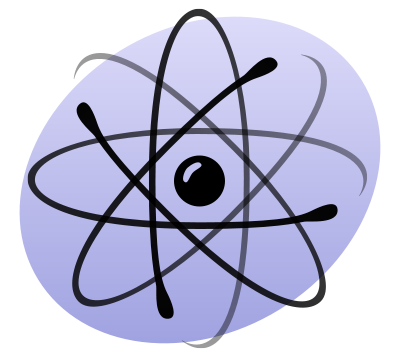
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PHYS2170: Semiconductor Physics

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# Abstract

This report details the phenomena observed a computer simulation of electrons in lattice structures. It was shown that for a two-well lattice decreased well separation increased electron wave interaction and decreased the magnitude of allowed energy levels. For a regular lattice a larger number of wells in the lattice increased the number of allowable electron energies and their magnitude. In an irregular lattice structure reducing the depth of a single well reduced the size of the gap separating allowed energies and altering the width of a single well an additional energy group is created which also reduced energy gaps.

# Introduction

Semiconductors exhibit unique conductive properties. Semiconductors have been utilised, most notably, to create computers which was possible through understanding their physical behaviours. These behaviours may be modelled using quantum mechanical systems. The Kronig-Penney Model approximates the potential energy of an electron in a conductive material (period lattice) using a series of equally spaced quantum wells (see Figure 1).

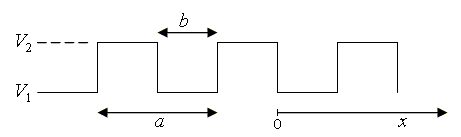


Figure 1: Kronig-Penney Model of an electron in a periodic lattice (source: Graz University of Technology)

This enables the use of Schrödinger’s Equation to model the interaction of electrons in structure of greater complexity such as molecules and solids. The model, by giving the allowed energies of the electrons, gives a crude approximation of the behaviour of a material. The magnitude of the energies and their spacing tells us how conductive or nonconductive a material would be (see Figure 2).

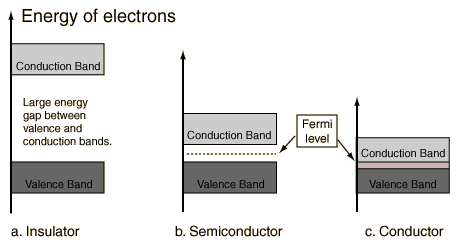


Figure 2: Energy bands of a material (Source: HyperPhysics)

The smaller the “band gap” between the valence and conduction band and the larger the conduction band the greater the conductivity of the material. The properties may be manipulated through “doping” which in the Kronig-Penny model is simulated by creating irregularities in the array of wells such that the wells are no longer periodic or square. Furthermore, by manipulating the number of wells or the separation of wells you may simulated different scenarios.

The solutions for Schrödinger’s Equation for a periodic structure are called “Bloch Functions” (see Equation 1) that describe the wavefunctions of particles in a periodically repeating environment.

The Kronig-Penney model determines the allowable energies using transcendental equation (see Equation 3) which may have a value of only ±1. Any energy that yields a value outside of this range is not allowed.

# Discussion

The Kronig-Penney model was used to calculate the energies for a periodic lattice of wells of depth 300eV and width 0.2nm. The allowable energies obtained are comparable to energies for a single well of the same width and depth, see Table 1 & 2.

|  |  |
| --- | --- |
| **Allowable Energy Level** | **Energy (eV)** |
| 1 | 9 |
| 2 | 37 |
| 3 | 83 |
| 4 | 149 |
| 5 | 323 |

Table 1: Allowable energy levels for a periodic lattice calculated using the Kronig-Penney Method. Depth 300eV and width 0.2nm.

|  |  |
| --- | --- |
| **Allowable Energy Level** | **Energy (eV)** |
| 1 | 7.59 |
| 2 | 30.28 |
| 3 | 67.8 |
| 4 | 119.56 |
| 5 | 184.33 |
| 6 | 258.57 |

Table 2: Allowable energy levels for a single well of depth 300eV and width 0.2nm.

The difference in results shows that that the Kronig-Penney Model is an approximation, despite this is can still be used to describe lattices structures.

## Part One – Two Square Wells

By simulating only two quantum wells the effect of altering their separation distance was observed. It showed a relationship between the magnitude of the energy levels and the proximity of 0the two wells, where greater separation increased magnitude (see Table 3 & Figure 5).

