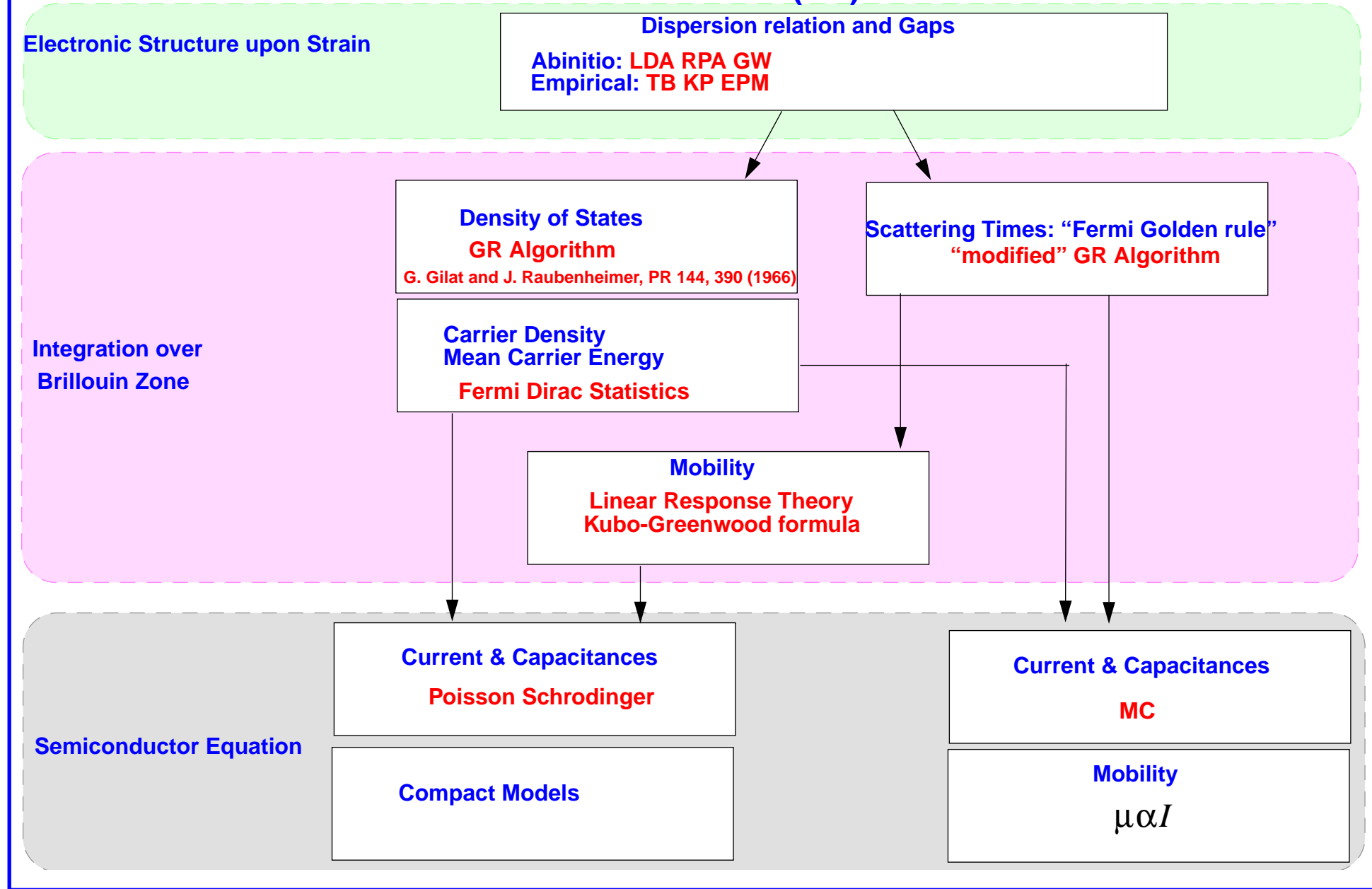
**Density of States**  
**GR Algorithm**  
G. Gilat and J. Raubenheimer, PR 144, 390 (1966)

