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Title: Quantum Dot as Absorbing Solar Cell Material

العنوان : النقاط المكماه كمواد امتصاص في الخلايا الضوئيه

A thesis presented in application for the M.Sc, in physics at University Shendi.

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حقوق الطبع

تمتلك الجامعة والطالب معاً حقوق الطبع الخاص بالأطروحات، ولا يجوز للطالب في أي حال من الأحوال إعادة طباعة الأطروحة أو إخراجها في شكل كتاب أو توزيعها دون مراجعة الجامعة أوالحصول على إذن خطي بذلك. كما تمتلك الجامعة كافة حقوق توظيف الأطروحات المُجازة فيأقسامها وتحت إشراف أساتذتها والاستفادة منها كمصادر مرجعية للمعلومات ولأغراض الإطلاع أوالإعارة وفق الأنظمة المعتمدة . وتعتبر الأطروحات الجامعية مكوناً أصيلاً وأساسياً من جُملة الإنتاج العلمي للجامعة متمثلةً في أساتذتها المشرفين على إعدادها وأقسامها وبرامجها الأكاديمية القائمة على برنامج الدراسة وتأهيل الطالب

توقيع الطالب	توقيع المشرف
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توقيع المشرف

محمد ياسين مصطفى

أستاذمساعد بقسم الفيزياء

كلية العلوم والتقانة

Dedication

I dedicate this research is my family especially to my brandies, husband and son. I extend dedication to those how have the interest to study quantum dot.

Acknowledgements

I would be so grateful to thank Assistant Professor, Mohamed Yassin Mustafa for his supervision, advices, encouragement, &moral support all through the research period.

I am also grateful for the financial support given by my husband Osama Ismail Al-fahal.

My thanks go to my mother Ekhlas Ahamed Mohamed, Who did so much by helping me in taking care of my son Mohamed.

Abstract

Quantum dots as nano-materials have been extensively investigated in the past several decades from growth to characterization to applications. As the basis of future developments in the field this thesis collects a series of state-of-the-art chapters on the current status of quantum dot devices and how these devices take advantage of quantum features. The chapters cover numerous quantum dot applications in solar cells. ***Quantum Dot Devices*** is appropriate for researchers of all levels of experience with an interest in epitaxial and/or colloidal quantum dots. It provides the necessary overview of this exciting field.

The third generation of solar cells includes those based on semiconductor quantum dots. This sophisticated technology applies nanotechnology and quantum mechanics theory to enhance the performance of ordinary solar cells. Although a practical application of quantum dot solar cells has yet to be achieved, a large number of theoretical calculations and experimental studies have confirmed the potential for meeting the requirement for ultra-high conversion. In this thesis, the methods used in and the results of various quantum dot solar cell designs were outlined, including quantum dot intermediate band solar cells, hot electron quantum dot solar cells, quantum-dot sensitized solar cells, colloidal quantum dot solar cells, hybrid polymer-quantum dot solar cells, and MEG quantum dot solar cells. Both theoretical and experimental approaches are described. ***Quantum Dot Solar Cells*** helps to connect the fundamental laws of physics and the chemistry of materials with advances in device design and performance.

In this thesis discussed Kronig – Penney model using a specific software program. Experiment was conducted where the calculated band gap of germanium

ملخص البحث

النقاط المكماه عباره عن مواد متناهيه الصغر في المدي (النانو) وقد بذل الباحثون جهداً مكثفاً خلال العقود القريبه المنصرمه للتحقق من كيفيه تنميتها ودراسه خصائصها واستخداماتها التطبيقيه. القاعده الاساسيه التي ينطلق منها هذا (المبحث) Thesis هو امعان النظر في كيفيه تطورها المستقبلي ومدى اسهامها في مجال التطبيقات (النانويه) , لذا اشتمل المبحث علي سلسله من الفصول توضح المستوي الضمني للاجهزه التقليديه الحاليه ومدى الاعتماد عليها لاستنباط الاجهزه ذات الخصائص النانويه. احتوت الفصول علي عدد من التطبيقات النانويه في مجال الخلايا الضوئيه.

