An Efficient Method for Calculating Host and Defect Deformation Potential Based on the Concept of Quantum Electronic Stress

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OUTLINE

- Intro to quantum electronic stress(QES)
  - Macroscopic view of mechanical lattice stress: Hooke's law
  - Microscopic view of mechanical lattice stress:
    Nielsen-Martin theorem and DFT formulation
  - Microscopic view of QES:
    DFT formulation---a quantum analog of Hooke's law

- Deformation potential (DP) of electron energy levels
  - Background: strain engineering of band structure
  - Calculation of DP
    conventional method and difficulties
    new method based on QES calculation

OUTLINE

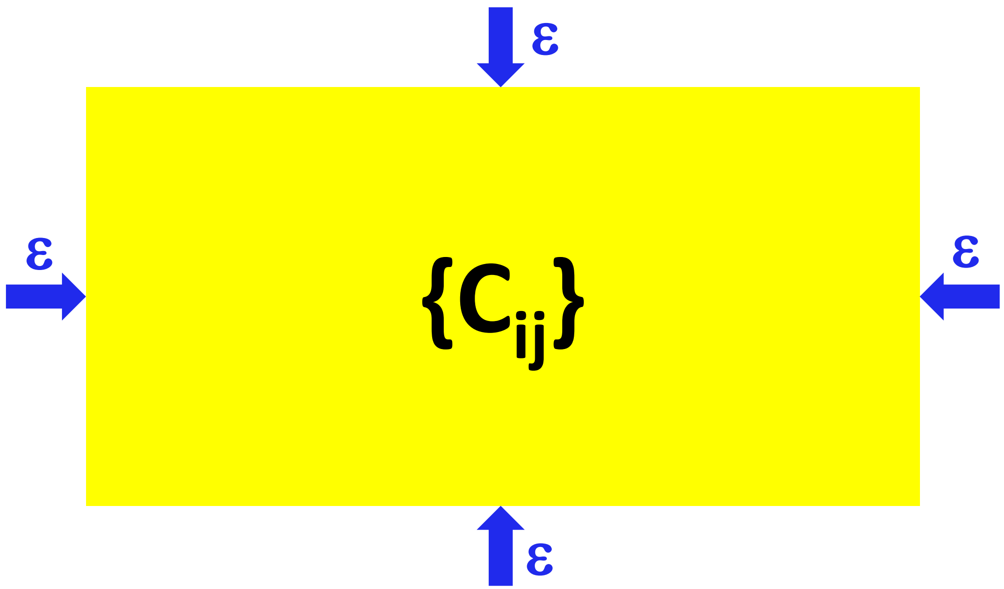
- Other physical manifestations of QES

  - Effect of strain on semiconductor doping:
    dopant size effect versus QES induced by carrier

  - QES induced phase transition:
    pulse-laser induced graphite-to-diamond transition

  - Surface/edge QES:
    quantum size effect induced surface stress oscillation
    quantum oscillation of graphene edge stress

Macroscopic view of mechanical lattice stress



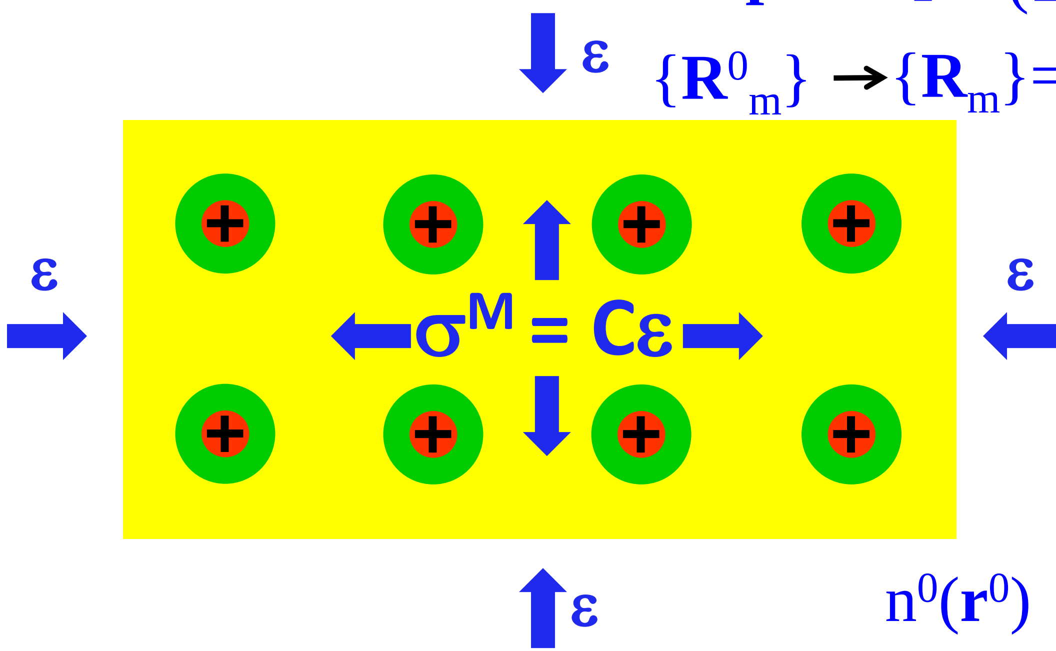
$$E = \frac{V}{2} C \varepsilon^2 \quad \Longrightarrow \quad \sigma^M \equiv \frac{1}{V} \frac{dE}{d\varepsilon} = C\varepsilon$$

Classical mechanical stress: Hooke's law

Microscopic view of mechanical lattice stress

$\mathbf{r}^0 \rightarrow \mathbf{r} = (1+\{\varepsilon_{ij}\})\mathbf{r}^0$

$\{\mathbf{R}^0{}_m\} \rightarrow \{\mathbf{R}_m\} = (1+\{\varepsilon_{ij}\})\{\mathbf{R}^0{}_m\}$

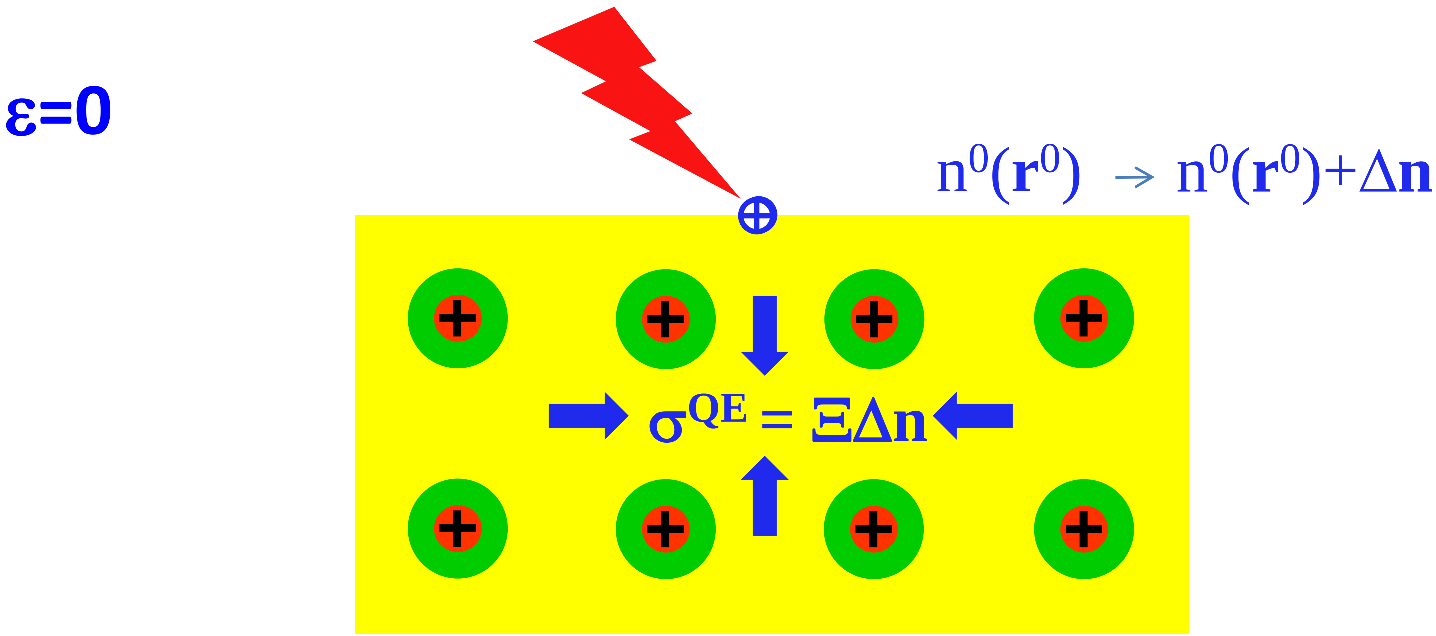


$n^0(\mathbf{r}^0) \rightarrow n(\mathbf{r})$

Quantum mechanical stress: Nielsen-Martin formula

Nielsen and Martin, PRL 50, 697(83); PRB 32, 3780 (85); 32, 3792 (85)