**Carrier Density**  
**Mean Carrier Energy**  
**Fermi Dirac Statistics**

**Scattering Times: "Fermi Golden rule"**  
**"modified" GR Algorithm**

**Mobility**  
**Linear Response Theory**  
**Kubo-Greenwood formula**

# OUTLOOK (4/4)



## Review for Electronic Band Structure Method

### Review for Electronic Band Structure

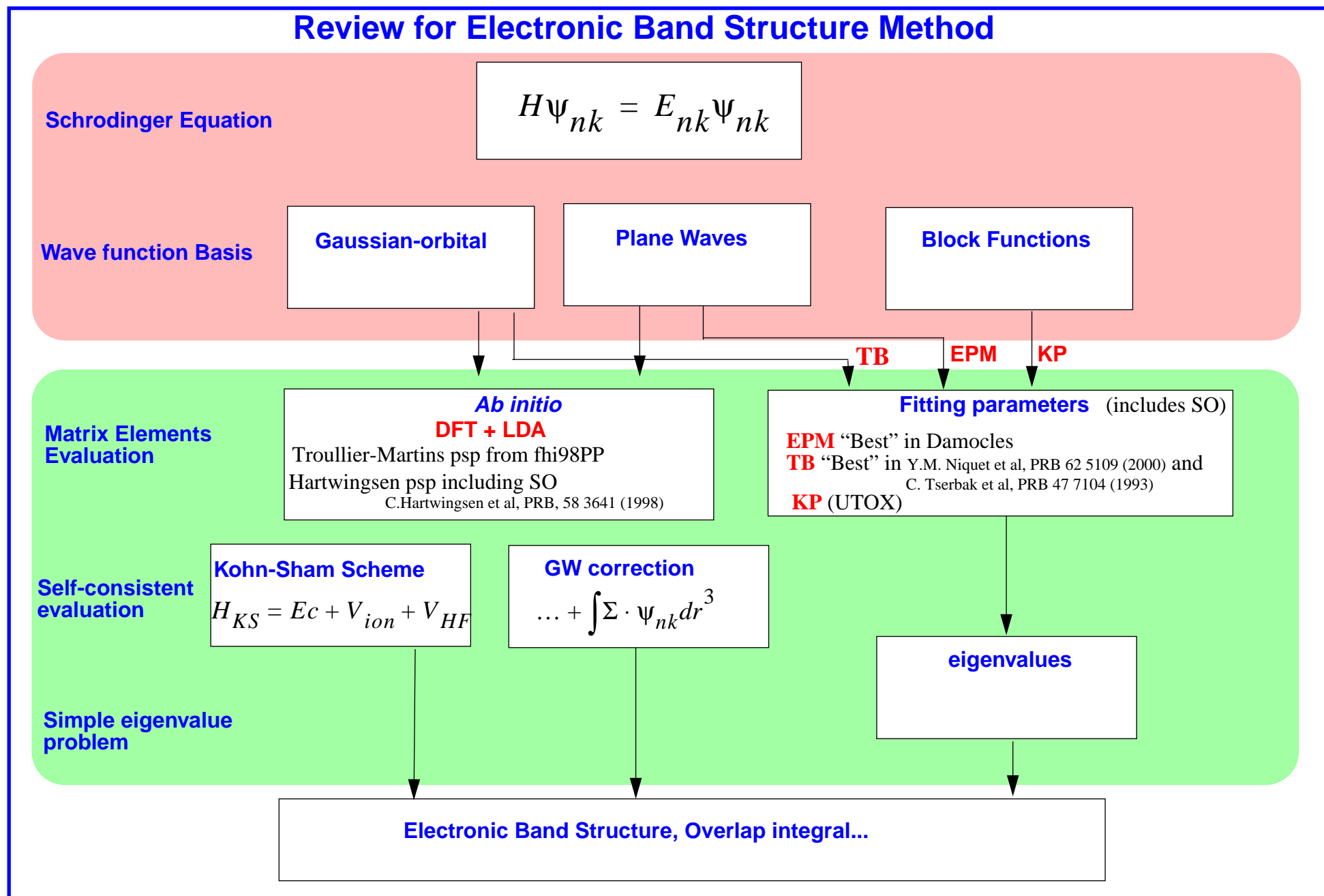
Ab initio vs Empirical methods

### Lower Dimension Aproximation

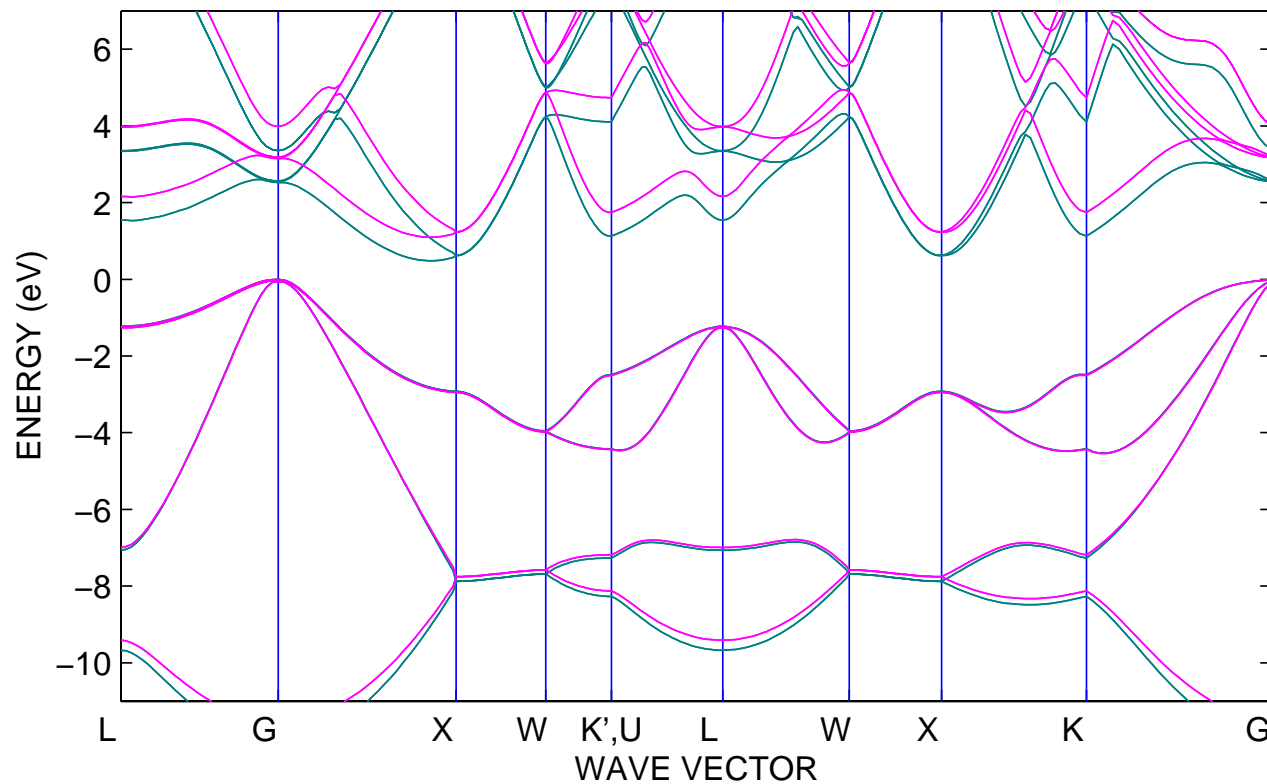
6X6 KP and Effective mass Hamiltonian

A strain example: Si on SiGe buffer

## Review for Electronic Band Structure Method



*Ab Initio:* **LDA KSS** vs **GW**



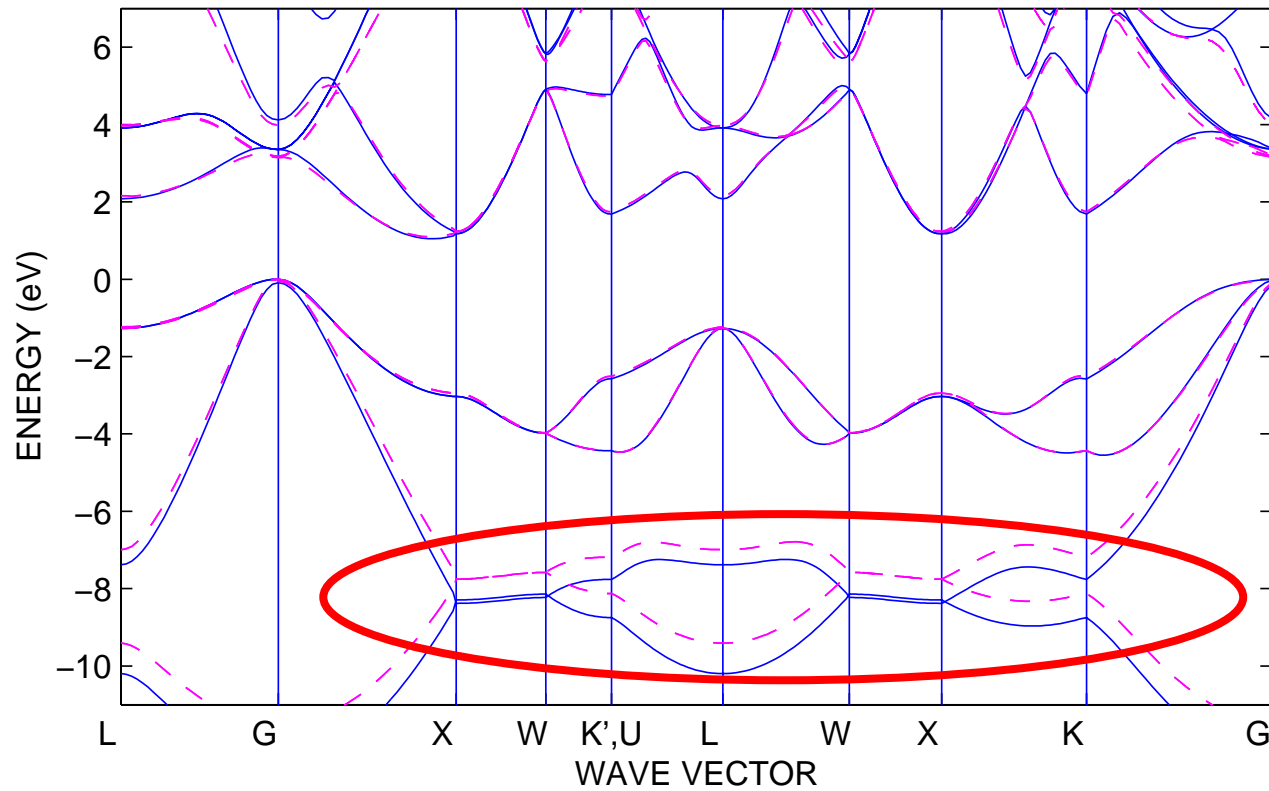
ABINIT V4.4.3

PSP: Hartwingsen psp (C.Hartwingsen et al, Phys. Rev. B, 58 3641 (1998))



# EPM (local)

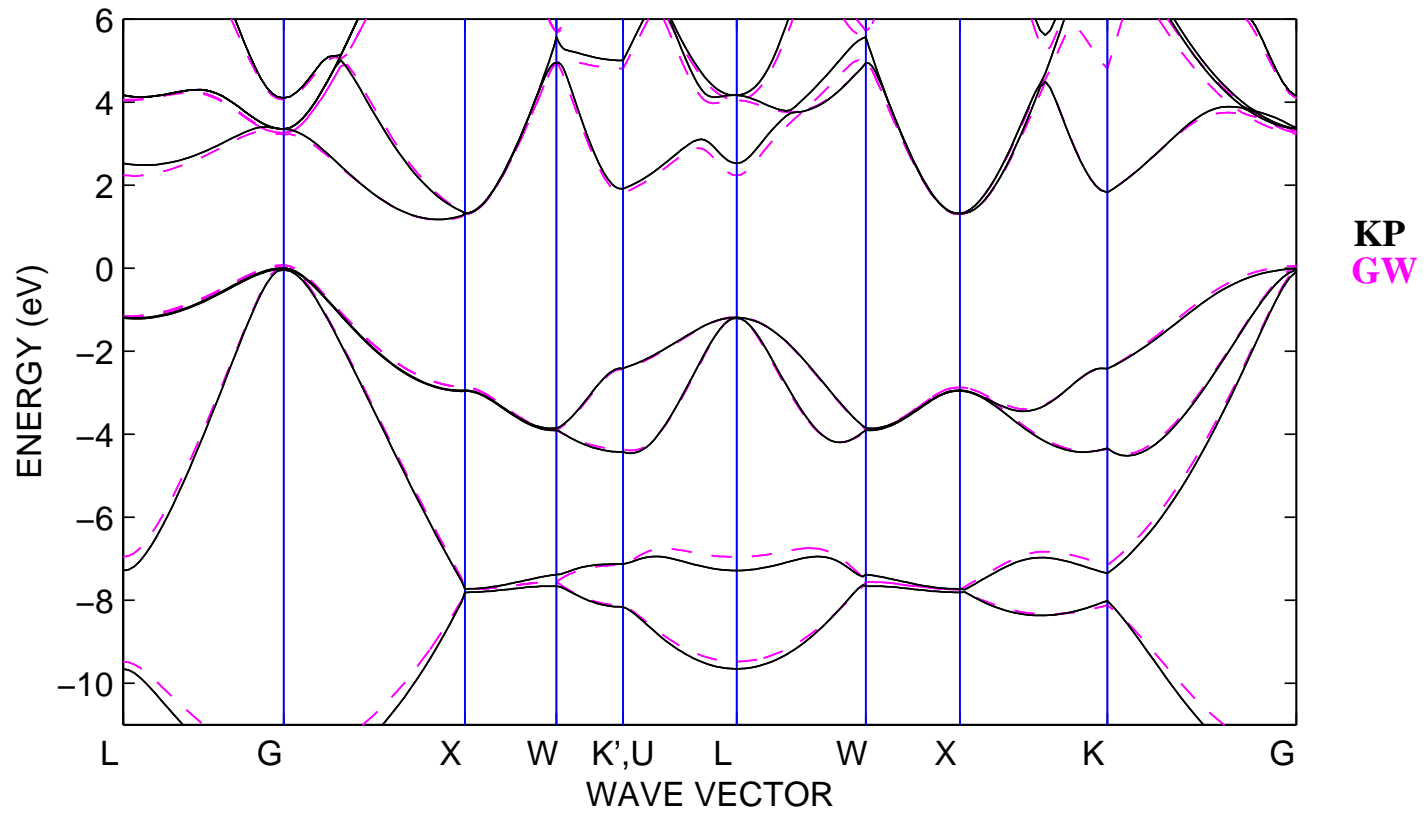
UTOX AFTER J.R. CHELIKOWSKY AND M.L. COHEN, PHYS. REV. B 14, 556 (1976)



“NON LOCAL EFFECT”