التفكير في الاجهزه (النانويه) المتناهيه الصغر يمثل جزء هاماً بالنسبه للباحثين علي مختلف خلفياتهم العلميه (المعرفيه) والعمليه خاصه في مجال تثبيت (زراعه) النقاط المكماه عن طريق التفاعل الكيماوى المحاليل السائبه Colloidal Solutions او استخدام التقنيات الحديثه في لصق النقاط المكماه بعد تجهيزها مختبريا علي هيئه (مداد) حبر قابل للرش او لعمليات الطباعه Epitaxial ونرى من الضروري التعرف علي هذه الجزئيه الآسره للعقول.

الجيل الثالث من الخلايا الضوئيه يشمل تلك التي تعتمد علي النقاط المكماه لاشباه الموصلات , ومن الناحيه النظريه يتم اعتماد نظريات التكميه لتعزيز ودراسه اداء هذه الخلايا الضوئيه. وعلي الرغم من ان تطبيقات الخلايا الضوئيه المصنعه من النقاط المكماه لم تصل الي الآن الي االمستوي التطبيقي التجاري ولكنه ما زال البحث جاريا علي قدم وساق في مجال التنظير والتجارب المختبريه التي اكدت علي امكانيه الاستفاده من النطاق الضوئي فوق البنفسجي (غير المرئي) والذي يمثل ثلثي طاقه الطيف الضوئي .

في هذا المبحث تم توضيح عده طرق مستخدمه في انتاج الخلايا الضوئيه المختلفه منها الخلايا الضوئيه ذات النطاق المتوسط Intermediate Quantum dot, وخلايا الالكترونات الساخنه hot electron, والخلايا الضوئيه رقيقه الشعور ذات الحساسيه العاليه quantum-dot sensitized solar cells, والخلايا السائله colloidal quantum dot solar cells, وخلايا المكوثرات المهجنه ذات النطاقات المتعدده hybrid polymer-quantum dot solar cells, والخلايا الضوئيه القادره علي توليد اكثر من الكترون واحد MEG quantum dot solar cells وجميع هذه الانواع قد تم وصفها والتعرق عليها للوصول للهدف المنشود الذي يساعدنا علي ربط القوانين الفيزيائيه والكيميائيه الاساسيه للمواد المتناهيه الصغر مما يساعد مستقبلا علي تسهيل النظر في عمليات التطور من ناحيتي الاداء والتصنيع (التصميم).

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Chapter seven

Pinch top nanotechnology guide to quantum dot fabrication

Abbreviations

NREL	National Renewable Energy Lab
SAQDs	Self assembled Quantum Dots
PL	Photo luminance
CCD	Charge compiled Device
SESAMs	Semiconductor saturable absorber
SQW	Single Quantum well
RHEED	Reflection high energy electron diffraction
TEM	Transmission electron microscope
CB	Conduction band
CV	Valence band
MBE	Molecular beam epitaxy
DOS	Density of states. *It has no correlation with DOS the disk operating system of Microsoft*

SC	Solar cell
QDs	Quantum dots

Greek Symbols

Note: The small Greek letter in the alphabet is used except where the notation (cap) is used where the capital version of the Greek letter is used.

Greek alphabet table

Greek Symbol		Greek Letter Name	Used to denote
Upper Case	Lower Case		
Α	α	Alpha	Angles, coefficients, attenuation constant, absorption factor, area
Β	β	Beta	Angles, coefficients, phase constant
Γ	γ	Gamma	Complex propagation constant (cap), specific gravity, angles, electrical conductivity, propagation constant
Δ	δ	Delta	Increment or decrement, determinant (cap), permittivity (cap), density, angles
Ε	ε	Epsilon	Dielectric constant, permittivity, electric intensity
Ζ	ζ	Zeta	Coordinates, coefficients
Η	η	Eta	Intrinsic impedance, efficiency, surface charge density, hysteresis, coordinates
Θ	θ	Theta	Angular phase displacement, angles, time constant, reluctance
Ι	ι	Iota	Unit vector
Κ	κ	Kappa	Susceptibility, coupling coefficient, thermal conductivity