Introduction of quantum electronic stress (QSE)



$$E = \mu \Delta N \quad \Longrightarrow \quad \sigma^{QE} \equiv \frac{1}{V}\frac{dE}{d\varepsilon} = \frac{1}{V}\frac{d\mu}{d\varepsilon}\Delta N = \Xi \Delta n$$

Quantum Analog of Hooke's law

Hu et al. Phys. Rev. Lett. 109, 055501(2012)

DFT formulation of quantum mechanical stress

Nielsen-Martin formula

Total energy functional of a solid

$$E\left[n(\vec{r}),\{\vec{R}_m\}\right] = E_e\left[n(\vec{r})\right] + E_{ext}\left[n(\vec{r}),\{\vec{R}_m\}\right] + E_I\left[\{\vec{R}_m\}\right]$$

Coordinate transformation,

$$\vec{r} = \left(I + \{\varepsilon_{ij}\}\right)\overrightarrow{r^0} \qquad \{\vec{R}_m\} = \left(I + \{\varepsilon_{ij}\}\right)\{\vec{R}_m^0\}$$

Ground-state electron density before and after:

$$n^0\left(\overrightarrow{r^0}\right) \Rightarrow n^{\varepsilon}\left(\vec{r}\right)$$

By definition:

$$\sigma_{ij}^{M} = \frac{1}{V}\frac{dE\left[n(\vec{r}),\{\vec{R}_m\}\right]}{d\varepsilon_{ij}}\Bigg|_{\substack{n^{\varepsilon} \\ \{\vec{R}_m\}}}$$

$$= \frac{1}{V}\left[\int\left(\frac{\partial\left(E_e + E_{ext}\right)}{\partial n(\vec{r})}\right)_{\substack{n(\vec{r}) \\ \{\vec{R}_m\}}}\frac{\partial n(\vec{r})}{\partial\varepsilon_{ij}}d\vec{r} + \sum_m \frac{\partial E_{ext}}{\partial\vec{R}_m}\frac{\partial\vec{R}_m}{\partial\varepsilon_{ij}} + \frac{\partial E_{Ion}}{\partial\varepsilon_{ij}}\right]_{\substack{n(\vec{r}) \\ \{\vec{R}_m\}}}$$

Hohenberg-Kohn theorem: $\left(\frac{\partial\left(E_e + E_{ext}\right)}{\partial n(\vec{r})}\right)_{\substack{n(\vec{r}) \\ \{\vec{R}_m\}}} = 0$

$$\sigma_{ij}^{M} = \frac{1}{V}\left[\frac{\partial E_R}{\partial\varepsilon_{ij}}\right]_{\substack{n^{\varepsilon}(\vec{r}) \\ \{\vec{R}_m\}}} ; \quad E_R = E_{ext} + E_{ion}$$

For simplicity, assuming hydrostatic strain, i.e. $\varepsilon_{ij}=\varepsilon\delta_{ij}$

$$E_R\left[n^{\varepsilon}(\vec{r}),\{\vec{R}_m\}\right]=E_R\left[n^{\varepsilon}(\vec{r}),\{\vec{R}_m^0\}\right]+\varepsilon\sum_m \vec{R}_m^0\cdot\left(\frac{\partial E_R}{\partial \vec{R}_m}\right)_{\vec{R}_m^0}+\frac{\varepsilon^2}{2!}\sum_m\left[\left(\vec{R}_m^0\cdot\frac{\partial}{\partial \vec{R}_m}\right)^2 E_R\right]_{\vec{R}_m^0}+\dots$$

Hooke's law: $\boldsymbol{\sigma^M = C\,\varepsilon}$

$$C=\sum_m\left[\left(\vec{R}_m^0\cdot\frac{\partial}{\partial \vec{R}_m}\right)^2 E_R\right]_{\vec{R}_m^0}$$

DFT formulation of QSE

The law of QSE

Total energy functional of a solid

$$E\left[n(\vec{r}),\{\vec{R}_m\}\right] = E_e\left[n(\vec{r})\right] + E_{ext}\left[n(\vec{r}),\{\vec{R}_m\}\right] + E_I\left[\{\vec{R}_m\}\right]$$

Electron density variation in the absence of strain:

$$n^*\left(\vec{r}^{\,0}\right) = n^0\left(\vec{r}^{\,0}\right) + \delta n\left(\vec{r}^{\,0}\right)$$

Ground-state electron density transform to excited density:

$$n^0\left(\overrightarrow{r^0}\right) \Longrightarrow n^*(\vec{r}^{\,0})$$

The differentials of energy functionals are

$$E_e\left[n^*(\vec{r})\right] = E_e\left[n^0(\vec{r})\right] + \delta E_e = E_e\left[n^0(\vec{r})\right] + \int_V \left(\frac{\partial E_e\left[n(\vec{r})\right]}{\partial n(\vec{r})}\right)_{n^0} \delta n(\vec{r})\, d\vec{r}$$

$$E_{ext}\left[n^*(\vec{r})\right] = E_{ext}\left[n^0(\vec{r})\right] + \delta E_{ext} = E_{ext}\left[n^0(\vec{r})\right] + \int_V \left(\frac{\partial E_{ext}\left[n(\vec{r})\right]}{\partial n(\vec{r})}\right)_{n^0} \delta n(\vec{r})\, d\vec{r}$$

The stress by definition is

$$\sigma_{ij}^{QE} = \frac{1}{V} \left. \frac{dE\left[n(\vec{r}), \left\{ \vec{R}_m \right\} \right]}{d\varepsilon_{ij}} \right|_{\substack{n=n^* \\ \varepsilon_{ij}=0}}$$

$$= \frac{1}{V} \left\{ \left. \frac{d\left(E_e + E_{ext} + E_{Ion} \right)}{d\varepsilon_{ij}} \right|_{\substack{n^0 \\ \varepsilon_{ij}=0}} + \left. \frac{d\left(\int_V \frac{\partial E_e}{\partial n} \delta n(\vec{r}) d\vec{r} + \int_V \frac{\partial E_{ext}}{\partial n} \delta n(\vec{r}) d\vec{r} \right)}{d\varepsilon_{ij}} \right|_{\substack{n^0 \\ \varepsilon_{ij}=0}} \right\}$$

$$= \frac{1}{V} \left\{ \int_V \left[\frac{\partial \left(\frac{\partial \left(E_e + E_{ext} \right)}{\partial n} \right)}{\partial \varepsilon_{ij}} \delta n(\vec{r}) + \frac{\partial \left(E_e + E_{ext} \right)}{\partial n} \frac{\delta n(\vec{r})}{\partial \varepsilon_{ij}} \right] d\vec{r} \right\}_{\substack{n^0 \\ \varepsilon_{ij}=0}}$$

We have the general expression of QES as

$$\sigma_{ij}^{QE} = \frac{1}{V}\left[\int_V \frac{\partial \mu}{\partial \varepsilon_{ij}} \delta n(\vec{r}) d\vec{r}\right]_{\substack{n^0 \\ \varepsilon_{ij}=0}} \quad ; \quad \mu = \partial_n^{'}\left(E_e + E_{ext}\right)$$

In a crystalline solid, to a good approximation, electron chemical potential and electron deformation potential are uniform, the QES can be simplified as

$$\sigma_{ij}^{QE} = \Xi_{ij}\Delta n; \quad \Xi_{ij} = \frac{\partial \mu}{\partial \varepsilon_{ij}}$$

The Law of QES --- a quantum analog of Hooke's law.

Hu et al. Phys. Rev. Lett. 109, 055501(2012)

Introduction of deformation potential (DP)

$$\delta U(r) = E_1 \Delta(r)$$

Band edge shift versus strain

Strain Engineering of band structure

TABLE III. Derivation of shift of energy bands with dilation from mobility data and comparison with shift of energy gap with dilation.