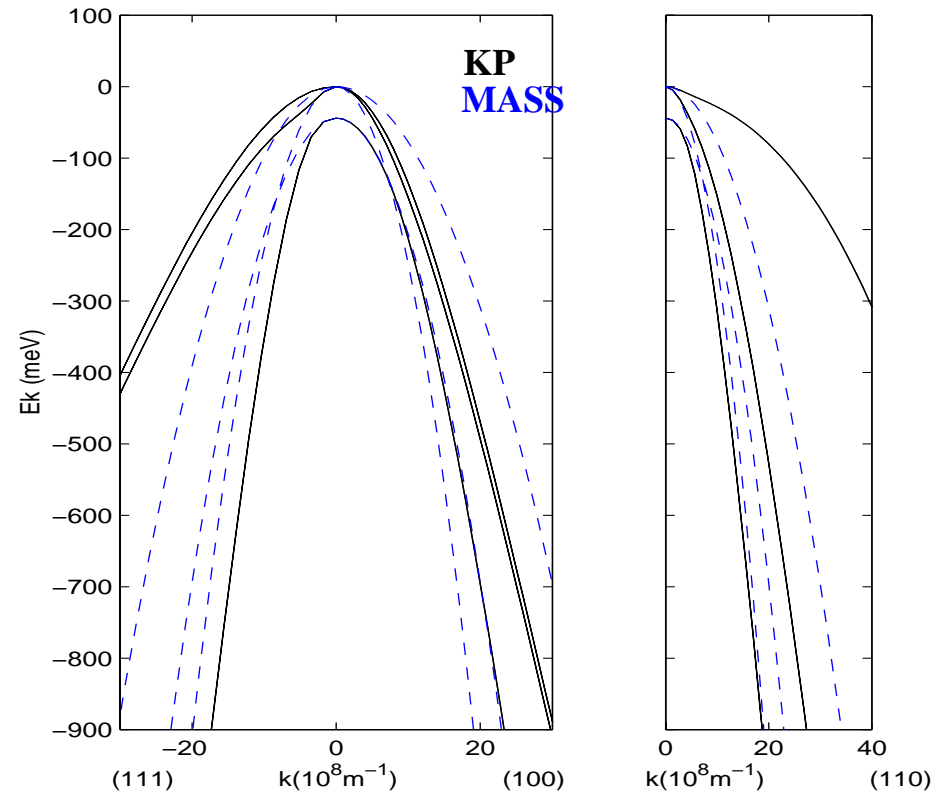
# KP

UTOX

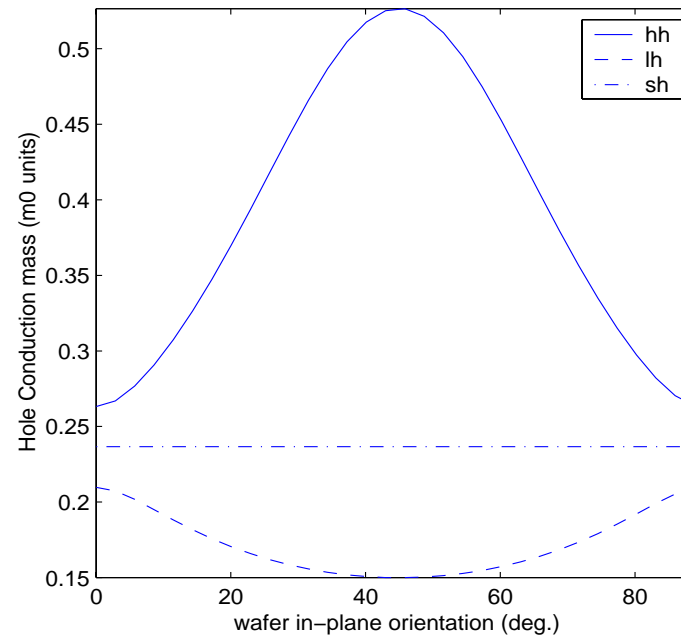


## Effective mass approximation for Electronic Band Structure

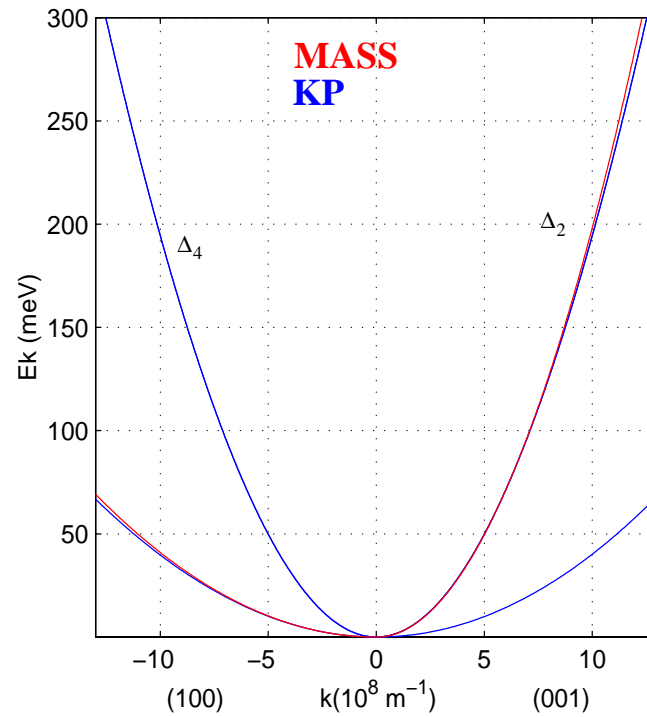
### Valence Bands: KP and Effective Mass Hamiltonian



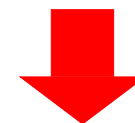
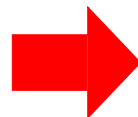
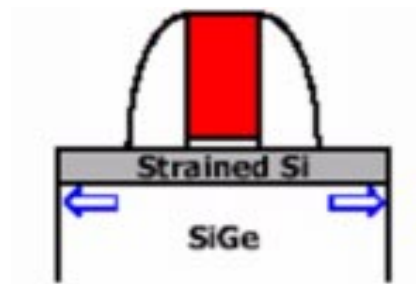
## Hole "curvature mass" for Effective Mass Hamiltonian



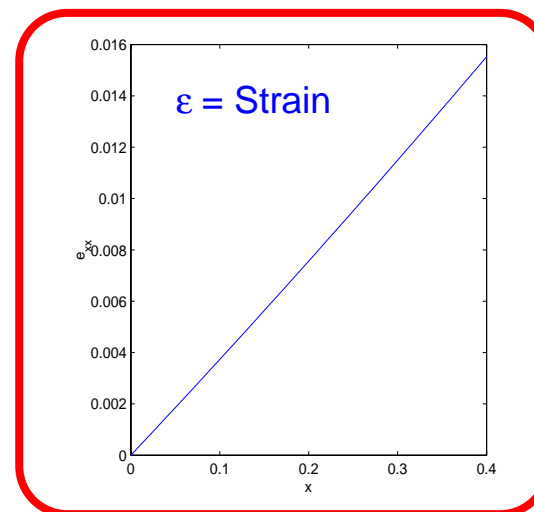
## Conduction Bands: KP and Effective Mass Hamiltonian



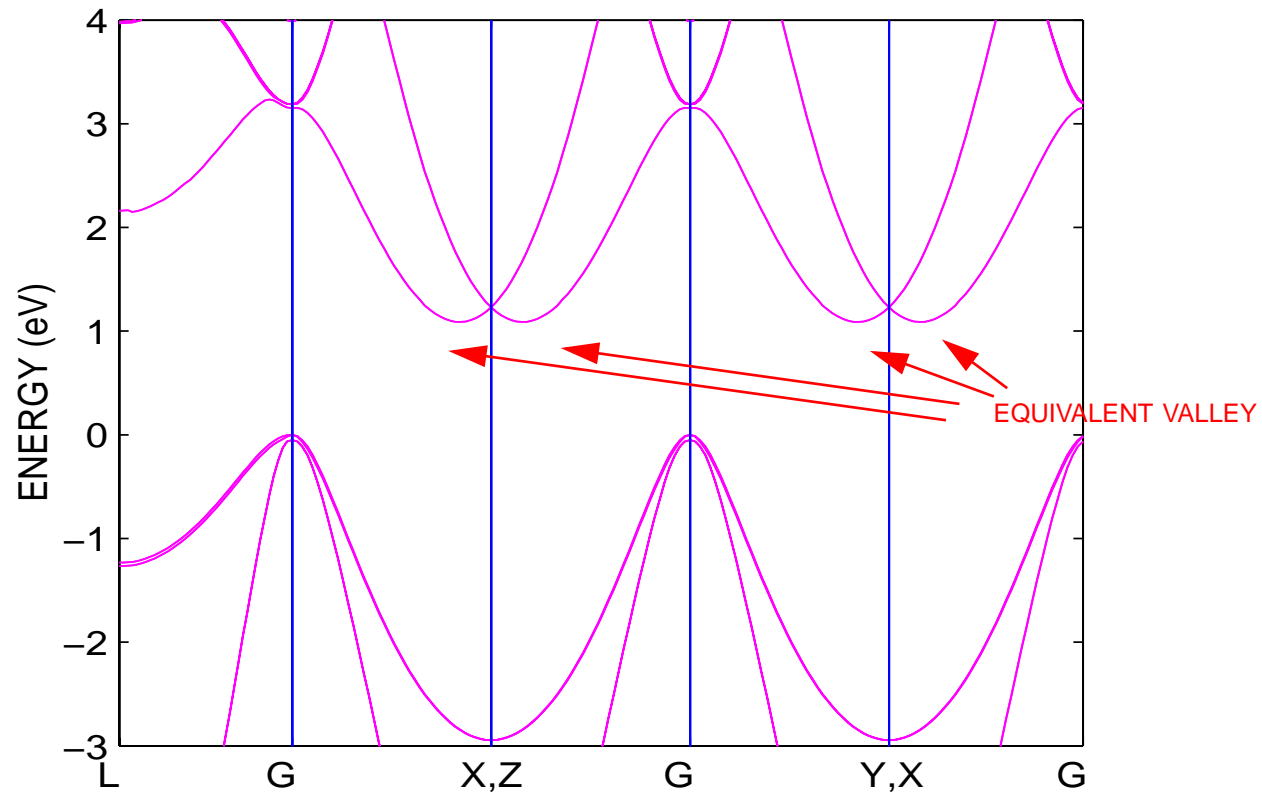
# STRAIN (STUDIED CASE)