Λ	λ	Lambda	Permeance (cap), wavelength, attenuation constant
Μ	μ	Mu	Permeability, amplification factor (in valves/ vacuum tubes), prefix for the micro multiplier.
Ν	ν	Nu	Reflectivity, frequency
Ξ	ξ	Xi	Coordinates
Ο	ο	Omicron	
Π	π	Pi	Universally used for 3.1416 . . . .
Ρ	ρ	Rho	Resistivity, volume charge density, coordinates
Σ	σ	Sigma	Summation (cap), surface charge density, complex propagation constant, electrical conductivity, leakage coefficient, deviation
Τ	τ	Tau	Time constant, volume resistivity, time-phase displacement, transmission factor, density
Υ	υ	Upsilon	
Φ	ϕ	Phi	Scalar potential (cap), magnetic flux, angles
Χ	χ	Chi	Electric susceptibility, angles
Ψ	ψ	Psi	Dielectric flux, phase difference, coordinates, angles
Ω	ω	Omega	Electrical resistance (cap), solid angle, angular velocity

Terminology

Nano-particles

Quantum dots are Nano-particles composed of periodic groups of III-V or II-VI semiconductor materials such as ZnS, ZnSe, CdS, CdSe, CdTe, InP, and others. Their reduced size induces a shift of the electronic excitations to higher energy, concentrating the oscillator strength into just a few transitions, conferring unique quantum-confined photonic and electronic properties. Although physically larger than organic dyes and fluorescent proteins, their cumulative optical properties offer great biological utility. With tunable core sizes, it is possible to attain a broad adsorption profile, narrow, size-dependent, and symmetric photoluminescence spectra depending of the constituent materials. QDs show also strong resistance to photo bleaching and chemical degradation, significant photo stability and high quantum yields.

Nanostructure is a structure of intermediate size between microscopic and molecular structures. Nanostructure detail is microstructure at nanoscale. In describing **nanostructures** it is necessary to differentiate between the numbers of dimensions on the nanoscale.

Nano-crystal is a material particle having at least one dimension smaller than 100 nanometers and composed of atoms in either a single- or poly-crystalline arrangement. More properly ,any material with a dimension of less than one micrometer should be referred to as nanoparticle not Nano-crystal.

Blue shift is any decrease in wavelength, with a corresponding increase in frequency, of electromagnetic waves; the opposite effect is referred to as red shift. In visible light, this shifts the color from the red end of the spectrum to the blue end.

Band gap generally refers to the energy difference (in electron volts) between the top of the valence **band** and the bottom of the conduction **band** in insulators and semiconductors. It is the energy range where no electron states can exist

Quantum dot

A quantum dot is a semiconductor nanostructure that confines the motion of conduction band electrons, valence band holes, or excitons (bound pairs of conduction band electrons and valence band holes) in all three spatial directions

Quantum wire is an electrically conducting **wire** in which **quantum** effects influence the transport properties.

Quantum well is a thin layer which can confine (quasi-)particles (typically electrons or holes) in the dimension perpendicular to the layer surface, whereas the movement in the other dimensions is not restricted. The confinement is a **quantum** effect.

Bulk semiconductors are characterized by a composition-dependent band gap energy (E_g), which is the minimum energy required to excite an electron from the ground state valence energy band into the vacant conduction energy band. With the absorption of a photon of energy greater than E_g, the excitation of an electron leaves an orbital *hole* in the valence band. The negatively charged electron and positively charged hole may be mobilized in the presence of an electric field to yield a current, but their lowest energy state is an electro-statically bound electron-hole pair, known as the *exciton*. Relaxation of the excited electron back to the valence band annihilates the exciton and may be accompanied by the emission of a photon, a process known as *radiative recombination*.

Density of states (DOS) of a system describes the number of **states** per interval of energy at each energy level that are available to be occupied.

DECLARATION

I hereby declare that I am the author of this thesis; that, unless otherwise stated, all references cited here have been consulted by me; that the work of which the thesis is a record has been done by me and that it has not been previously accepted for higher degree

Sheema Abdeldaiem

Statement

I certify that Sheema Abdeldaiem remains under my supervision as a research student for M.Sc Degree, that all conditions of ordinance & regulations related to the degree of Master of Science have been satisfied.

M.Y.Mustafa

Chapter one

Introduction

1-1 Solar Cell History:

1839 – The photovoltaic effect was discovered by Alexandre-Edmond Becquerel, who was a French physicist. This was "the beginning" of the solar cell technology. Becquerel's experiment was done by illuminating two electrodes with different types of light. The electrodes were coated by light sensitive materials, AgCl or AgBr, and carried out in a black box surrounded by an acid solution. The electricity increased when the light intensity increased.

