

# SILICON GERMANIUM AND VEGARD'S LAW

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## 1. INTRODUCTION

Silicon Germanium,  $\text{Si}_{1-x}\text{Ge}_x$ , is a compound with high functioning properties (discovered after being dropped on the floor!) used in semiconductor technologies. The band gap of  $\text{Si}_{1-x}\text{Ge}_x$  can be altered by the altering fractional content of germanium, allowing for the production of compounds with better high frequency performance and improved charge mobility[1].

We can investigate these properties by creating models of the **band structure** of different fractional compositions of  $\text{Si}_{1-x}\text{Ge}_x$ . From this the **band gap energy** and **effective mass** of electrons can be found and we can learn more about the current carrying capabilities of these compounds.

## 3. DETERMINING THE BAND GAP

Between the **valence** and **conduction** bands exists a region of '**forbidden energies**' due to the fact that electrons cannot exist at these energies. The compound  $\text{Si}_{1-x}\text{Ge}_x$  can have a variable band gap as germanium has a smaller band gap than silicon. Vegard's law predicts that the band gap will decrease following a quadratic curve empirically described by[3],

$$E_{g,\text{SiGe}} = \begin{cases} 1.17 - 0.47x + 0.24x^2, & x < 0.85 \\ 5.88 - 9.58x + 4.43x^2, & x > 0.85 \end{cases} \quad (3)$$

The split in values is due to the position of the band gap changing from the (1,0,0) where it is found in silicon to the (1,1,1) direction where it is found in germanium.

Figure 1 illustrates the relationship between germanium composition and band gap energy[4]. As expected there is a change in the trend at  $x = 0.85$  where the value for the band gap increases and falls back into a decreasing linear trend. However, in comparison to empirical data based on Vegard's law the values do not agree, instead following a linear trend. This shows that the linear interpolation method used in Vegard's law is not accurate. This can be corrected by including a factor known as the **bowing factor**.