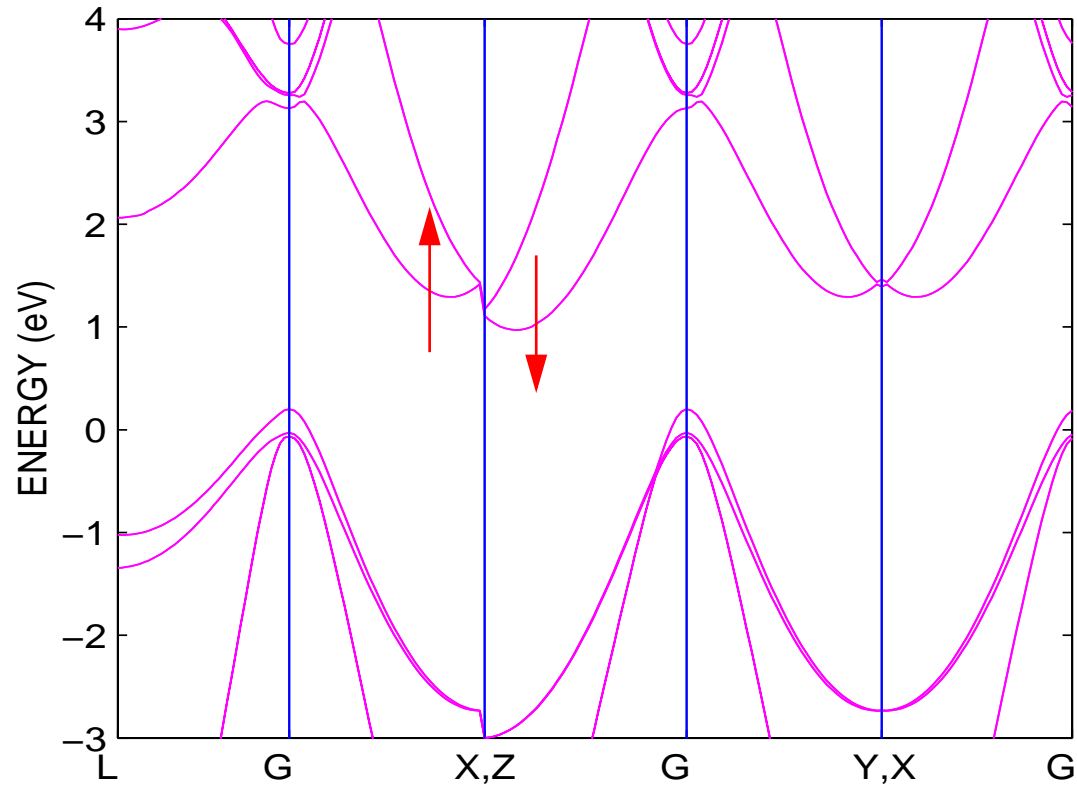
SiGe lattice larger than Si lattice



### RELAXED SILICON

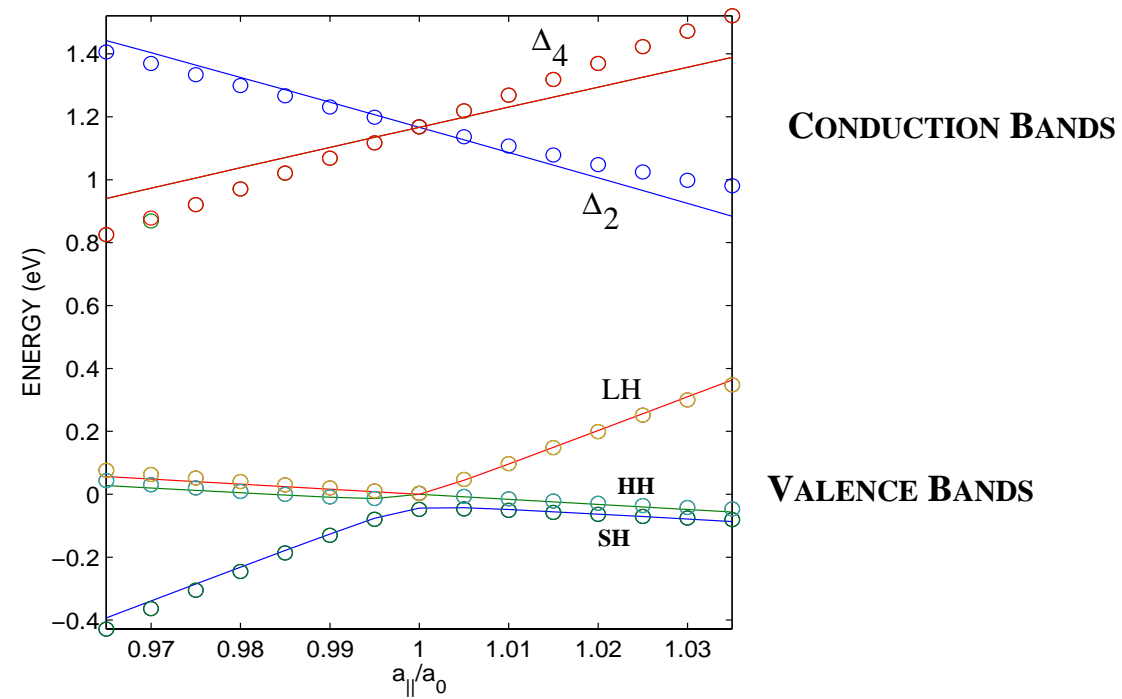


### 2% TENSILE

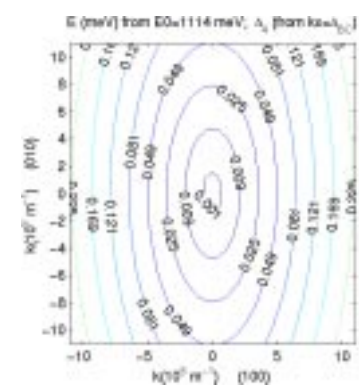
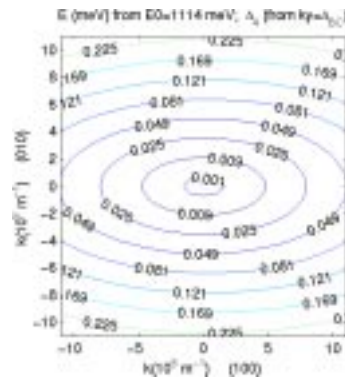
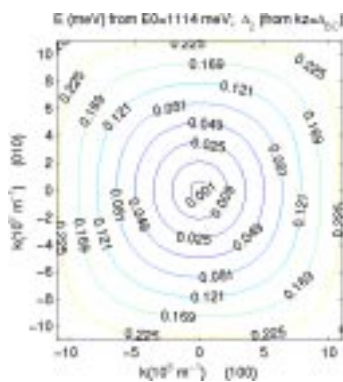
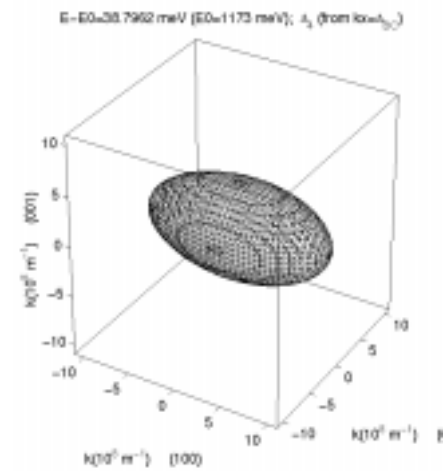
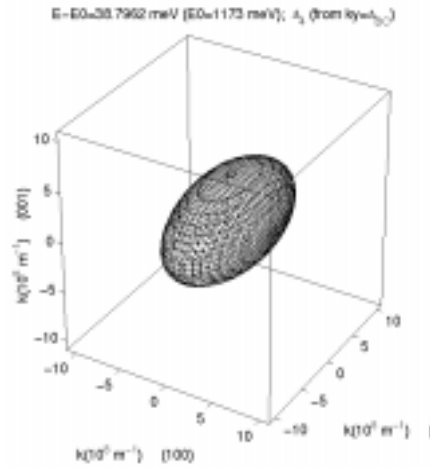
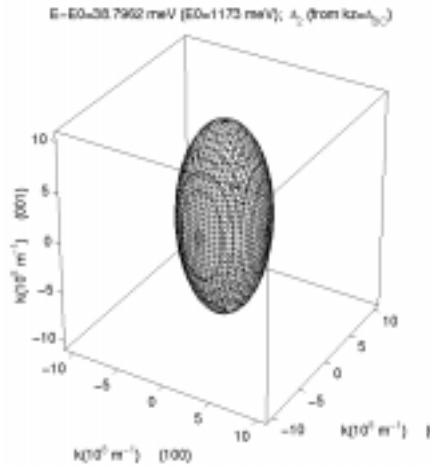




# ENERGY SHIFT VS. STRAIN

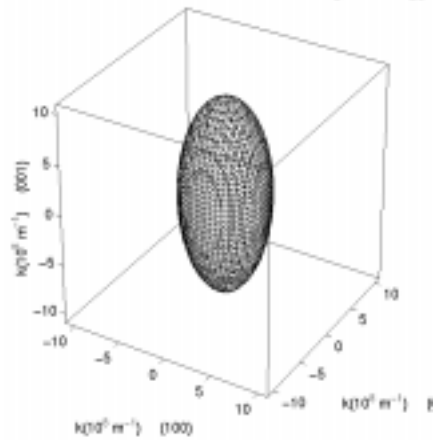


# CONDUCTION BANDS (RELAXED)

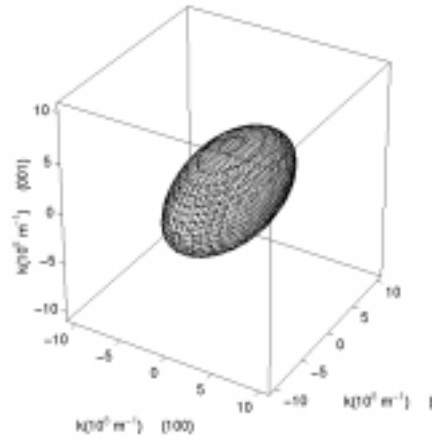


# CONDUCTION BANDS (1% TENSILE)

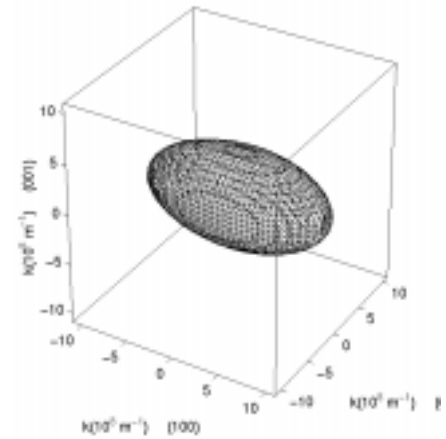
E=60.38.7962 meV (E0=1070 meV); 1% Tensile;  $\lambda_2$  (from  $k_x=k_{x0}$ )



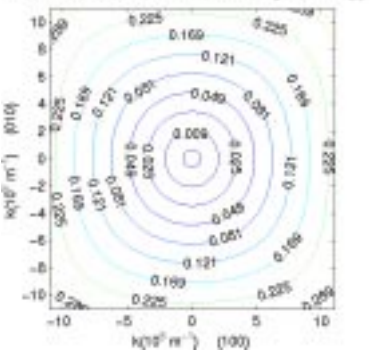
E=60.38.7962 meV (E0=1244 meV); 1% Tensile;  $\lambda_3$  (from  $k_y=k_{y0}$ )



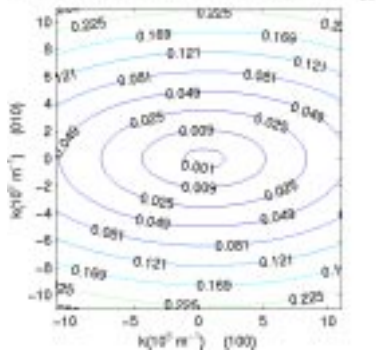
E=60.38.7962 meV (E0=1244 meV); 1% Tensile;  $\lambda_1$  (from  $k_x=k_{x0}$ )



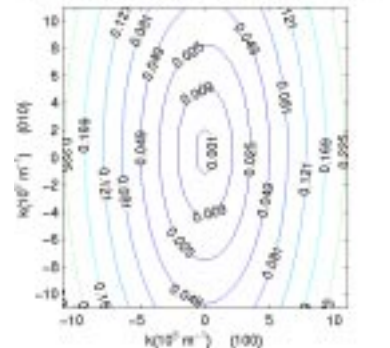
E (meV) from E0=049 meV; 1% Tensile;  $\lambda_2$  (from  $k_x=k_{x0}$ )



E (meV) from E0=1241 meV; 1% Tensile;  $\lambda_3$  (from  $k_y=k_{y0}$ )

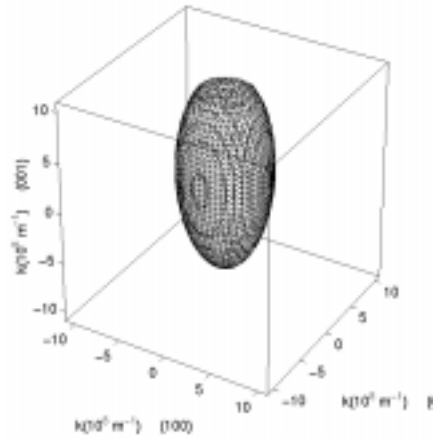


E (meV) from E0=1241 meV; 1% Tensile;  $\lambda_1$  (from  $k_x=k_{x0}$ )

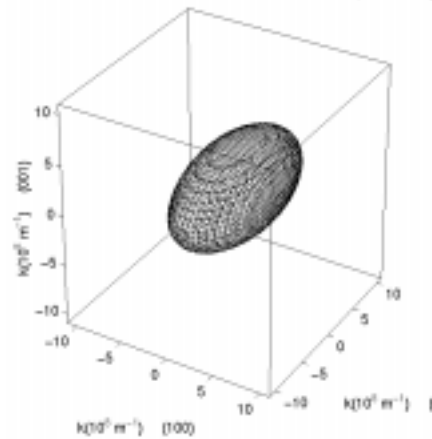


# CONDUCTION BANDS (1% COMPRESSIVE)

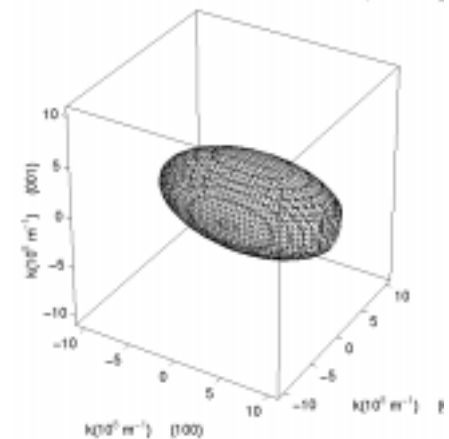
$E_0=38.7962$  meV ( $E_0=1272$  meV); 1% Compressive;  $\Delta_0$  (from  $k_x=0$ )