	Diamond	Silicon	Germanium	Tellurium
(1) $c_{ii} \times 10^{-12}$ c.g.s., (110)	10.8	2.0	1.55	0.50
(2) μ_n (electrons) (295°K)	900	300	3500	530
(3) μ_p (holes) (295°K)	>200	100	1700	530
(4) $\mu_n T^{3/2}$	45×10^5	15×10^5	180×10^5	27×10^5
(5) $\mu_p T^{3/2}$	$>10\times10^5$	5×10^5	86×10^5	27×10^5
(6) $\lvert E_{1c}\rvert$ (ev)	8.8	6.5	1.7	2.4
(7) $\lvert E_{1v}\rvert$ (ev)	<30	11.3	2.4	2.4
(8) $\lvert E_{1c}\rvert + \lvert E_{1v}\rvert$ (ev)	<39	17.8	4.1	4.8
(9) E_{1G} (ev)	?	~ -30	~ -5	$+4.0$

Bardeen et. al., Phys. Rev. 80, 72 (1950).

First-principles calculation of DP

$$D_n^{i,j} = \frac{\partial E_n}{\partial \varepsilon_{ij}}$$

Advantage:

easy to handle different types of strain

Disadvantage:

- time consuming
- uncertain reference energy
  - supercell of superlattice
  - all-electron: core level

CaRdona et al., PRB 35, 6182(87), Van de Walle et al., PRL 62, 2028(89), Li et al., APL 88, 042104(2006)

An ad-hoc approach for calculating band edge DP from QES

1. Calculating quantum mechanical stress at n^0, using Nielsen-Martin formula:

$$\sigma^M(n^0)$$

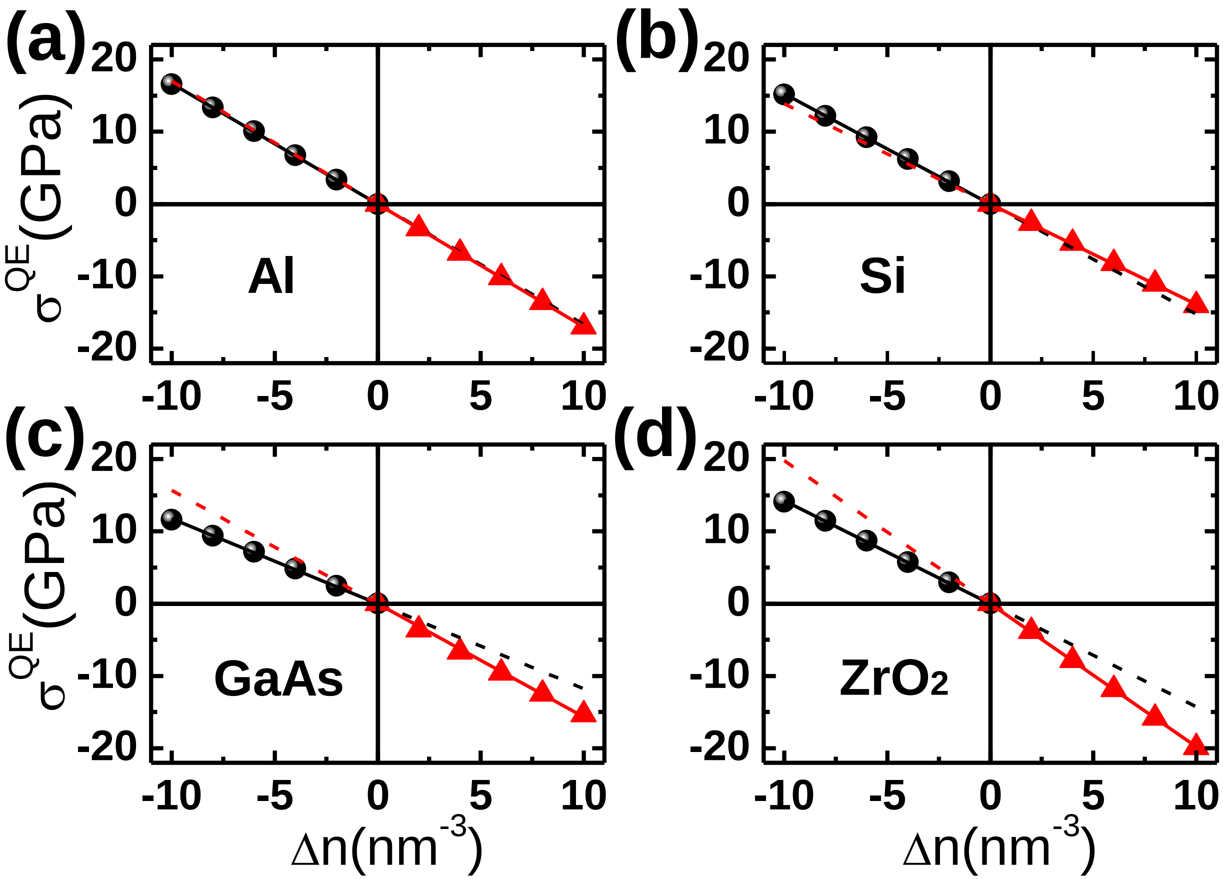
2. Calculating quantum mechanical stress at n^*, using Nielsen-Martin formula:

$$\sigma^M(n^*)$$

3. Take the difference:

$$\sigma^{QE} = \sigma^M(n^*) - \sigma^M(n^0)$$

QES induced by charge carriers



-10.52 eV

CBM: -8.9 eV

VBM: -9.39 eV

-12.36 eV

-8.87 eV

-12.36 eV

-8.87 eV

Calculation of band-edge DP from QES induced by charge carriers

For metals (e-h symmetry):

$$\Xi^e = \Xi^h = \frac{\partial E_F}{\partial \varepsilon}$$

For semiconductor (e-h asymmetry):

$$\Xi^e = \frac{\partial E_{CBM}}{\partial \varepsilon} \neq \Xi^h = \frac{\partial E_{VBM}}{\partial \varepsilon}$$

The larger the band gap, the larger the DP difference.

An elaborate approach for calculating DP of all energy levels

From DFT Kohn-Sham equation:

$$\left[-\nabla^2+\hat{U}_{el}(\vec{r})+\hat{V}_{ext}(\vec{r})+\hat{V}_{xc}(\vec{r})\right]\phi_i\left(\vec{r}\right)=E_i\phi_i\left(\vec{r}\right)$$

$$E_i=\int\phi_i^*\left(\vec{r}\right)\left[-\nabla^2+\hat{U}_{el}(\vec{r})+\hat{V}_{ext}(\vec{r})+\hat{V}_{xc}(\vec{r})\right]\phi_i\left(\vec{r}\right)d\vec{r}$$

$$\Xi^i_{\alpha\beta}=\frac{\partial E_i}{\partial\varepsilon_{\alpha\beta}}$$?

$$\sigma^{QE} = \Xi(\Delta n)$$

hint →

$$\Xi \sim \frac{\Delta\sigma}{\Delta n} \sim \frac{\partial\sigma}{\partial n}$$

$$\partial n \sim \partial f$$

f is occupation number

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Proof that $\partial E/\partial n_i = \epsilon_i$ in density-functional theory

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(Received 14 June 1978)

Introducing a set of occupation numbers $\{f_i\}$,

$$\rho(\vec{r}) = \sum_i f_i \phi_i^*(\vec{r}) \phi_i(\vec{r})$$

$$\tilde{E}_t = \tilde{T} + E_{el}[\rho] + E_{ext}[\rho] + E_{xc}[\rho]$$

$$\frac{\partial \tilde{E}_t}{\partial f_i} = E_i$$

$$\Xi_{\alpha\beta}^{i} = \frac{\partial E_i}{\partial \varepsilon_{\alpha\beta}} = \frac{\partial^2 \tilde{E}_t}{\partial f_i \partial \varepsilon_{\alpha\beta}} = \frac{\partial^2 \tilde{E}_t}{\partial \varepsilon_{\alpha\beta} \partial f_i} = \frac{\partial \sigma_{\alpha\beta}}{\partial f_i}$$

The reciprocal-space expression for the total energy (LDA)

$$E_t = \sum_{\vec{k},\vec{G},i} \left|\phi_i\left(\vec{k}+\vec{G}\right)\right|^2 \left(\vec{k}+\vec{G}\right)^2 + \frac{1}{2}(4\pi)\sum_{\vec{G}\neq 0} \frac{\left|\rho\left(\vec{G}\right)\right|^2}{\vec{G}^2} + \sum_{\vec{G}} \varepsilon_{xc}\left(\vec{G}\right)\rho^*\left(\vec{G}\right)$$

$$+ \sum_{\vec{G}\neq 0,\mu} S_\mu\left(\vec{G}\right) V_\mu^L\left(\vec{G}\right)\rho^*\left(\vec{G}\right)$$

$$+ \sum_{\vec{k},\vec{G},\vec{G}',i,l,\mu} S_\mu\left(\vec{G}-\vec{G}'\right)\Delta V_{l,\mu}^{NL}\left(\vec{k}+\vec{G},\vec{k}+\vec{G}'\right)\phi_i\left(\vec{k}+\vec{G}\right)\phi_i^*\left(\vec{k}+\vec{G}'\right)$$

$$+\left[\sum_\mu \alpha_\mu\right]\left[\frac{1}{\Omega}\sum_\mu Z_\mu\right] + \Omega^{-1}\gamma_{Ewald}$$