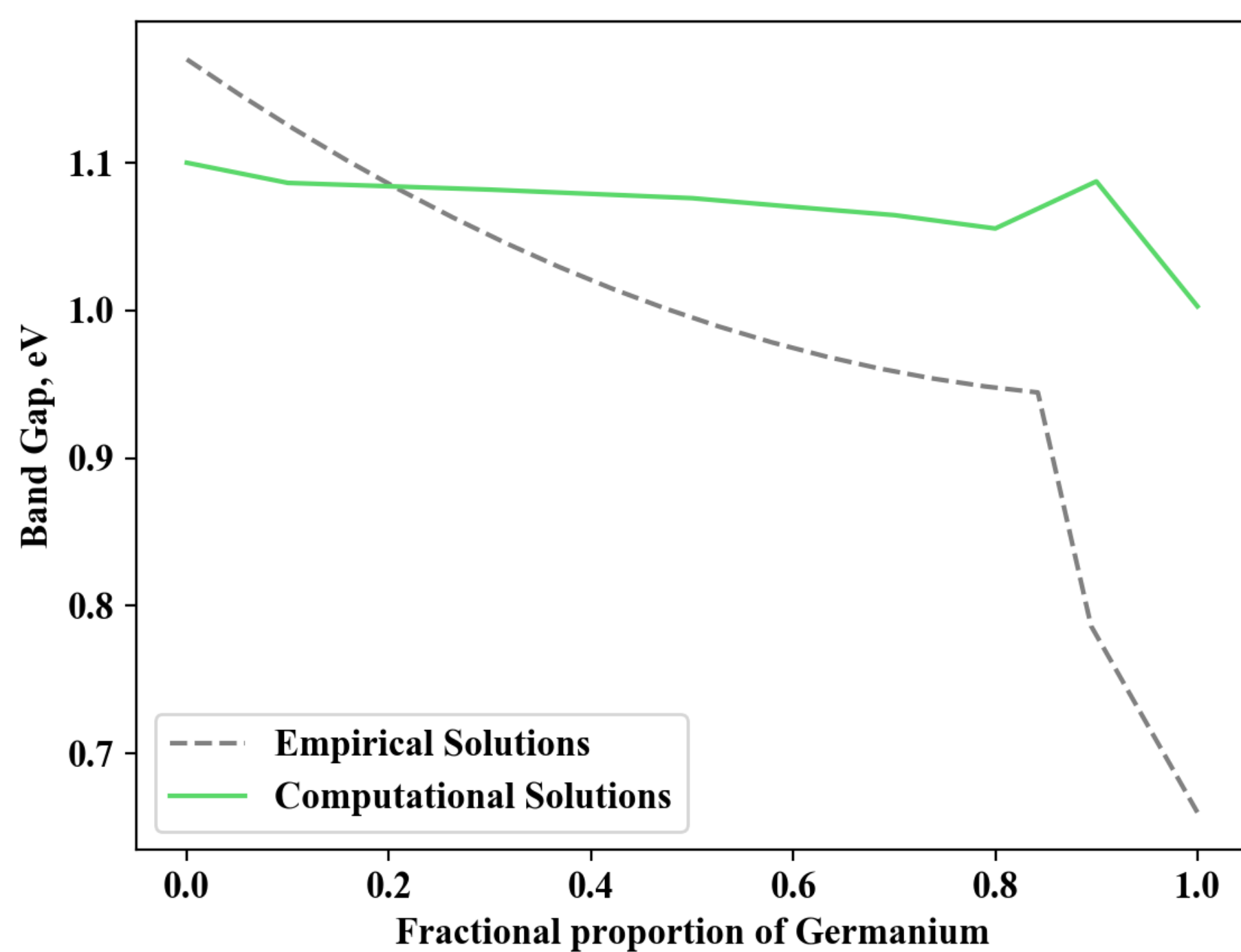


Figure 1: Variation of band gap energy with fractional composition of germanium

Decreasing the band gap proportionally decreases the energy required to excite electrons into the conduction band (allowing them to conduct). This makes these compounds useful in transistors, as they can be sensitive to more specific applied voltages.

## 5. CONCLUSIONS & FURTHER WORKS

This project has applied Vegard's law to find the properties of  $\text{Si}_{1-x}\text{Ge}_x$  and found the limitations of the linear interpolation method. Future investigations will focus on

- Implementing the bowing factor to correct the trend for the band gap relation.
- Correcting the effective mass curvature approximations to be in 2 dimensions and applying this method to the valence band to find the effective mass of holes.
- Investigating the carrier (electron or hole) concentration of the valence and band gaps.

## 2. CREATING THE BAND STRUCTURE

To find the allowed energies of the electrons within the lattice (and hence the band structure) of the compounds we solve the **Schrödinger equation**,

$$\frac{-\hbar^2}{2me} \nabla^2 \psi_{\mathbf{k}}(\mathbf{r}) + V(\mathbf{r})\psi_{\mathbf{k}}(\mathbf{r}) = E_{\mathbf{k}}\psi_{\mathbf{k}}(\mathbf{r}) \quad (1)$$

where  $\psi_{\mathbf{k}}$  represents the Bloch wave-function of the electron. Plotting energies against wave vectors,  $k$ , shows a functional relationship of different bands of energies for different electron states known as the band structure.

When the two compounds are mixed **Vegard's law**[2] suggests that their properties can be linearly interpolated via their proportions,

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

where  $\zeta$  represents a physical property that varies between materials. In this case we have interpolated the **lattice constant**,  $a$  and the **pseudopotential form factors**, that are encapsulated in the above potential term,  $V$ .

## 4. FINDING THE EFFECTIVE MASS

The **effective mass**,  $m^*$ , is evaluated from the curvature of the conduction energy band via the equation,

$$m^* = \hbar^2 \left[ \frac{d^2 E}{dk_i dk_j} \right]^{-1} \quad (4)$$

This was determined two ways:

- Modelling the Band Structure:** By modelling the values of energy of the conduction band,  $E$ , as a second order polynomial of wave vector,  $k$ , the curvature can be found as the coefficient of the  $k^2$  term.
- Using Finite Differences:** This method approximates the second order derivative using central difference.

Effective mass has a small dependence on the composition of germanium and then undergoes a transition where the location of the conduction band minimum changes and the material goes from being 'silicon like' to 'germanium like'[5]. The results plotted in Figure 2 show a linear relationship implying that the method of interpolation has created a band structure with varying curvature. This is likely

due to the fact that we have only modeled the curvature in one direction in each case. The results deviate more for the finite difference method as the approximation assumed that the energy surface is **isotropic**. The effective mass is in fact **anisotropic** so when being excited to the conduction band the electron will also gain momentum as the band gap is indirect. As momentum is a vector quantity variation of energy in both the  $k_x$  and  $k_y$  direction must be considered.