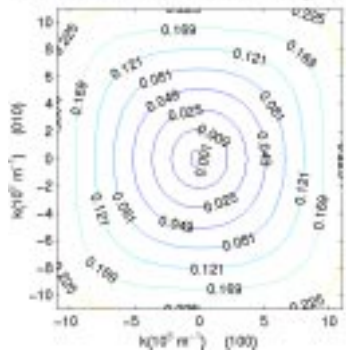
$E_0=38.7962$  meV ( $E_0=1096$  meV); 1% Compressive;  $\Delta_0$  (from  $k_y=0$ )



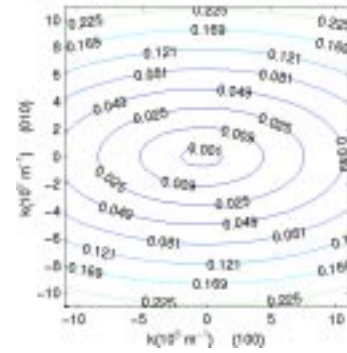
$E_0=38.7962$  meV ( $E_0=1096$  meV); 1% Compressive;  $\Delta_0$  (from  $k_x=0$ )



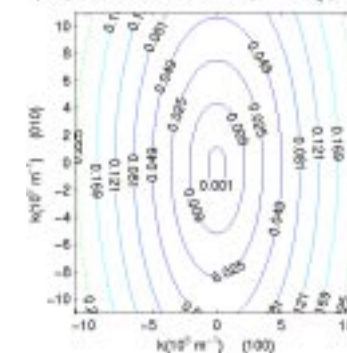
(meV) from  $E_0=1235$  meV; 1% Compressive;  $\Delta_0$  (from  $k_x=0$ )



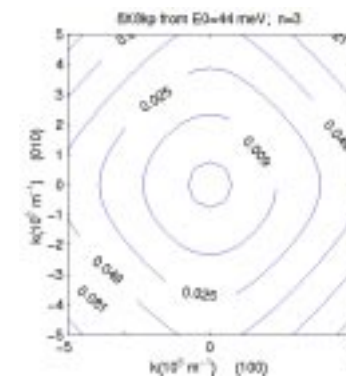
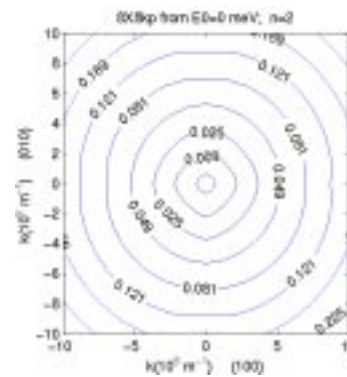
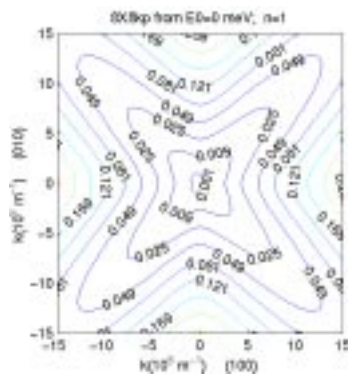
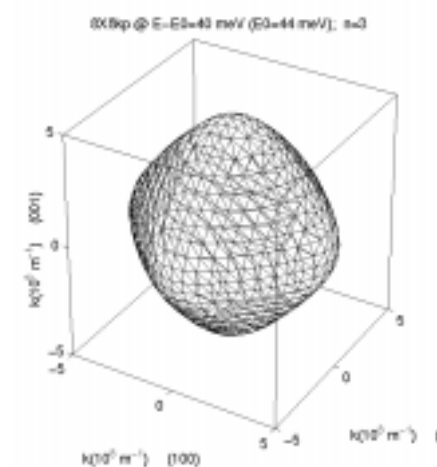
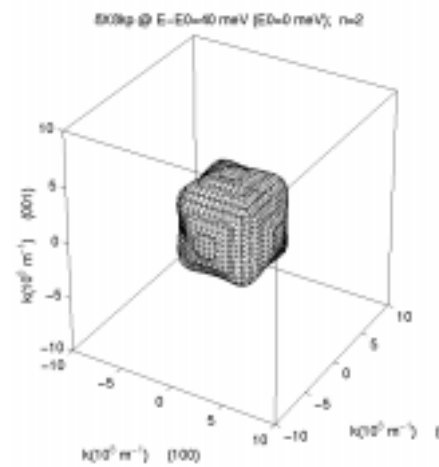
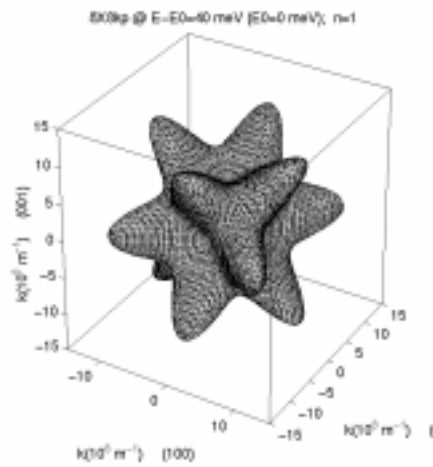
(meV) from  $E_0=985$  meV; 1% Compressive;  $\Delta_0$  (from  $k_y=0$ )



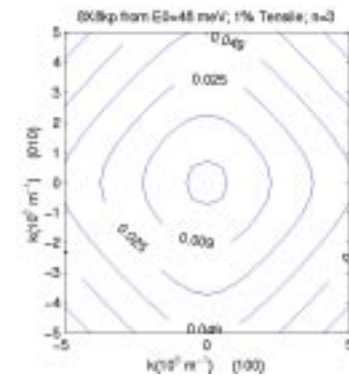
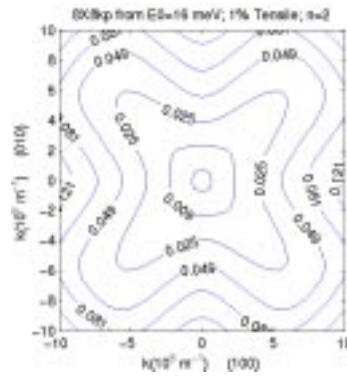
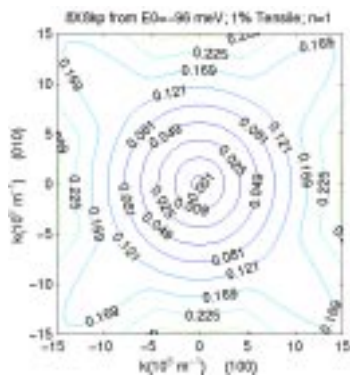
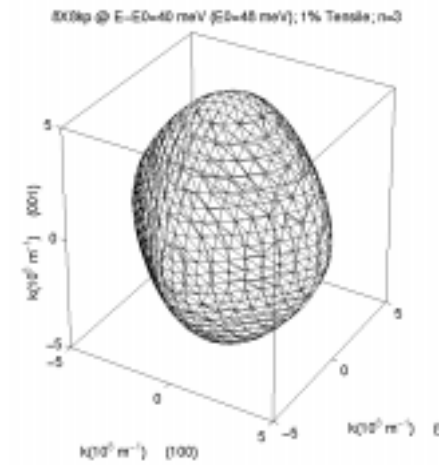
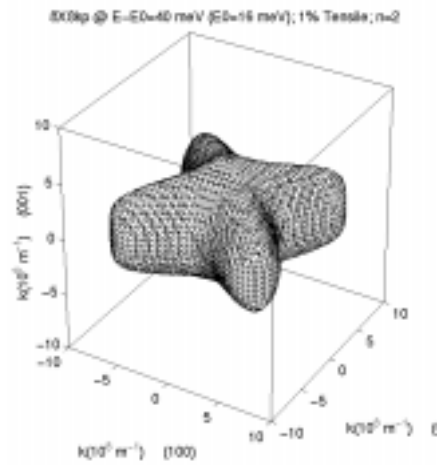
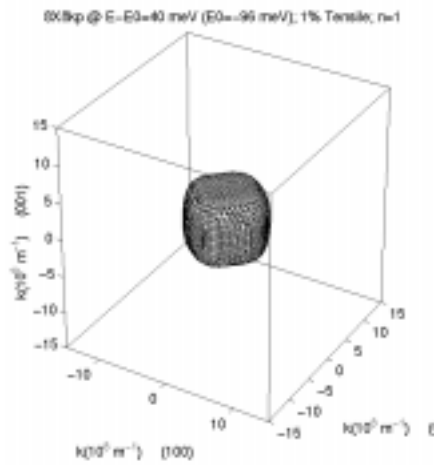
(meV) from  $E_0=985$  meV; 1% Compressive;  $\Delta_0$  (from  $k_x=0$ )



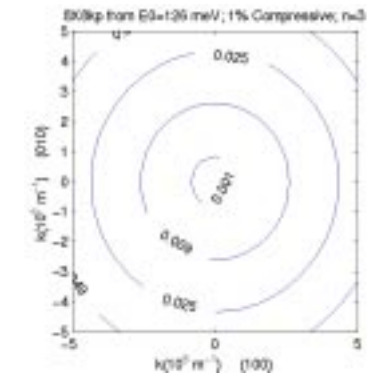
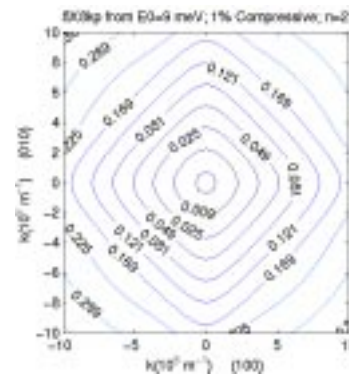
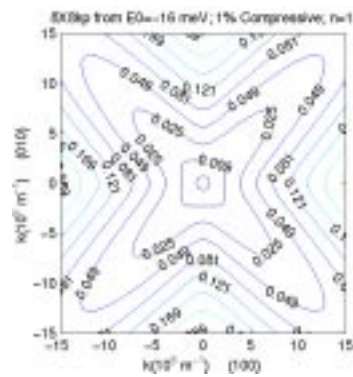
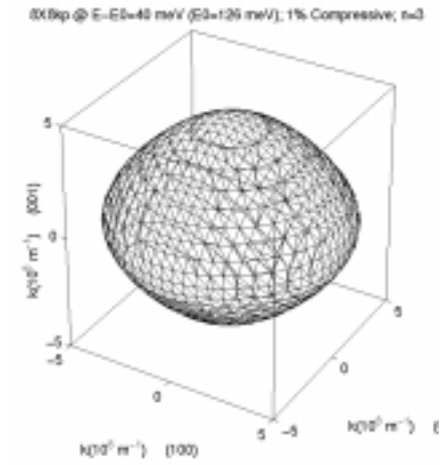
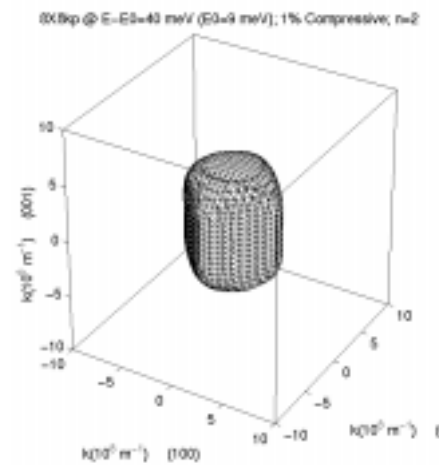
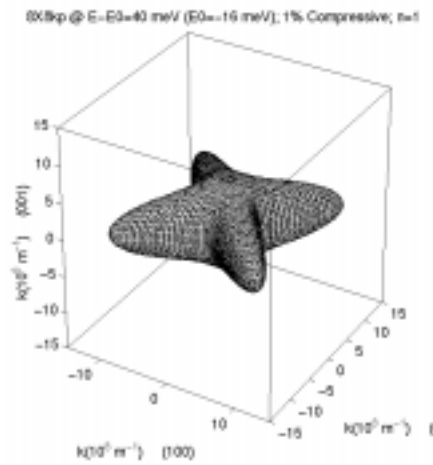
# VALENCE BANDS (RELAXED)



