Tight-Binding (TB) parameterization of semiconductors using Genetic Algorithms

Objective

- To generate TB parameters for various semiconductors and various temperatures and validate them by matching with experiment.

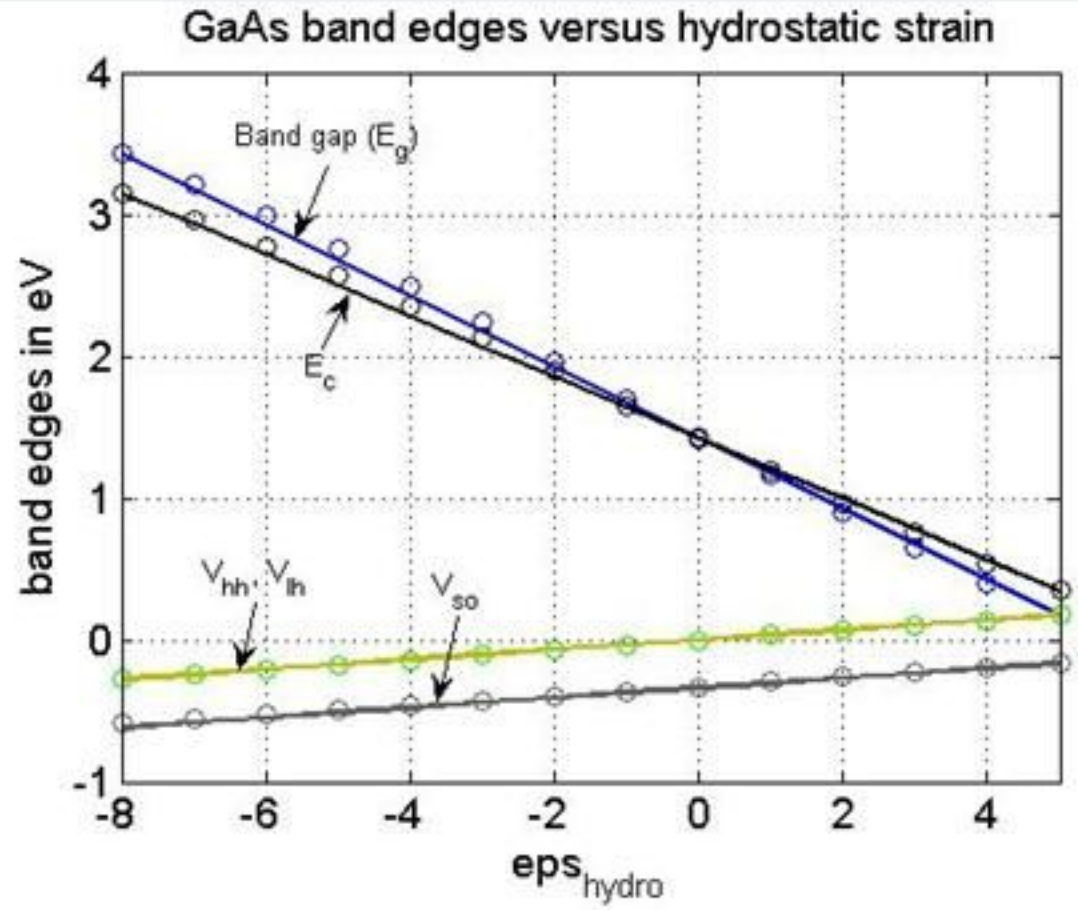
Approach

a) Generation of parameters

- Reverse-engineering → band gaps, masses, energies obtained from experiment and theory are used to 'fit' or optimize TB parameters.
- Genetic Algorithms are used for this non-trivial optimization.
- Variation of energies with strain included from theory.

b) Validation of parameters

- TB parameters obtained are fed into NEMO3D which simulates dots, wells, etc.
- Parameters validated when optical gap/absorption spectrum of simulated device matches experiment as closely as possible.



Result

- TB parameters generated for InAs, GaAs, Si and AlAs at 4K and AlAs at 300K generated.
- TB strain parameters for InAs and GaAs at 300K corrected for better fits at high strain.

Impact

- Found discrepancy in previous InAs and GaAS TB parameters at high strain.
- Different strain models valid for different temperatures.

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