1905 – Albert Einstein published his paper about the photoelectric effect. There he claimed that light consists of "packets" or quanta of energy, which we now call photons. This energy varies only with its frequency (electromagnetic waves, or the "color of the light"). This theory was very simple, but revolutionary, and it explained very well the absorption of the photons regarding to the frequency of the light.

1930s – Walter Schottky, Neville Mott and some others developed a theory of metal-semiconductor barrier layers.

1950s – Bell Labs produce solar cells for space activities.

1999 – Spectrolab, Inc. and the National Renewable Energy Laboratory develops a photovoltaic solar cell that converts 32.3 percent of the sunlight that hits it into electricity. The high conversion efficiency was achieved by combining three layers of photovoltaic materials into a single solar cell. The cell performed most efficiently when it received sunlight concentrated to 50 times normal. To use such cells in practical applications, the cell is mounted in a device that uses lenses or mirrors to concentrate sunlight onto the cell. Such "concentrator" systems are mounted on tracking systems that keep them pointed toward the sun.

1999 – The National Renewable Energy Laboratory achieves a new efficiency record for thin-film photovoltaic solar cells. The new measurement is of 18.8 percent efficiency.

2000 – Two new thin-film solar modules, developed by BP Solarex, break previous performance records. The company's 0.5-square-meter module achieves 10.8 % conversion efficiency—the highest in the world for thin-film modules of its kind. And its 0.9-square-meter module achieved 10.6% conversion efficiency and a power output of 91.5 watts — the highest power output for any thin-film module in the world.

1-2 Research problem:

The research problem is related to the fact that no intensive research on the means by which one can increase the efficiency of the solar cell by absorbing most of the whole sun radiation spectrum.

1-3 Literature Review:

Researchers have demonstrated a way to use quantum dots to significantly reduce the amount of energy that solar cells lose to heat, paving the way for future cells that are twice as efficient as today's technology. From the literature review there after will show how they did it.

New research shows next-generation solar cells could more than double the efficiency of conventional silicon cells. **When it comes to turning sunlight into electricity,** today's technology leaves lots of room for improvement. The most efficient solar cells on the market, which are made of silicon, convert less than 20 percent of the light that hits them into electricity, and the theoretical maximum efficiency of these cells is around 31 percent.

One reason for this low efficiency is that much of the incoming light contains energy that is too high for solar cells to capture, so it's lost as heat. Now researchers have shown that it's possible to harvest that energy before it escapes, meaning that engineers could one day develop next-generation solar cells with efficiencies of up to 66 percent.

When light hits a solar cell; a fraction of its energy is absorbed, exciting electrons in the cell's material and knocking them free. An electric field then forces the free electrons to flow in a specific direction, producing electric current. The energy that is absorbed is determined by what scientists call the band gap, a limited range of energies, the cell’s material can capture.

But sunlight is composed of particles, called photons, representing a very broad range of energies. The energy from photons too high to be absorbed takes the form of high-energy electrons—or, as scientists called them, "hot electrons"–and is lost as heat. However, if one could remove the hot electrons before they cool, says study author Xiao yang Zhu, a chemistry professor at University of Texas at Austin, "then you essentially shut down this heat-loss pathway, and you increase efficiency by more than a factor of two."

To accomplish this, the group used nanoscale (less than 100 nanometers, or10^{-9} meters) crystals of a compound called lead selenide. Like silicon, lead selenide is a semiconductor, meaning it absorbs light energy within a certain band gap, or range of energies. But semi conducting nano crystals, also known as **quantum dots**, exhibit very different properties than their larger counterparts. For one thing, they can hold on to a hot electron for a longer period of time, stretching out the amount of time it takes for the electron to cool. In fact, previous research has shown that **quantum dots** can increase the life time of hot electrons by as much as 1000 times.

Once a hot electron is confined within a **quantum dot**, and then comes the hard part: removing it so its energy can be harvested. The electron likes to stay inside the **quantum dot**, Zhu says, "So we needed to find something that would attract it out." For this role, the researchers chose titanium oxide, a well-studied compound known for its ability to accept new electrons. Then came the really hard part: arranging the lead selenide **quantum dots** and titanium dioxide in such a way that their chemical interactions would induce electron transfer.