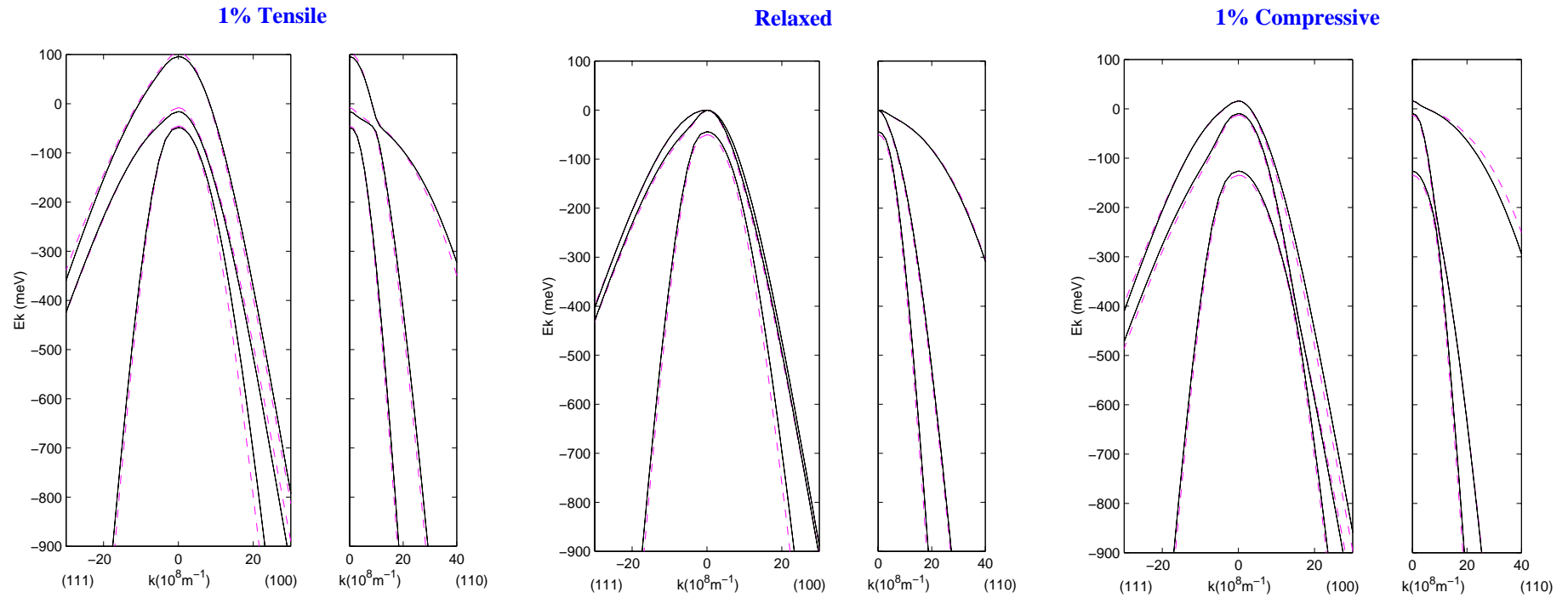
# VALENCE BANDS (1% TENSILE)



# VALENCE BANDS (1% COMPRESSIVE)



# VALENCE BANDS





# INTEGRATION OVER BRILLOUIN ZONE

Electronic Structure

Dispersion relation and Gaps

Abinitio: LDA RPA GW  
Empirical: TB KP EPM

1

Density Of States and DOS masses

2

Carrier Density

3

Scattering Rates

# DENSITY OF STATES

Electronic Structure

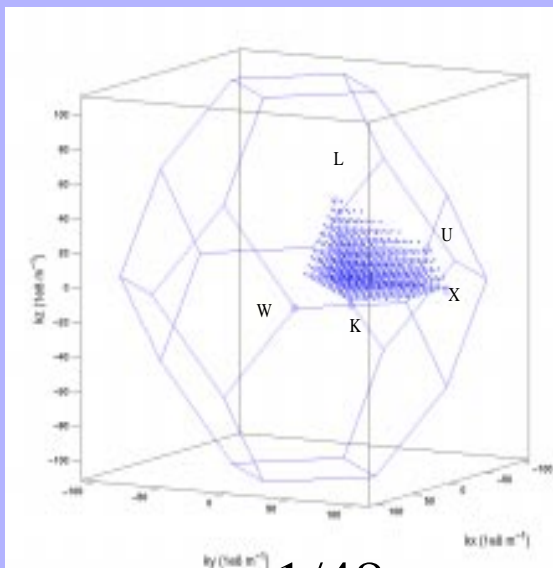
Dispersion relation and Gaps  
 Abinitio: LDA RPA GW  
 Empirical: TB KP EPM

INTEGRATION

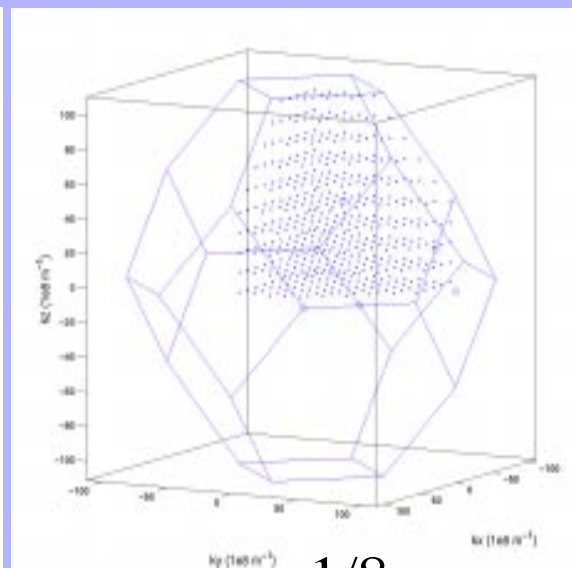
$$\rho_E(E) = \sum_n \sum_{\mathbf{k} \in BZ} \delta[E - E_n(\mathbf{k})]$$

G. Gilat and J. Raubenheimer, PR 144, 390 (1966)

SYMMETRIES

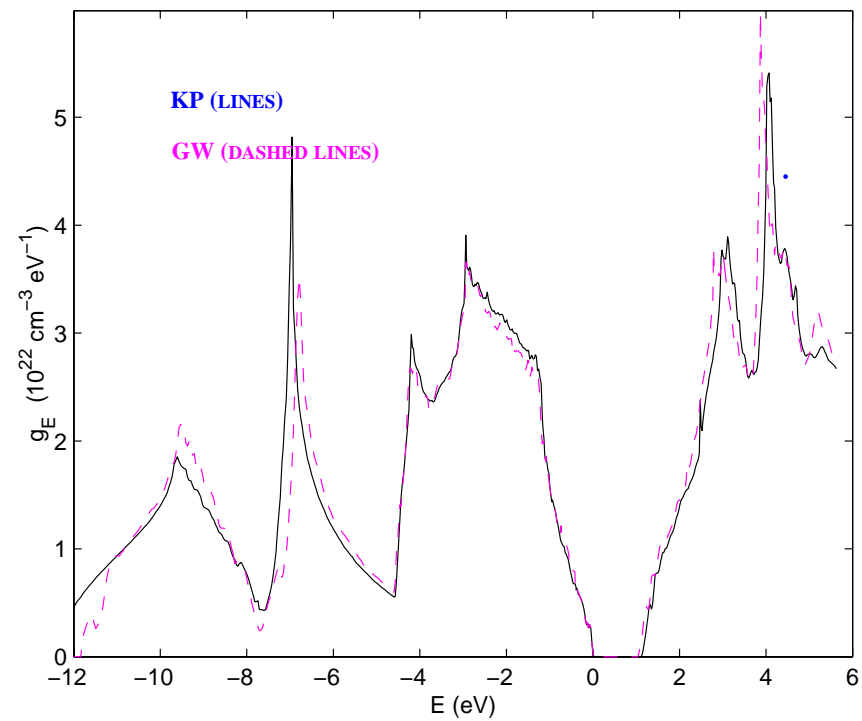
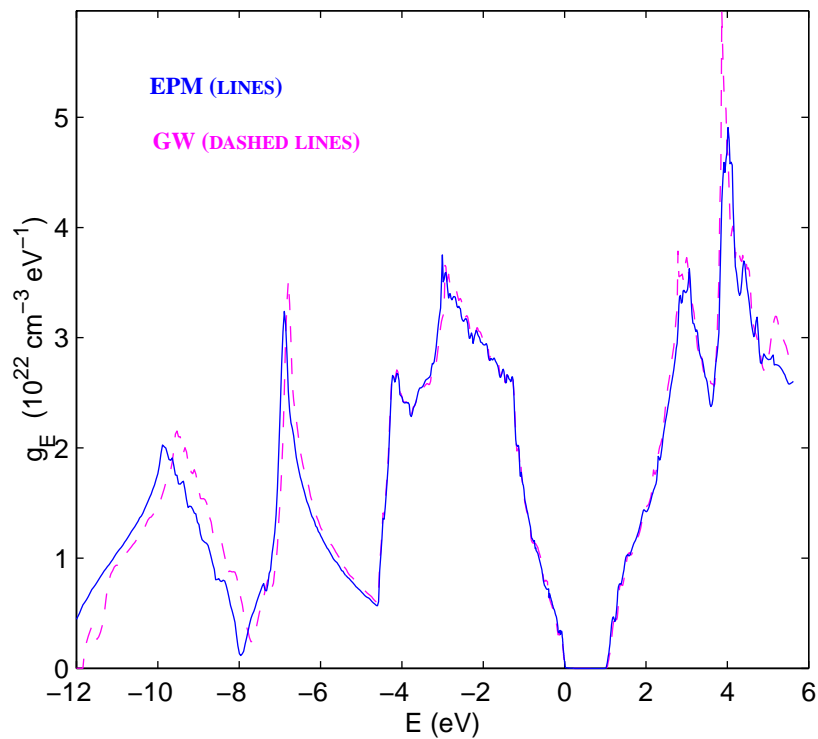