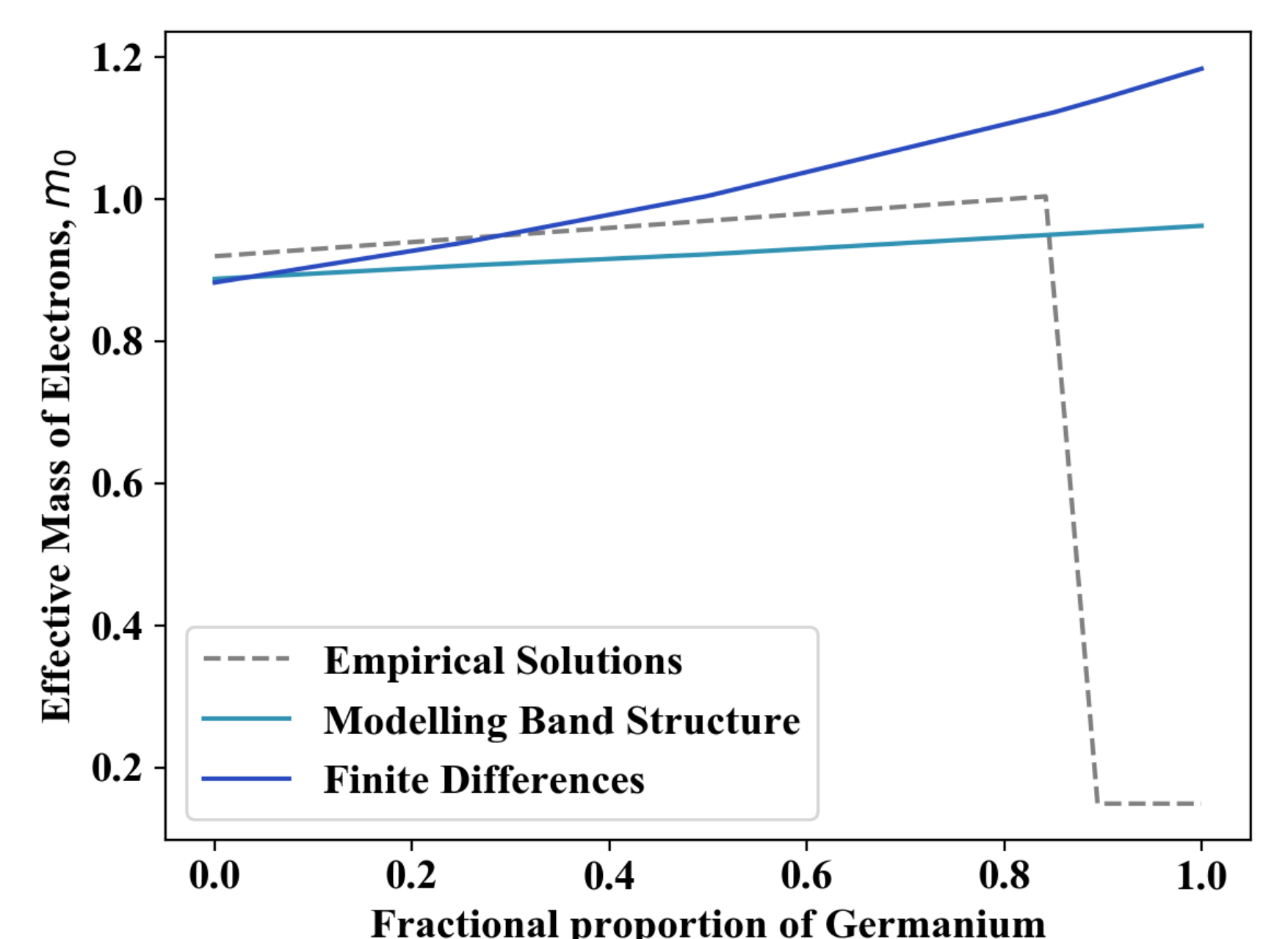


Figure 2: Variation of effective mass with fractional composition of germanium