

Theory of Idealized and Imperfect Antimonide-Based Superlattices.

M. R. Kitchin and M. Jaros.

Department of Physics,
The University of Newcastle upon Tyne,
Newcastle upon Tyne,
NE1 7RU, U.K.

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Outline of talk

- Modelling Antimonide superlattices: Why and how
- Optical properties:
 1. Interface bonds: Effects on absorption
 2. Alloy disorder: Emission linewidth
- Dynamical properties:
 1. Defect scattering: Cross-section vs. position and size
 2. Interface islands: Configuration and adjacent impurities
- Conclusions

Introduction

- Applications: IR photonics and ultra-fast electronics
- Outline of problem
 1. Atomic defects: Carrier scattering
 2. Microscopic disorder: Optical processes
 3. Interface configuration: Gaps and transition strengths
- What we do
 1. Seek links: microscopic configuration and device performance
 2. Apply empirical pseudopotential method (EPM)
 3. Model atomistic disorder
 4. Employ scattering theory

Strained Empirical Pseudopotentials ^a

- Describes atomic potentials of heterostructures
- Differentiates between interface bonding types
- Includes biaxial strain model
- Atomistic disorder e.g. isovalent defects, alloy materials
- Accounts for lattice relaxation around defects
- Band structure: Input to optical and scattering calculations

^aSee Shaw *et al*, J. Vac. Sci. Technol. B 18(4) 2088 (2000)

Alloys e.g. $\text{Ga}_{1-x}\text{In}_x\text{Sb}$

- Virtual Crystal Approximation: VCA
 1. Properties weighted average of constituents
 $\Rightarrow E_g(x) = xE_g^{\text{InSb}} + (1 - x)E_g^{\text{GaSb}}$
 2. Does not account for disorder
- Random Alloy Model: RND
 1. Cation potentials set to those of In or Ga
 2. Random number algorithm models disorder
 3. Check that fractions x and $(1 - x)$ correct

Scattering Theory

Compute dynamical properties

- Cross-section, σ
- Lifetime, $\tau \propto \sigma^{-1}$

1st Order (Born Approximation)

$$\sigma(\mathbf{k}) \propto \sum_{\mathbf{k}'} |\langle \phi_{\mathbf{k}'} | V | \phi_{\mathbf{k}} \rangle|^2 \rho_{\mathbf{k}'}(E_{\mathbf{k}}) \quad (1)$$

n th Order (T-matrix)

$$\sigma(\mathbf{k}) \propto \sum_{\mathbf{k}'} |\langle \phi_{\mathbf{k}'} | V | \Psi_{\mathbf{k}} \rangle|^2 \rho_{\mathbf{k}'}(E_{\mathbf{k}}) \quad (2)$$

Isolated Anion and Cation Defects

Study the effect of **isovalent**, substitutional defects such as Sb ions at As sites in the InAs (written Sb_{As}).

Consider the variation of the scattering cross-section from these defects at all possible sites within the perfect superlattice unit cell.

Full relaxation of the lattice around the defects can be included using valence force field approach. Results shown with and without relaxation for comparison.

Effect of Defect Position and Lattice Relaxation

Anion defects

Hole scattering essentially follows envelope function peaking in centre of valence well. Under relaxation of the lattice the position dependence of cross-section is radically changed.

Electron scattering follows envelope function only when relaxation effects included. Mechanism behind this phenomenon is investigated as part of ongoing research.

Cation defects

Hole scattering follows envelope function again. Relaxation increases cross-section slightly though leads to no significant qualitative change.

Electron process follows envelope function again. Relaxation drastically reduces the cross-section in the InAs conduction well.

Conclusion

- Interface bonds show significant influence on optical properties.
- Alloy layer disorder shows large effect on emission lineshape.
- Carrier scattering at isolated defects was generally greatest when defect/carrier overlap was largest.
- Anomalous role of lattice relaxation identified. Need microscopic models and further investigation.
- Scattering cross-section increases with the square of the number of atoms in a defect cluster for both holes and electrons.
- Lifetime exhibited non-linear dependence on combinations of anion and cation defects.

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