Transforming the scaling of [**r** to (1+ ε)**r**] to [**G** to (1-ε)**G**]

$$\sigma_{\alpha\beta} = \Omega^{-1}\frac{\partial E_t}{\partial \varepsilon_{\alpha\beta}} = \sum_{\vec{k},\vec{G},i}\left|\phi_i\left(\vec{k}+\vec{G}\right)\right|^2\left(\vec{k}+\vec{G}\right)_\alpha\left(\vec{k}+\vec{G}\right)_\beta + \frac{1}{2}(4\pi)\sum_{\vec{G}\neq 0}\frac{\left|\rho\left(\vec{G}\right)\right|^2}{\vec{G}^2}\left[\frac{2G_\alpha G\beta}{G^2}-\delta_{\alpha\beta}\right]$$

$$+\delta_{\alpha\beta}\sum_{\vec{G}}\left(\varepsilon_{xc}\left(\vec{G}\right)-V_{xc}\left(\vec{G}\right)\right)\rho^*\left(\vec{G}\right)$$

$$-\sum_{\vec{G}\neq 0,\mu}S_\mu\left(\vec{G}\right)\left[\frac{\partial V_\mu^L}{\partial\left(G^2\right)}2G_\alpha G_\beta + V_\mu^L\left(\vec{G}\right)\delta_{\alpha\beta}\right]\rho^*\left(\vec{G}\right)$$

$$+\sum_{\vec{k},\vec{G},\vec{G}',i,l,\mu}S_\mu\left(\vec{G}-\vec{G}'\right)\frac{\partial \Delta V_{l,\mu}^{NL}\left(\vec{k}+\vec{G},\vec{k}+\vec{G}'\right)}{\partial\varepsilon_{\alpha\beta}}\phi_i\left(\vec{k}+\vec{G}\right)\phi_i^*\left(\vec{k}+\vec{G}'\right)$$

$$-\delta_{\alpha\beta}\left[\sum_\mu \alpha_\mu\right]\left[\frac{1}{\Omega}\sum_\mu Z_\mu\right] + \Omega^{-1}\frac{\partial \gamma_{Ewald}}{\partial \varepsilon_{\alpha\beta}}$$

Adding the occupation numbers $\{f_i\}$, the electron density becomes

$$\rho\left(\vec{r}\right)=\sum_i f_i\phi_i^*\left(\vec{r}\right)\phi_i\left(\vec{r}\right)=\sum_i f_i\rho_i\left(\vec{r}\right)$$

$$\rho\left(\vec{G}\right)=\sum_i f_i\rho_i\left(\vec{G}\right)$$

Then the total energy can be expressed as

$$\tilde{E}_t = \sum_{\vec{k},\vec{G},i} f_i \left| \phi_i \left(\vec{k} + \vec{G} \right) \right|^2 \left(\vec{k} + \vec{G} \right)^2 + \frac{1}{2}(4\pi) \sum_{\vec{G}\neq 0} \frac{\left[\sum_i f_i \rho_i^* \left(\vec{G} \right) \right] \left[\sum_j f_j \rho_j \left(\vec{G} \right) \right]}{\vec{G}^2}$$

$$+ \sum_{\vec{G},i} f_i \varepsilon_{xc} \left(\vec{G} \right) \rho_i^* \left(\vec{G} \right) + \sum_{\vec{G}\neq 0,\mu,i} f_i S_\mu \left(\vec{G} \right) V_\mu^L \left(\vec{G} \right) \rho_i^* \left(\vec{G} \right)$$

$$+ \sum_{\vec{k},\vec{G},\vec{G}',i,l,\mu} f_i S_\mu \left(\vec{G} - \vec{G}' \right) \Delta V_{l,\mu}^{NL} \left(\vec{k} + \vec{G}, \vec{k} + \vec{G}' \right) \phi_i \left(\vec{k} + \vec{G} \right) \phi_i^* \left(\vec{k} + \vec{G}' \right)$$

$$+ \left[\sum_\mu \alpha_\mu \right] \left[\frac{1}{\Omega} \sum_\mu Z_\mu \right] + \Omega^{-1} \gamma_{Ewald}$$

The expression for stress is

$$\tilde{\sigma}_{\alpha\beta} = \sum_{\vec{k},\vec{G},i} f_i \left|\phi_i\left(\vec{k}+\vec{G}\right)\right|^2 \left(\vec{k}+\vec{G}\right)_\alpha \left(\vec{k}+\vec{G}\right)_\beta$$

$$+\frac{1}{2}(4\pi)\sum_{\vec{G}\neq 0} \frac{\left[\sum_i f_i \rho_i^*\left(\vec{G}\right)\right]\left[\sum_j f_j \rho_j\left(\vec{G}\right)\right]}{\vec{G}^2}\left[\frac{2G_\alpha G\beta}{G^2} - \delta_{\alpha\beta}\right]$$

$$+\delta_{\alpha\beta}\sum_{\vec{G},i} f_i \left(\varepsilon_{xc}\left(\vec{G}\right) - V_{xc}\left(\vec{G}\right)\right)\rho_i^*\left(\vec{G}\right)$$

$$-\sum_{\vec{G}\neq 0,\mu,i} f_i S_\mu\left(\vec{G}\right)\left[\frac{\partial V_\mu^L}{\partial\left(G^2\right)} 2G_\alpha G_\beta + V_\mu^L\left(\vec{G}\right)\delta_{\alpha\beta}\right]\rho_i^*\left(\vec{G}\right)$$

$$+\sum_{\vec{k},\vec{G},\vec{G}',i,l,\mu} f_i S_\mu\left(\vec{G}-\vec{G}'\right)\frac{\partial \Delta V_{l,\mu}^{NL}\left(\vec{k}+\vec{G},\vec{k}+\vec{G}'\right)}{\partial \varepsilon_{\alpha\beta}}\phi_i\left(\vec{k}+\vec{G}\right)\phi_i^*\left(\vec{k}+\vec{G}'\right)$$

$$-\delta_{\alpha\beta}\left[\sum_\mu \alpha_\mu\right]\left[\frac{1}{\Omega}\sum_\mu Z_\mu\right] + \Omega^{-1}\frac{\partial \gamma_{Ewald}}{\partial \varepsilon_{\alpha\beta}}$$

Now we can obtain the DP for energy level *i* as

$$\Xi^{i}_{\alpha\beta} = \left(\frac{\partial \tilde{\sigma}_{\alpha\beta}}{\partial f_i}\right)_{f_i = 1\, or\, 0} = \sum_{\vec{k},\vec{G}} \left|\phi_i\left(\vec{k}+\vec{G}\right)\right|^2 \left(\vec{k}+\vec{G}\right)_\alpha \left(\vec{k}+\vec{G}\right)_\beta$$

$$+\frac{1}{2}(4\pi)\sum_{\vec{G}\neq 0} \frac{\rho_i^*\left(\vec{G}\right)\rho\left(\vec{G}\right)+\rho^*\left(\vec{G}\right)\rho_i\left(\vec{G}\right)}{\vec{G}^2}\left[\frac{2G_\alpha G_\beta}{G^2}-\delta_{\alpha\beta}\right]$$

$$+\delta_{\alpha\beta}\sum_{\vec{G}}\left(\varepsilon_{xc}\left(\vec{G}\right)-V_{xc}\left(\vec{G}\right)\right)\rho_i^*\left(\vec{G}\right)$$

$$-\sum_{\vec{G}\neq 0,\mu} S_\mu\left(\vec{G}\right)\left[\frac{\partial V_\mu^L}{\partial\left(G^2\right)}2G_\alpha G_\beta + V_\mu^L\left(\vec{G}\right)\delta_{\alpha\beta}\right]\rho_i^*\left(\vec{G}\right)$$

evaluate numerically

$$+\sum_{\vec{k},\vec{G},\vec{G}',l,\mu} S_\mu\left(\vec{G}-\vec{G}'\right)\frac{\partial \Delta V_{l,\mu}^{NL}\left(\vec{k}+\vec{G},\vec{k}+\vec{G}'\right)}{\partial \varepsilon_{\alpha\beta}}\phi_i\left(\vec{k}+\vec{G}\right)\phi_i^*\left(\vec{k}+\vec{G}'\right)$$