Not only was the transfer successful, it was also very fast. If verified, this result makes highly efficient **quantum dots** solar cells more realistic, according to Tianquan Lian, a chemistry professor at Emory University who was not part of this study, and whose research revolves around the use of nano materials for solar energy conversion. This is the first demonstration that, in principle, the vital electron transfer step is possible, he says.

The ultimate goal, Zhu says, is called a "hot-carrier solar cell," which could convert up to 66 percent of incoming light into electricity. But many scientific and engineering steps remain before such a cell can be commercially developed. One challenge is to figure out how to transfer the hot electrons to a conducting wire. "This is science that has really striking implications, but implication is not application yet," Zhu says, adding, "I'll be extremely happy if, in my lifetime, I see [hot-carrier cells] on roofs."

Silicon had six decades to get where it is today, and even silicon hasn't reached the theoretical limit yet. You can't hope to have an entirely new technology beat an incumbent in just four years of development," said Professor Vladimir Bulović in the release.

The researchers still need to determine why these films are so stable and there's still a long way to go before they are commercially viable. But they now hold the National Renewable Energy Lab (NREL) record for quantum dot solar efficiency.

1-4 Aim of the work:

The aim of this work is to find how to increase the performance of solar cells by using quantum dots and other related techniques. Some experimental work and computer programmers were made for this purpose.

1-5resentation of the thesis:

This work consists of seven chapters. Chapter one is the introduction, chapter two traditional solar cells, chapter three spectrum of solar radiation, chapter four quantum dots, chapter five energy band, chapter six density of states, chapter seven pinch top nanotechnology guide to quantum dot fabrication.

Chapter tow

Traditional solar cells

2-1 Semiconductors fundamentals:

Since the development of the first transistor in 1948, semiconductors components come into use of every conceivable kind in the field of electricity. Semiconductor components are generally made of germanium or silicon. More recently components of other substances, such as gallium and arsenic (gallium arsenide) have been used.

Atoms consist of a nucleus surrounded by electron shells which are occupied by varying numbers of electrons. Semiconductor materials possess four valiancy (outer shell) electrons when germanium or silicon atoms are bounded in a crystal lattice; all their valiancy atoms are bounded. This form of boding is known as atomic bonding .Unlike metal, semiconductor therefore initially have no free electrons. The atoms of Semiconductors form regular crystal lattice.

If semiconductors are cooled to a temperature 0K, they don't conduct current at all. The explanation for this loss of conductivity is that all valiancy electrons have been used up to bond the atoms in their crystal lattice, leaving no free electrons to conduct the current.

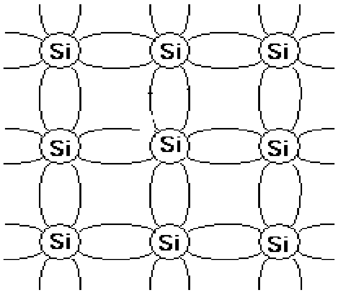


Figure (2-1): structures of silicon crystals

When semiconductors are heated they begin to conduct current .A temperature 0K already represents a considerable degree of heating for semiconductors, since the temperature difference between 0K and 0C is 273 K .The conductivity of the semiconductors are also found to increase exponentially with rise in temperature. When atoms are heated they are no longer at rest, but vibrate in all directions. Bonds with the neighboring atoms are destroyed and valiancy electrons are freed from their atoms. Therefore: The ***conductivity of semiconductors is temperature dependant***.

If a voltage is applied to any semiconductor the free electrons migrate towards the positive charge potential, each electron leaving behind vacant referred to as a hole; the positive charge of the atomic nucleolus predominates , so the hole is considered to be positively charged , its charge is exactly as large as the negative electron charge. Some new electrons occupy the vacant holes again and the atoms become electrically neutral, this process is termed ***recombination***. Since each recombined electron leaves a hole behind, the holes appear to migrate through the crystal towards the negative potential of the voltage source.

For the sake of simplicity, assume that holes also help to conduct current though the semiconductor crystal. Charge transfer of this kind is called **p-type** conduction as opposed to electrons **n-type** conduction. Therefore conduction observed in a pure semiconductor at room temperature is known as ***intrinsic*** conduction. ***Intrinsic*** conduction in a pure semiconductor is produced by heating and depends on temperature attained .Both electrons and holes contribute to intrinsic conduction.