1/48



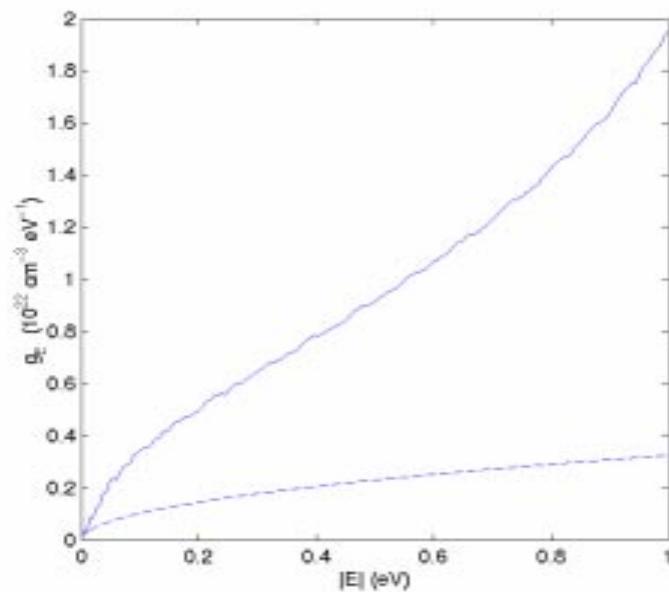
1/8

## DENSITY OF STATES

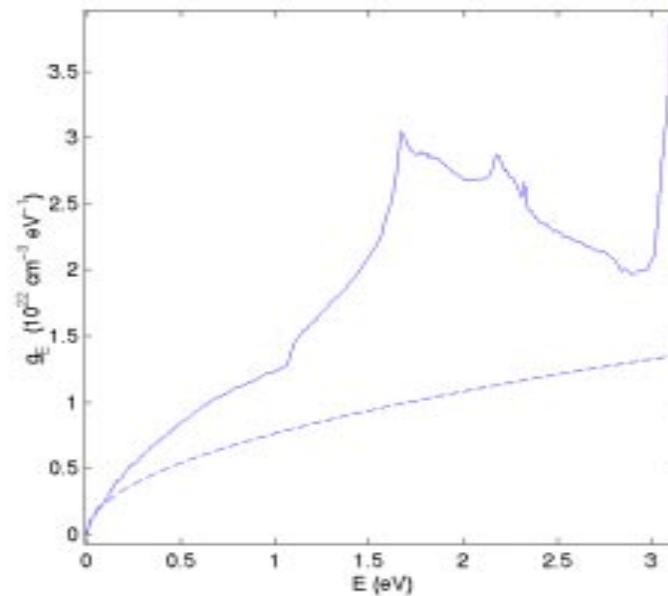


## DENSITY OF STATES (FB VS. EFF MASSES)

### HOLES



### ELECTRONS



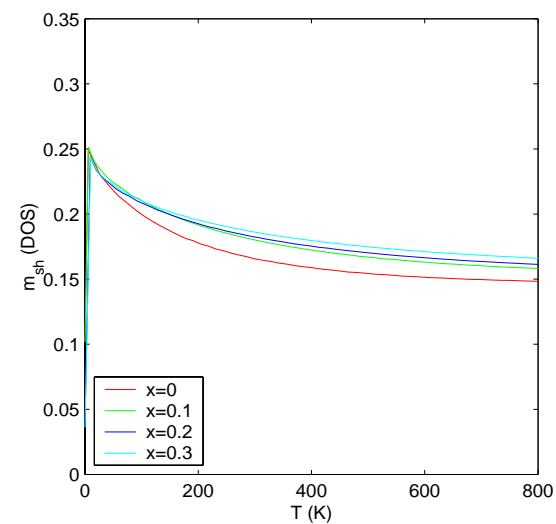
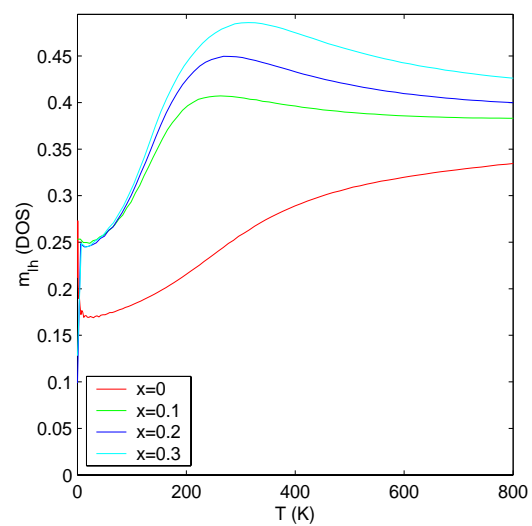
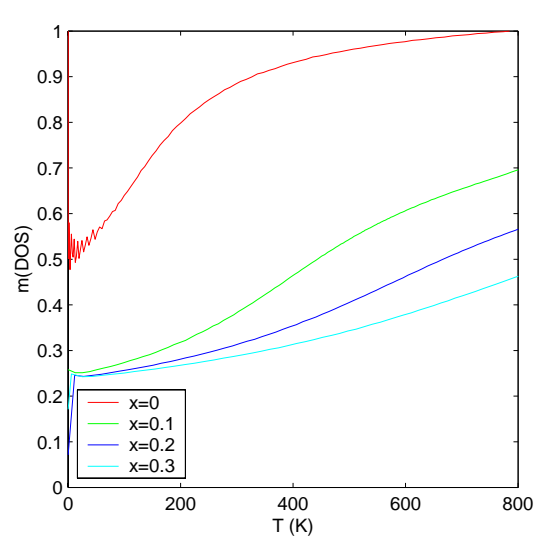
## MASSES

**Table 1 Experimental and theoretical band gap, conduction band curvature masses and valence band Luttinger parameters for Silicon.**

	Exp. <sup>a</sup>	k.p	GW <sup>c</sup>	EPM <sup>d</sup>
$E_g$ (eV)	1.170	1.17	1.1	1.17
$m_t$ ( $m_0$ )	0.191	0.194	0.191	0.21
$m_l$ ( $m_0$ )	0.916	0.916	0.921	0.916
$\gamma_1$	4.27	4.27 <sup>b</sup>	4.27	4.27
$\gamma_2$	0.32	0.315 <sup>b</sup>	0.315	0.315
$\gamma_3$	1.458	1.386 <sup>b</sup>	1.386	1.3867

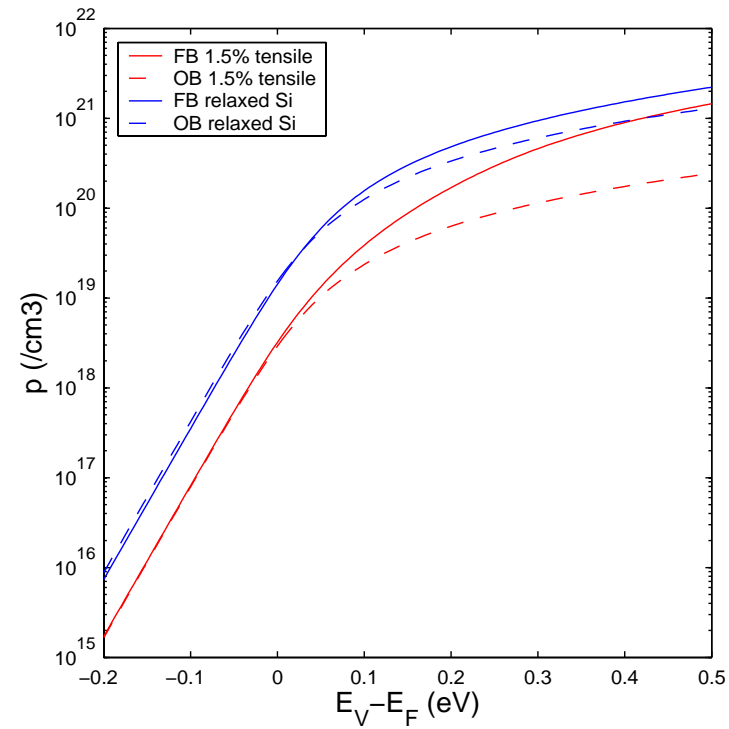
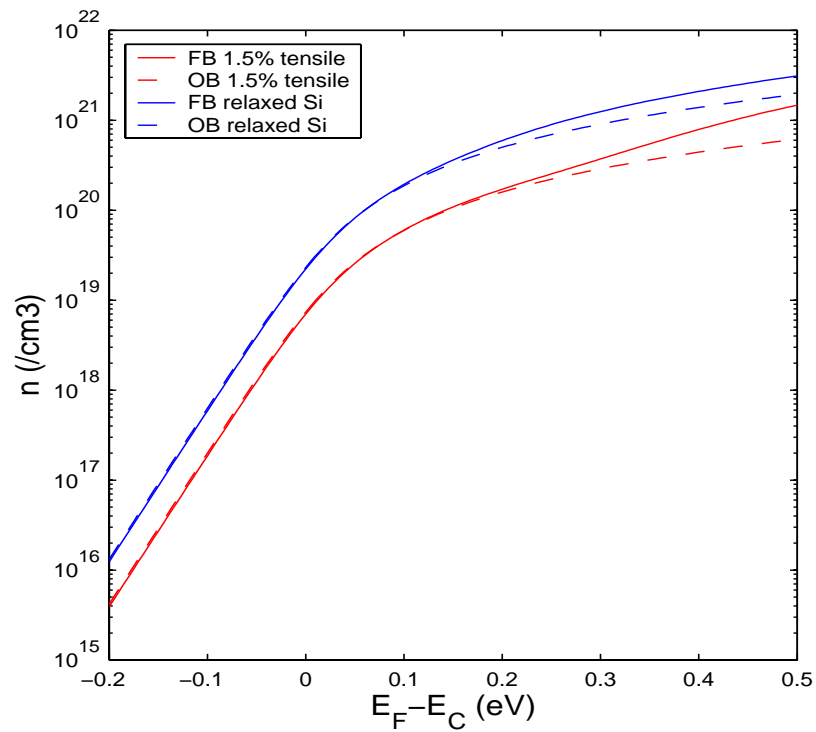
<sup>a</sup> Ref. [11]; <sup>b</sup> Fit for the 6-level k.p; <sup>c</sup> with ABINIT V4.3.3 [3]; <sup>d</sup> Ref. [17].