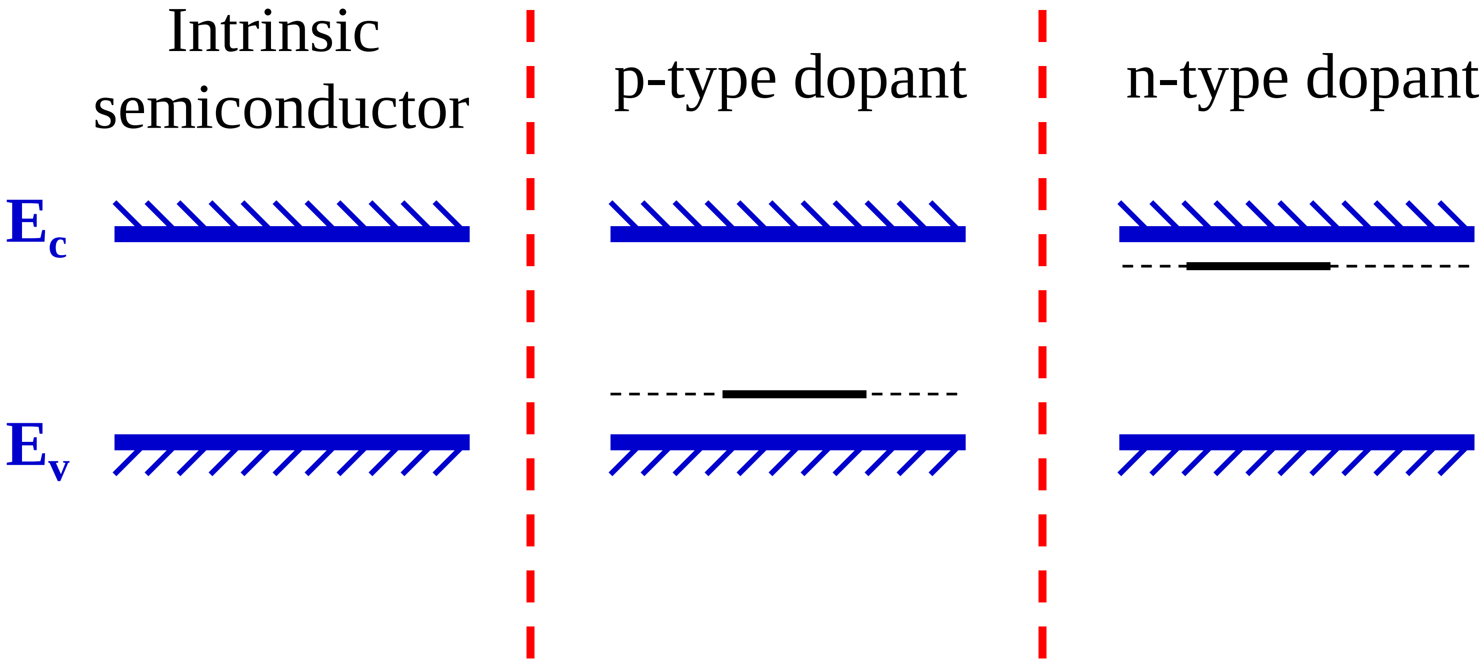
$$\Delta V_j^{NL} = \sum_{nm} D_{nm}^j \left| \beta_n^j \right\rangle \left\langle \beta_m^j \right|$$

j is the ionic site, β is the projector function.

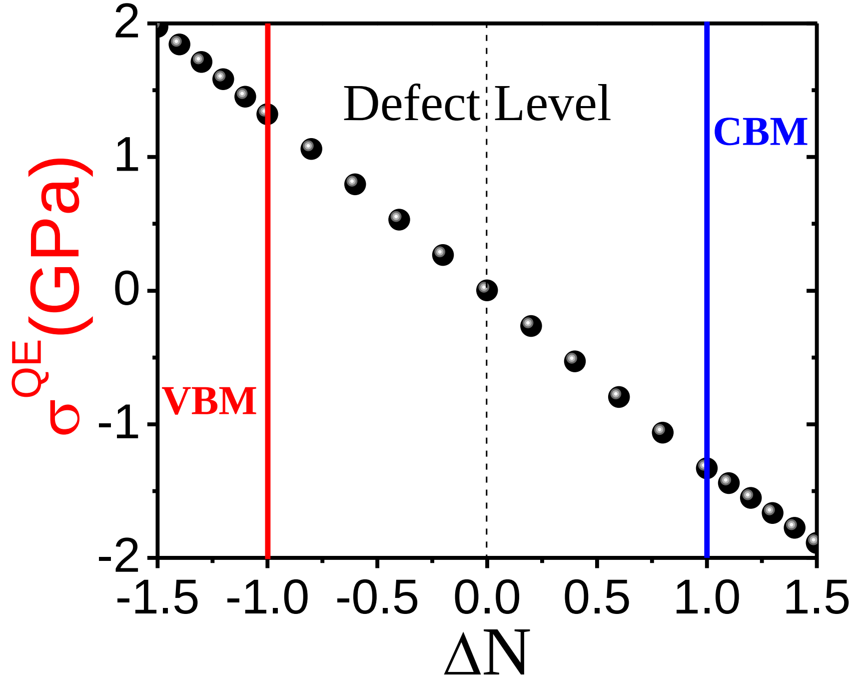
$$\frac{\partial \beta_n^j \left(\vec{k} + \vec{G} \right)}{\partial \varepsilon_{\alpha\beta}} = -\frac{\partial \beta_n^j \left(\vec{k} + \vec{G} \right)}{\left(\vec{k} + \vec{G} \right)_\alpha} \left(\vec{k} + \vec{G} \right)_\beta - \delta_{\alpha\beta} \beta_n^j \left(\vec{k} + \vec{G} \right)$$

Filippetti,PRB, 61, 8433(2000)