In order to make semiconductor components, a semiconductor material whose conductivity is largely unaffected by temperature and greatly in excess of their intrinsic conductivity is needed. To obtain these qualities, impurity atoms possessing either three or five outer shell electrons are introduced into crystal lattice of a semiconductor, in a process known as ***doping.*** The following figure shows the lattice structures of two doped silicon crystals .Doping disturbs the regular crystal structure, creating what is so called ***impurities***, but the crystal remains electrically neutral.

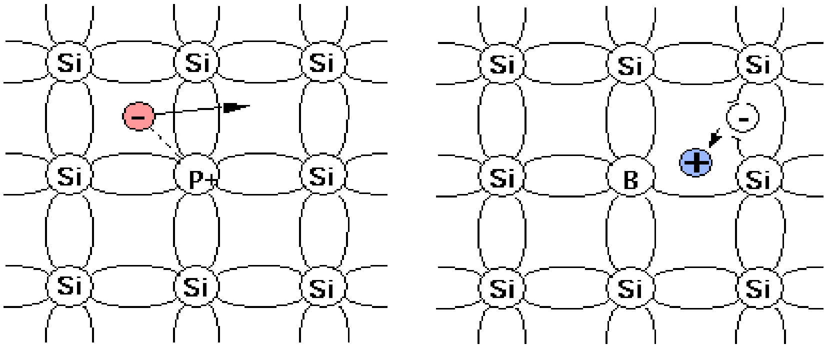


Figure (2-2): figure shows the lattice structures of tow doped silicon crystal.

Doping with Pentavalent impurity atoms increases electrical conductivity by releasing free electrons and it is referred to as ***n-type*** semiconductor .Thus the current is conducted via the electrons. In contrast, silicon is doped with trivalent impurity atoms some electrons of the outer shells are not induced in the crystal structure, because there is no partner electron available on the outer shell of impurity atom. This type of doping also creates impurity in the crystal lattice structure, and can pick up electrons, holes are then produced which increases electrical conductivity via holes. Semiconductor doped in this way is termed a ***p-type*** semiconductor.

In practice semiconductors are doped in such away their intrinsic conduction is negligible by comparison with their extrinsic conduction .Since extrinsic conduction is not temperature dependant, the conductivity of doped semiconductors is largely unaffected by temperature .

2-2 Semiconductor diode:

Semiconductors components are generally made in such a way that ***p-type*** material is in close contact with ***n-type*** material. The interface between the two is termed ***p-n junction***. As indicated by the following figure

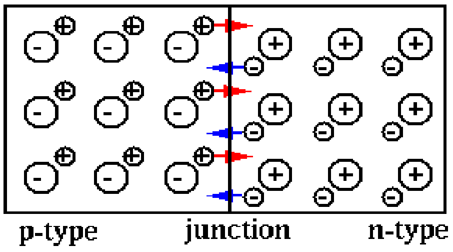


Figure (2-3): p-n junction

Holes and electrons in a narrow layer on either side of the contact surface attempt to migrate to crystal structure on opposite sides as indicated by the arrows .This type of migration referred to as ***diffusion*** .Electrons diffuse to the p-type part of the crystal encounter holes and recombine with them. The same occurs with the holes which diffuse to the n-type part of the crystal and encounter electrons. A layer free of mobile charge carriers is created due recombination of holes and electrons.

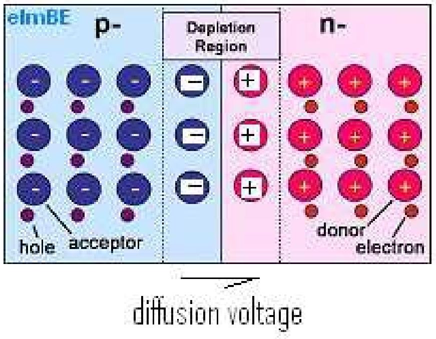


Figure (2-4): shows p-n junction and diffusion voltage

Current cannot normally flow though this zone, which is known as the ***barrier; blocking or depletion layer*** .Diffusion transfers negative charge carriers to the ***p-doped*** part and positive charges to the ***n-doped*** part of the crystal .Thus diffusion causes the p-type material in depletion layer to become negatively charged and the n-type positively charged .A potential known as the ***diffusion voltage*** is created. As a result, holes and electrons are repelled and can no longer diffuse. The depletion layer does not attempt to extend itself further into the crystal. The diffusion voltage is approximately 0.2 …0.4 volts in germanium and 0.5 …0.8 in silicon.

