

# Benchmarking of bulk SiGe and strained SiGe/(100)Si bandstructure using Tight-binding VCA model

## Objective:

- SiGe alloy an attractive material for pMOS devices.
- Benchmarking of bulk relaxed SiGe and compressively strained SiGe/Si using tight-binding (TB) VCA model.

## Approach:

- **Bulk** :simple VCA is employed for the tight-binding Hamiltonian<sup>1</sup>,

$$d_{\text{SiGe}} = (1-x)d_{\text{Si}} + x d_{\text{Ge}} \quad (1)$$

$$H_{\text{SiGe}} = (1-x)H_{\text{Si}} + x H_{\text{Ge}} \quad (2)$$

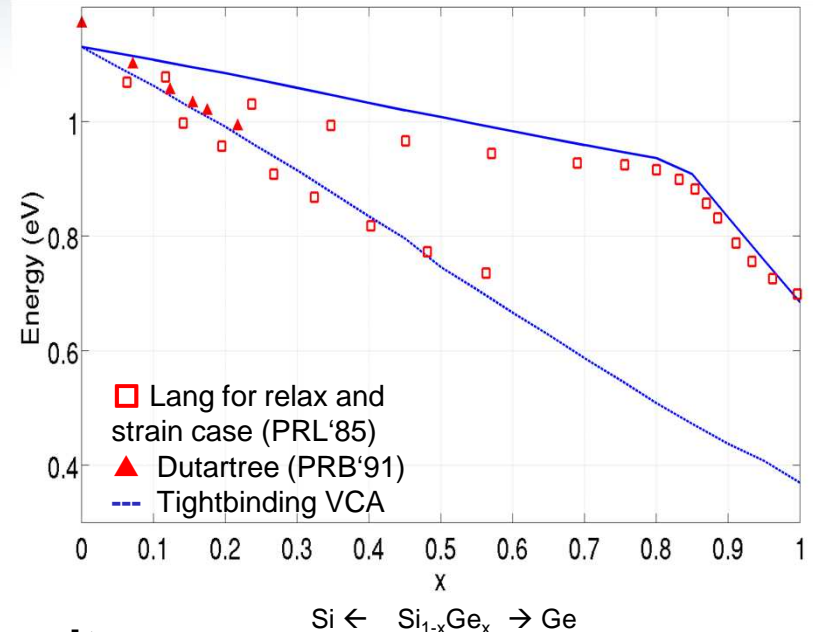
- **Strain** :two center integrals varied as follows,

$$V_{\text{SiGe}} = (1-x) \cdot (d_{\text{Si}}/d_{\text{SiGe}})^{\eta} V_{\text{Si}} + x \cdot (d_{\text{Ge}}/d_{\text{SiGe}})^{\eta} V_{\text{Ge}} \quad (3)$$

- Diagonal shifts<sup>2</sup> introduced for onsite parameters for strain.

[1] T. B. Boykin, G. Klimeck and F. Oyafuso, *Phys. Rev. B*, vol. 69, 115201/1-10, Mar. 2004

[2] T. B. Boykin et al, *Phys. Rev. B, Condens. Matter*, vol. 66, no. 12, p. 125 207, Sep. 2002



## Result:

- TB results benchmarked for SiGe relaxed and compressively strained SiGe/(100) cases with experimental data.

## Impact:

- Results published in ISDRS (Wash.DC, Dec 2009).
- A. Paul S. Mehrotra Elec. Dev. Lett. April 2010.