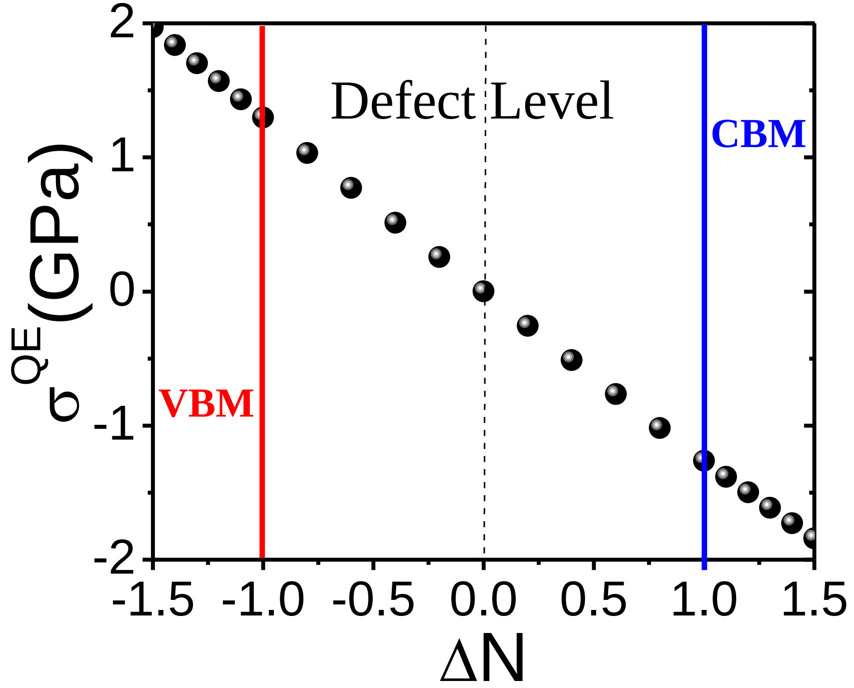
DP of defect level in semiconductor



Ad-hoc QES calculation of defect level DP in Si



BSi_{63}



NSi_{63}

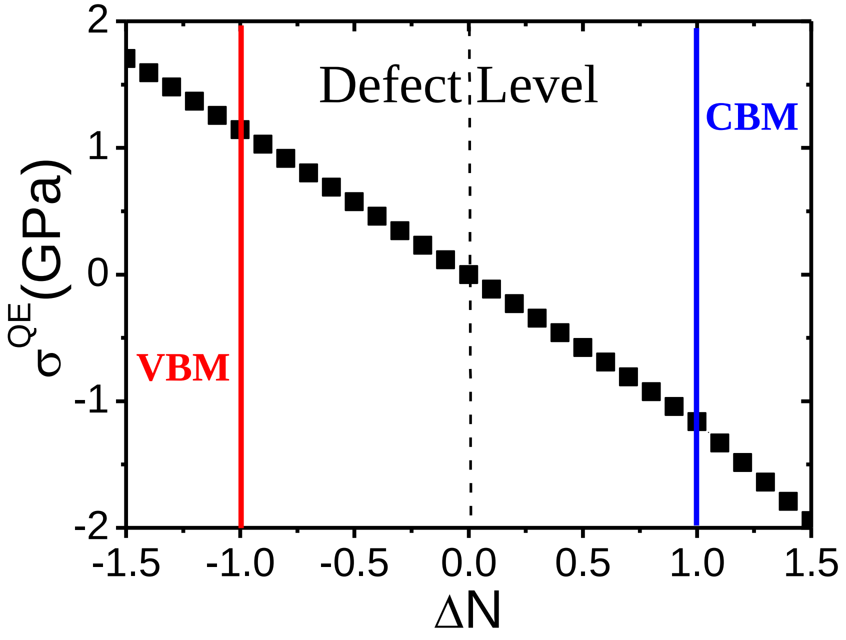
DP of defect level in Si

	Ξ^{CBM}(eV)	Ξ^{def}(eV)	Ξ^{VBM}(eV)
B	8.66	10.29	10.12
Al	8.56	10.17	10.03
Ga	8.54	10.14	9.99
N	8.96	9.87	10.41
P	8.93	8.85	10.34
As	8.93	8.85	10.30
Pure Si	8.59		10.30

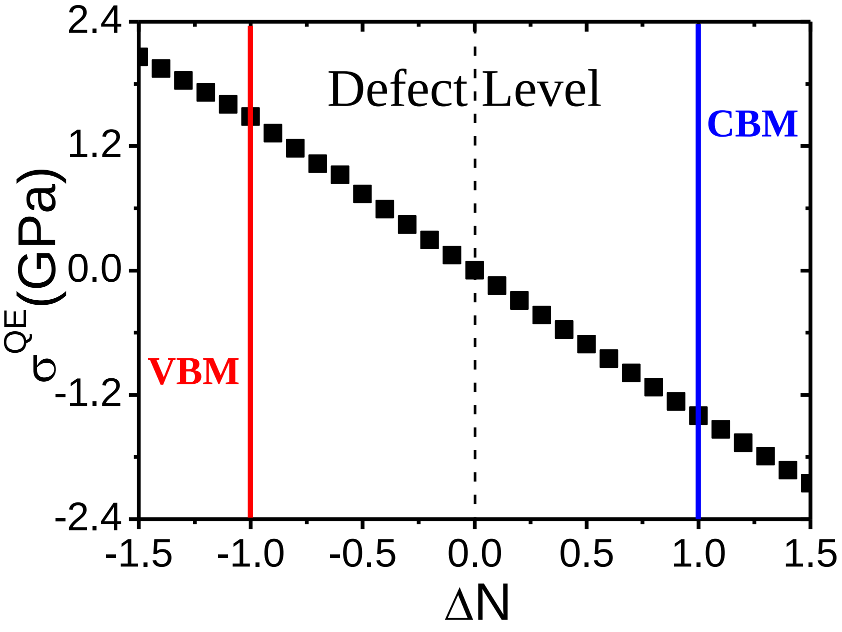
p doping

n doping

Ad-hoc QES calculation of defect level DP in GaAs



$ZnGa_{31}As_{32}$



$SeGa_{32}As_{31}$

DP of defect level in GaAs

	Ξ^{CBM}(eV)	Ξ^{def}(eV)	Ξ^{VBM}(eV)
Zn_Ga	13.88	10.13	9.90
Si_Ga	11.56	12.55	10.25
Ge_Ga	12.11	12.82	10.23
Sn_Ga	11.62	12.95	10.21
Si_As	13.90	10.20	9.96
Ge_As	13.93	10.20	9.92
Sn_As	13.97	10.17	9.95
Se_As	11.60	12.90	10.26
GaAs	14.26		10.66

n dopping

p dopping

Physical manifestations of QES

Effect of strain on semiconductor doping

Stress induced by dopant size vs. charge state

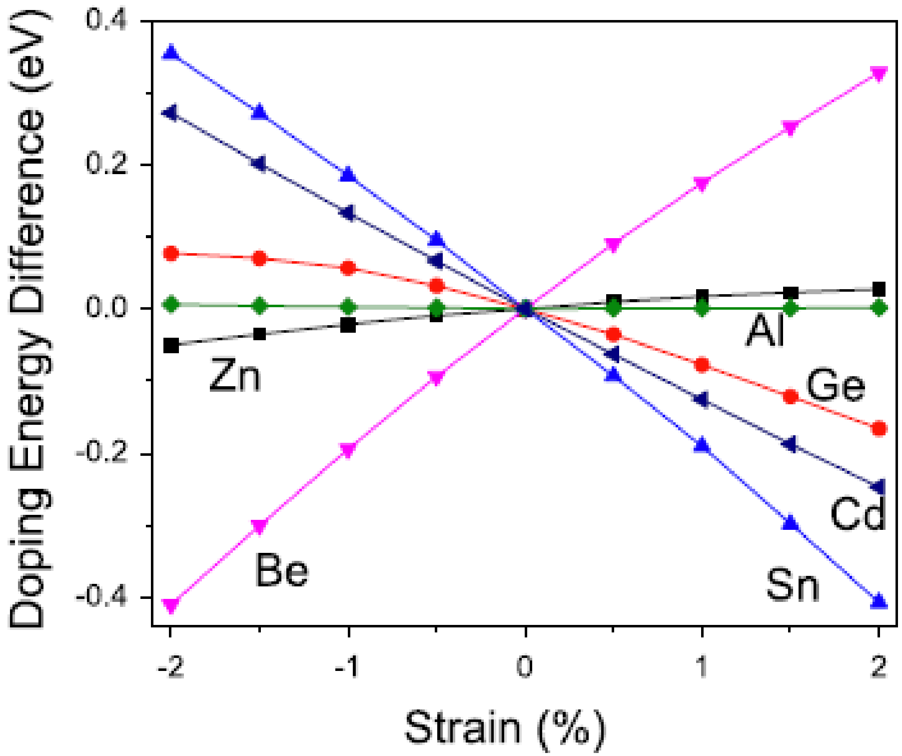
Dopant induced volume change in GaP: $\Delta V = \Delta V_i + \Delta V_e$

Dopant	ΔV (Å^3)	ΔV_i	ΔV_e	p/n	R (Å)
Ga	0	0	0	Neutral	1.225
Zn	−1.46	0	−1.46	*p*	1.225
Al	0.21	0.26	−0.05	Neutral	1.230
Cd	8.66	10.17	−1.51	*p*	1.405
In	9.54	10.17	−0.63	Neutral	1.405
Ge	4.54	0	4.54	*n*	1.225
Be	−12.88	−11.78	−1.1	*p*	0.975
Sn	13.25	10.17	3.08	*n*	1.405
Zn + Ge	−0.2	0	−0.2	Neutral	1.225

n-dopant: compressive QES; p-type: tensile QES

Zhu, et al. PRL, 105, 195503(20010)

Effect of strain on semiconductor doping



To reduce QES:

Small n-dopant
Large p-dopant
co-doping

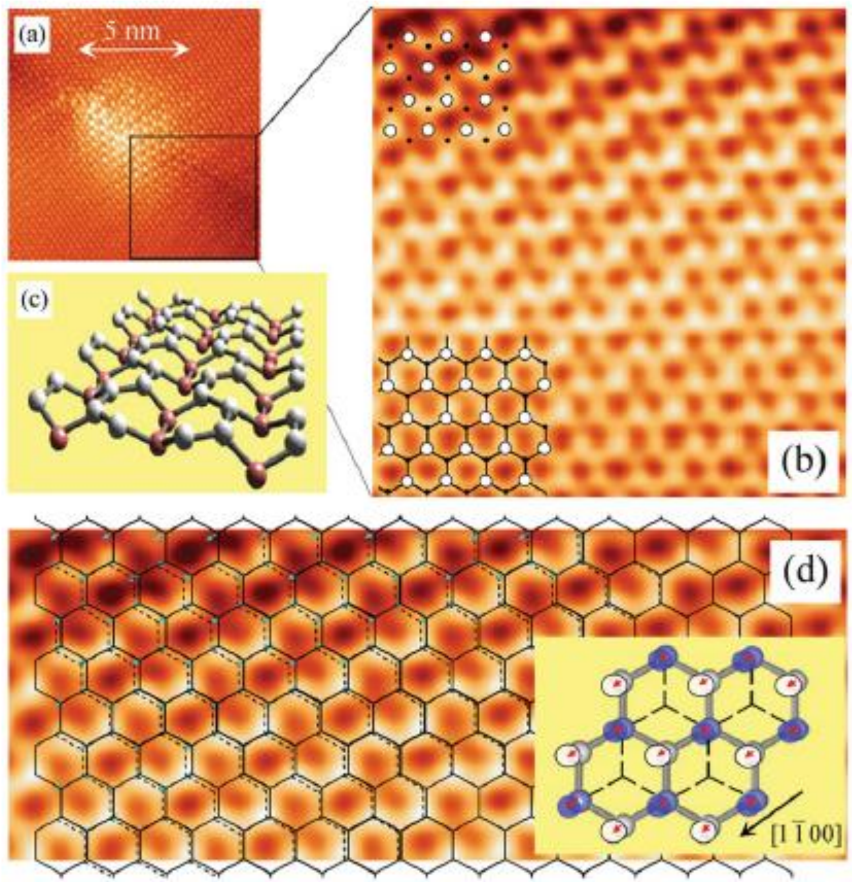
Strain enhancement:
unbounded

Charge state?

Zhu, et al. PRL, 105, 195503(2010)

QES induced structural phase transition:

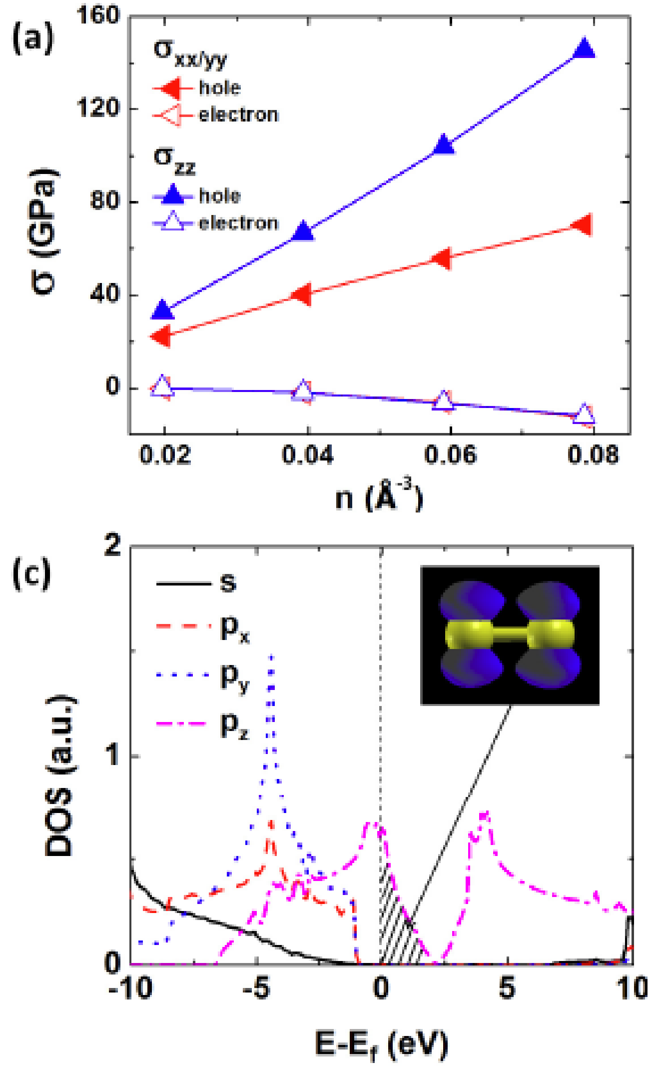
Graphite-diamond transition by pulse laser excitation



J. Kanasaki, et al. PRL, 102, 087402(2009)

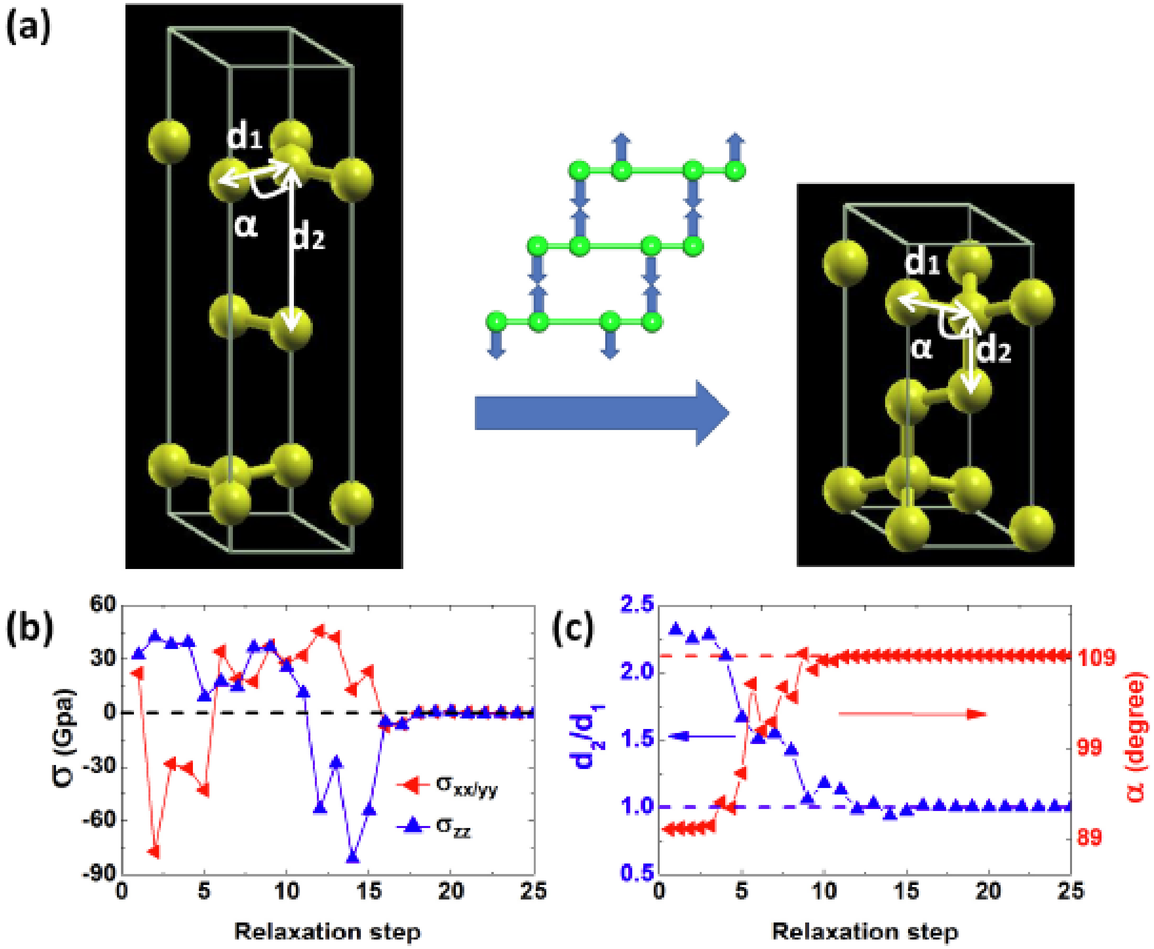
QES induced structural phase transition:

Graphite-diamond transition by pulse laser excitation



QES induced structural phase transition:

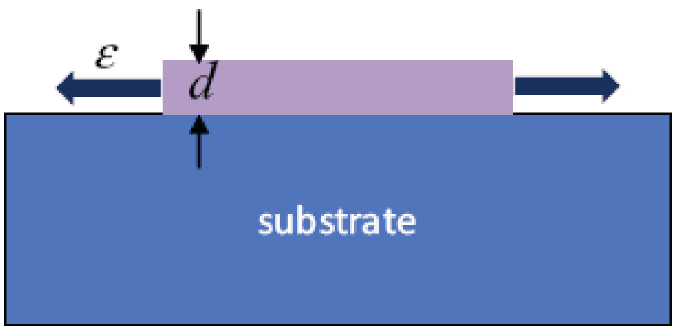
Graphite-diamond transition by pulse laser excitation