This semiconductor component (diode) transmit current in one direction, so it has the valve effect, in this case it is known as passive diode, because it needs to be biased by an external potentials .in addition to the semiconductor components already described there are another components whose function depend upon ***light radiation***, magnetic fields or any other variable .these are known as active diodes .but our aim is interested in ***light radiation*** ones to build our solar cells.

2-3 Solar cells:

Solar cells convert light energy into electrical energy. They are referred to as photoelectric cells or photovoltaic cells. The light falling on the ultra thin n-doped layers destroys individual bonds producing holes and electrons. See fig. below;

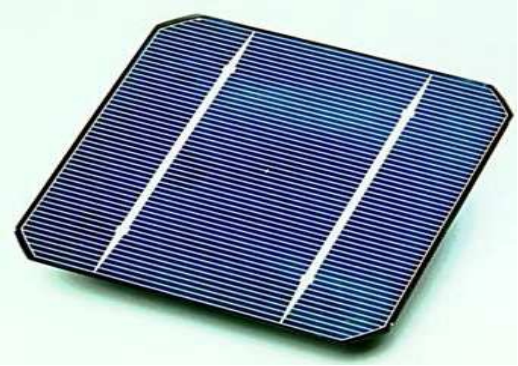


Figure (2-5): Solar cell component

Holes and electrons moves in different directions under the influence of diffusion potential. In consequence the n-layer is charged negatively and the p-layer is charged positively inducing voltage between the contacts of the solar cell. The voltage and currents in the cell depends on the intensity of illumination.

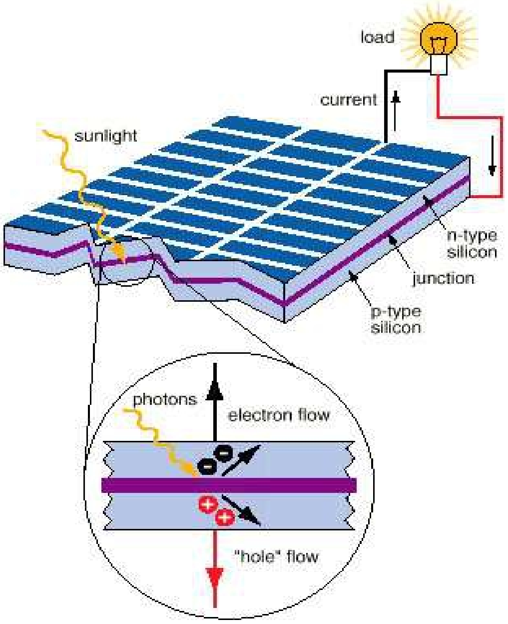


Figure (2-6): the Photovoltaic Effect in a Solar Cell

In practice, solar cells are linked in the same way as voltaic cells to produce higher powers .typical values for a solar cell are;

Shot circuit current I k = 138mA

No load voltage V0/c = 600mV

Maximum power P max = 63mW

Efficiency η =11

2-4 Electricity generation

The basic idea of a solar cell is to convert light energy into electrical energy. The energy of light is transmitted by *photons*, small packets or quanta of light. Electrical energy is stored in electromagnetic fields, which in turn can make a current of electrons flow.

When photons are absorbed by matter in the solar cell, their energy excites electrons higher energy states where the electrons can move more freely. Perhaps most well-known example of this is the photoelectric effect, where photons give electrons in a metal enough energy to escape the surface. In an ordinary material, if the electrons are not given enough energy to escape, they would soon relax back to their ground states. In a solar cell however, the way it is put together prevents this from happening. The electrons are instead forced to one side of the solar cell, where the build-up of negative charge makes a current flow through an external circuit. The current ends up at the other side (or *terminal*) of the solar cell, where the electrons once again enter the ground state, as they have lost energy in the external circuit.