**This behaviour may be due to increased wave interaction at closer distances. When the waves interact more destructive interference is created which lowers their magnitude.**

**Furthermore, at 0nm and 0.01nm separation the number of allowable energies reduced to 3. Why?**

The wavefunctions for the double well were similar to those in the single well of the same dimensions (see figures 3&4).

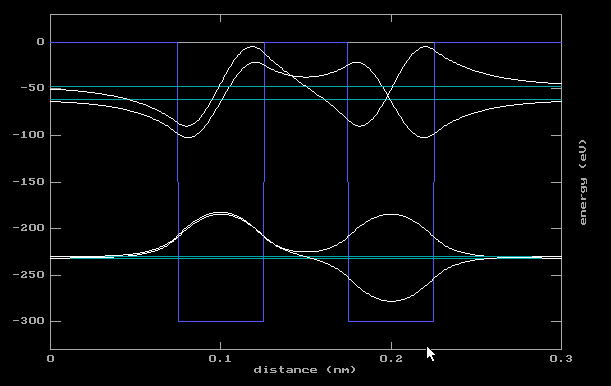


Figure 3: Wavefunctions for a double well of depth 300eV, width 0.2nm and separation 0.1nm

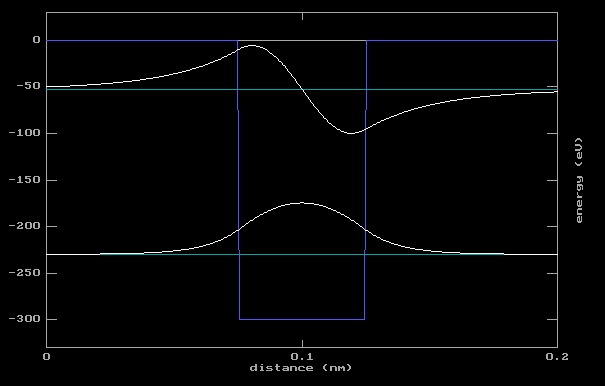


Figure 4: Wavefunctions for a single well of depth 300eV and width 0.2nm

It looks like the waves in the double well are the same as in the single well but have continued propagating through the wells, repeating periodically. There are four energy levels in the double-well lattice, two of which mirror exactly the shape of the single well and two others that are the inverse of the single well shapes.

Bloch’s theorem states that each wavefunction is an energy eigenstate [1] (i.e. corresponding to an eigenvalue of a wavefunction) and that each wave may be described by a Bloch function (see equation 1). Bloch functions may be used to calculate the predicted behaviour of electron’s in a periodic lattice helping to understand the properties of the material they reside in.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Separation (nm)** | **0** | **0.01** | **0.05** | **0.1** | **Single Well** |
| **1** | 24.6 | 60.96 | 69.52 | 70.29 | 7.59 |
| **2** | 96.65 | 97.88 | 71.09 | 70.31 | 30.28 |
| **3** | 208.44 | 251.71 | 241.73 | 246.92 | 67.8 |
| **4** | **-** | - | 258.81 | 249.1 | 119.56 |

Table 5: Allowed energies for a two-well lattice of depth 300eV and width 0.05nm with varying separation.

Figure 5: Allowed energies for a two-well lattice of depth 300eV and width 0.05nm with varying separation.

## Part Two – Regular Lattice of Wells

A regular lattice of a greater number of wells allowed for a greater number of allowable energy levels. The energy levels were discretely grouped into two “bands” and the number of energy levels in each band were directly proportional to the number of wells.

The Kronig-Penney model that is being used to generate this data may be translated to a more practical interpretation. That is, the number of wells represents the number of atoms, and the energy levels represent the electrons that each additional atom’s presence permits.

The two distinct groupings of energy levels (atoms) represent the conduction and valence bands of the material in which the electrons reside. Therefore, by increasing the number of atoms in the material you are increasing its current carrying capacity. The separation of the two bands ( aka “band gap”) influences the conductivity of the material.

## Part Three – Irregular Lattice of Wells

## Part Four – Stationary States in One Dimension

# Conclusion

# Bibliography

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| --- | --- |
| [1] | F. Bloch, "Über die Quantenmechanik der Elektronen in Kristallgittern", 1928. |
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