Surface QES induced by quantum confinement in metal thin film

$$\sigma^{T} = \sigma^{iS} + \sigma^{MS}(d)$$

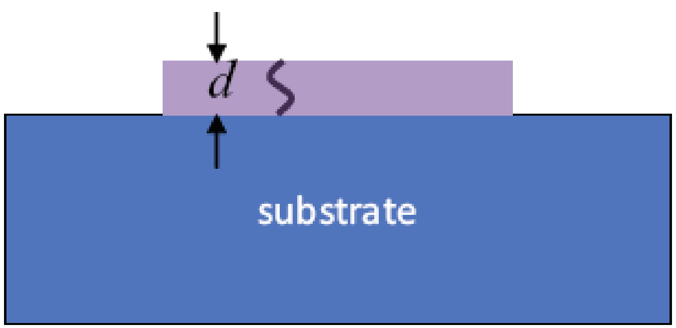
(a)



$$\sigma^{MS}(d) = C\varepsilon d$$

$$\sigma^{T} = \sigma^{iS} + \sigma^{QS}(d)$$

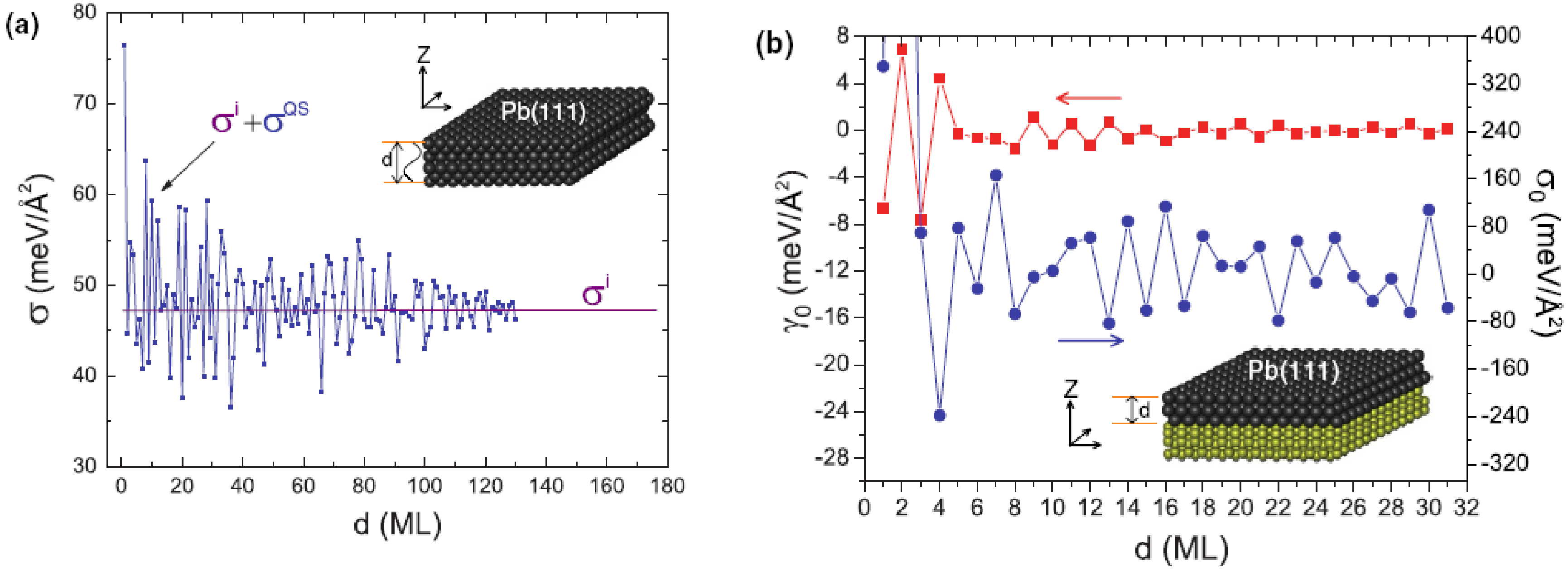
(b)



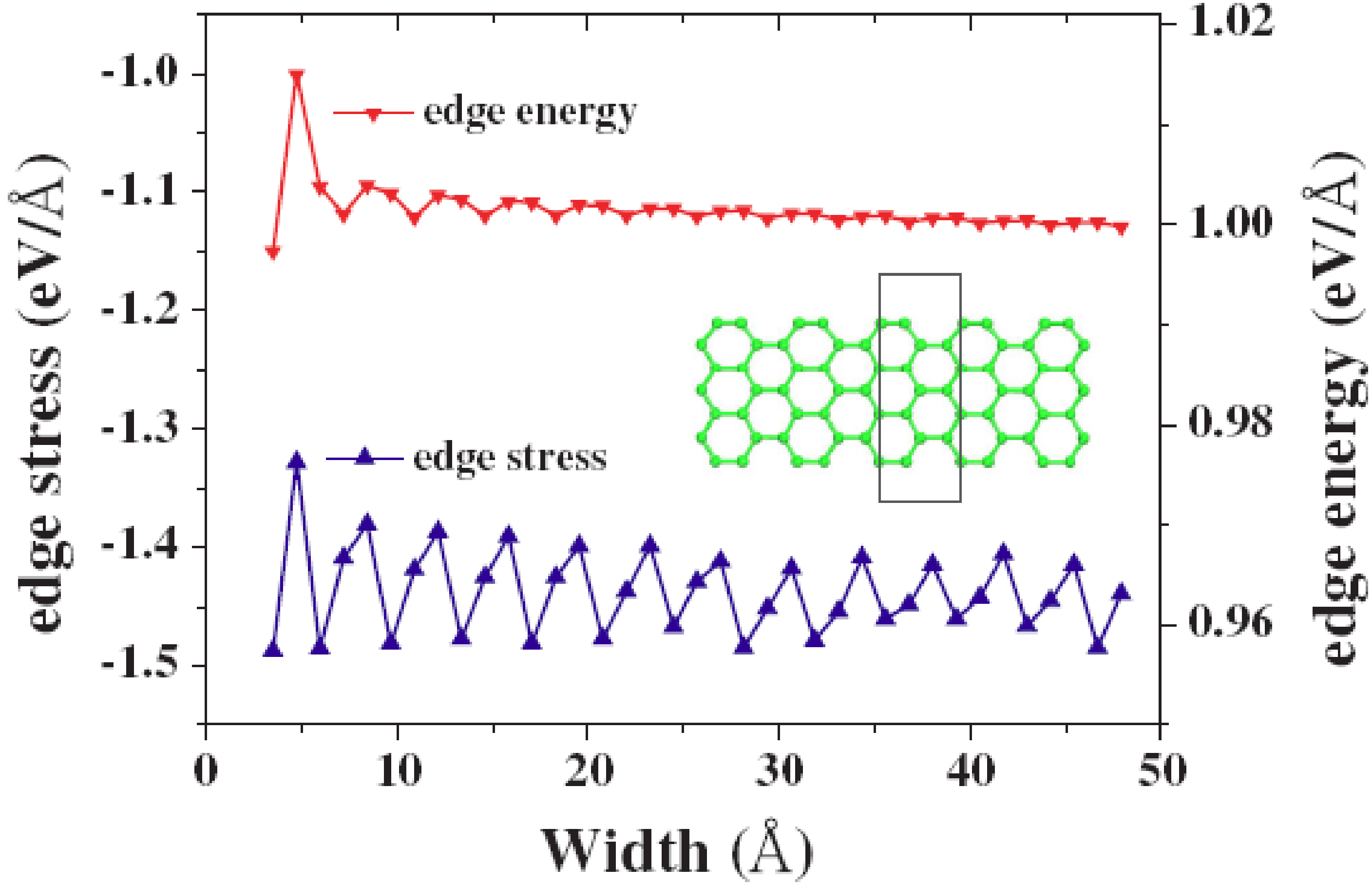
$$\sigma_{ij}^{QE} = \frac{1}{V}\int_{V} \frac{\partial \mu}{\partial \varepsilon_{ij}} \delta n(\vec{r})\, d\vec{r}$$

$$\sigma_{ij}^{QS} = \frac{1}{d}\int \frac{\partial \mu}{\partial \varepsilon_{ij}}(z)\delta n(z)\, dz$$

Surface QES Induced by Quantum Confinement in Thin Metal Film



Edge QES in Graphene



B. Huang, et al. PRL, 102, 166404(2009)

Summary

- Concept and DFT formulation of quantum electronic stress
  - A quantum analog of Hooke's law: $\sigma_{ij}^{QE} = \Xi_{ij} \Delta n$
  - DFT formulation and code implication (VASP):

    QES and DP of electronic levels

- Physical manifestation of QES
  - Effect of strain on doping
  - QES induced phase transition:

    in analogy to pressure induced transition
  - Surface/Edge QES

    nanostructure stability and growth

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