## DOS MASSES IN SI/SiGE (VALENCE BANDS)



KP (UTOX)

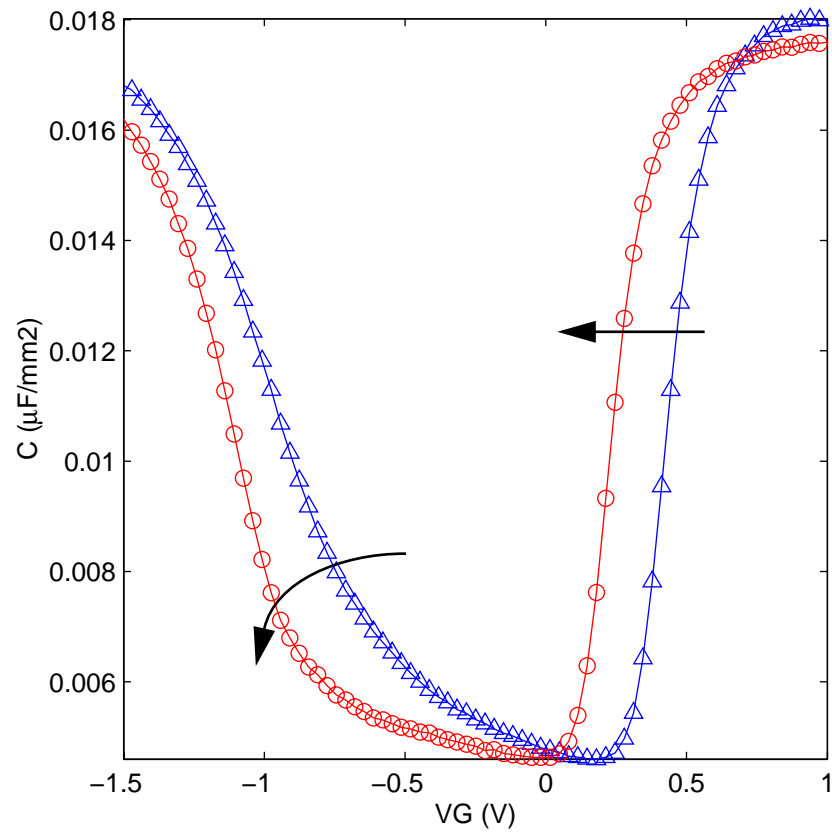
## CARRIER DENSITY VS. STRAIN:



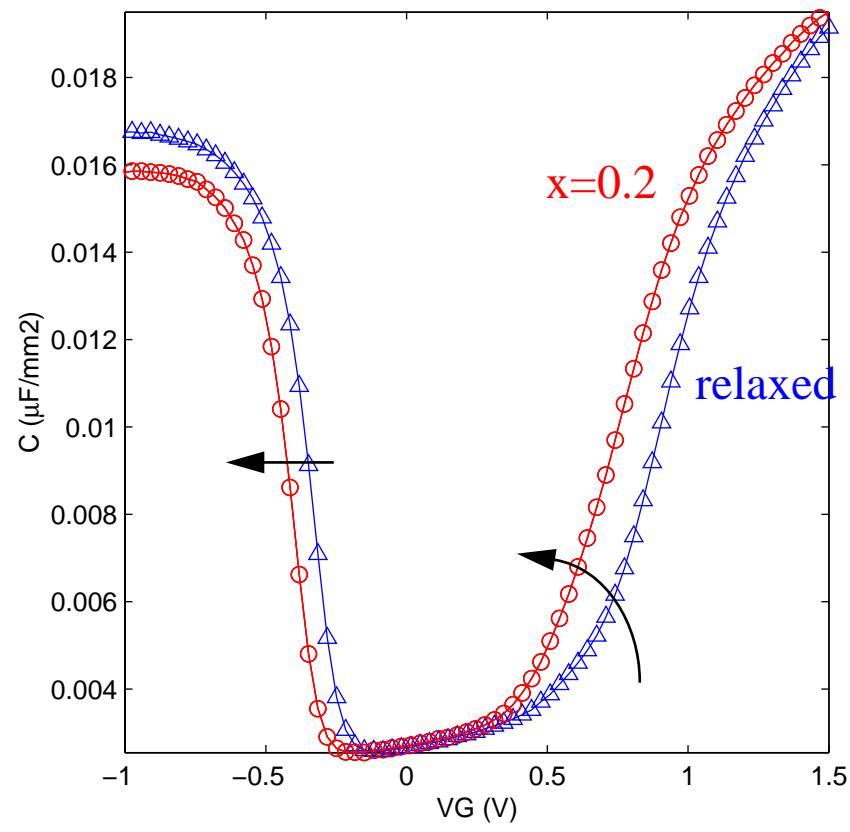
UTOX AFTER M. V. FISCHETTI ET AL. IN DAMOCLES

# CAPACITANCE (MEASUREMENTS)

NMOS

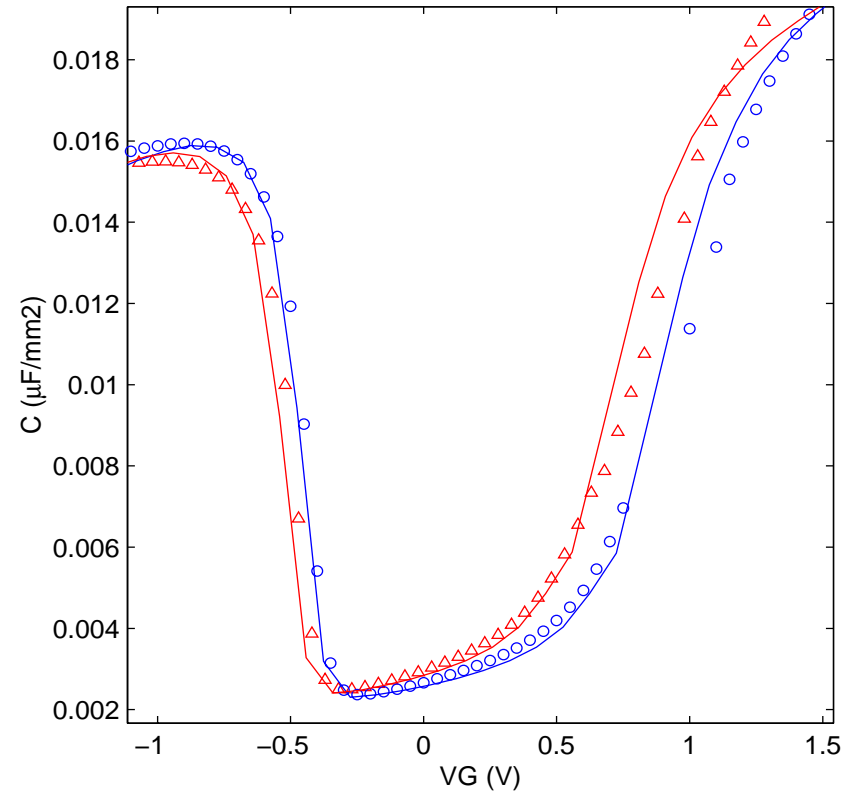
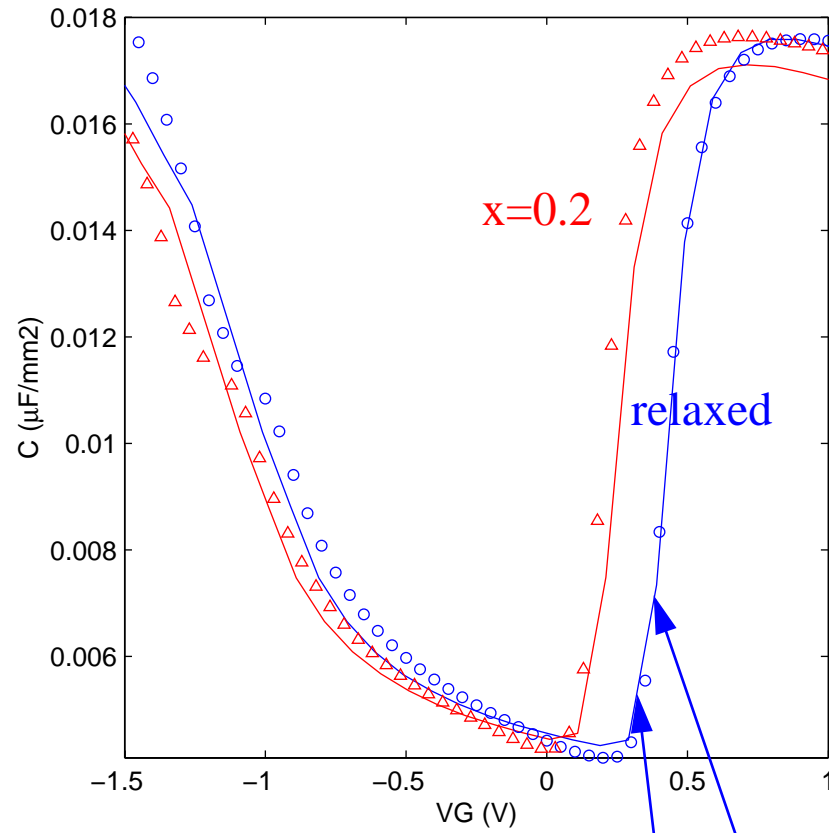


PMOS



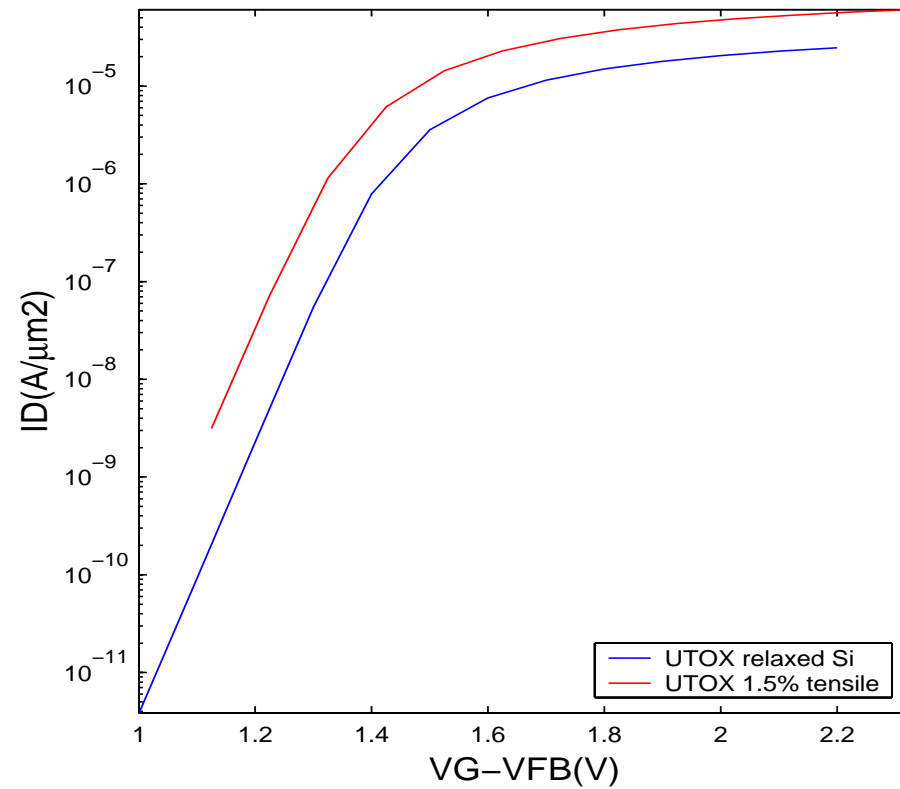


# CAPACITANCE (SIMULATED CURVES)



○ Charge Sheet Model — Density Gradient

# CURRENT (LOW FIELDS)



## CONCLUSIONS

- **Methods for Band Structure**
- **STRAINED SILICON Band Structure**
- **DOS and Scattering times**
- **Capacitances**