Two important quantities to characterize a solar cell are

- Open circuit voltage (V_{oc}): The voltage between the terminals when no current is drawn (infinite load resistance)
- Short circuit current (I_{sc}): The current when the terminals are connected to each other (zero load resistance)

The short circuit current increases with light intensity, as higher intensity mean more photons, which in turn mean more electrons. Since the short circuit current I_{sc} is roughly proportional to the area of the solar cell, the short circuit current density,

$$\mathbf{J_{sc} = I_{sc}/A,} \qquad (2\text{-}1)$$

Current density used often to compare solar cells. [9]

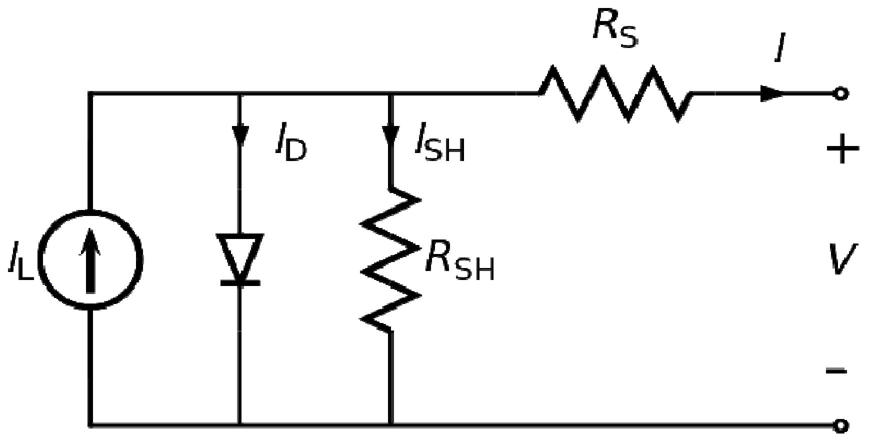


Figure (2-7): The equivalent circuit of a solar cell

To understand the electronic behavior of a solar cell, it is useful to create a model which is electrically equivalent, and is based on discrete electrical components whose behavior is well known. An ideal solar cell may be modeled by a current source in parallel with a diode; in practice no solar cell is ideal, so a shunt resistance and a series resistance component are added to the model.[8] (seefig.11above)

2-5 Characteristic equation

From the equivalent circuit it is evident that the current produced by the solar cell is equal to that produced by the current source, minus that which flows through the diode(internal resistance, minus that which flows through the shunt resistor(leakage) :[7][5]

$$I = I_L - I_D - I_{SH} \qquad (2\text{-}2)$$

Where:

- I = output current (ampere)
- I_L = photo generated current (ampere)
- I_D = diode current (ampere)
- I_{SH} = shunt current (ampere).

The current through these elements is governed by the voltage across them:

$$V_j = V + IR_S \qquad (2\text{-}3)$$

Where:

- V_j = voltage across both diode and resistor R_{SH} (volt)

- V = voltage across the output terminals (volt)
- I = output current (ampere)
- R_S = series resistance (Ω).

By the Shockley diode equation, the current diverted through the diode is:

$$I_D = I_0 \left\{ \exp\left[\frac{qV_j}{nkT}\right] - 1 \right\} \text{[6]} \qquad (2\text{-}4)$$

Where:

- I_0 = reverse saturation current (ampere)
- n = diode ideality factor (1 for an ideal diode)
- q = elementary charge
- k = Boltzmann's constant
- T = absolute temperature
- At 25°C, $kT/q \approx 0.0259$ volt.

By Ohm's law, the current diverted through the shunt resistor is:

$$I_{SH} = \frac{V_j}{R_{SH}} \qquad (2\text{-}5)$$

Where:

- R_{SH} = shunt resistance (Ω).

Substituting these into the first equation produces the characteristic equation of a solar cell, which relates solar cell parameters to the output current and voltage:

$$I = I_L - I_0 \left\{ \exp\left[\frac{q(V + IR_S)}{nkT}\right] - 1 \right\} - \frac{V + IR_S}{R_{SH}}. \qquad (2\text{-}6)$$

An alternative derivation produces an equation similar in appearance .The two alternatives are identities; that is, they yield precisely the same results.

In principle, given a particular operating voltage *V* the equation may be solved to determine the operating current *I* at that voltage.

Since the parameters I_0, n, R_S, and R_{SH} cannot be measured directly, the most common application of the characteristic equation is nonlinear to extract the values of these parameters on the basis of their combined effect on solar cell behavior.

2-6 Open-circuit voltage and short-circuit current

When the cell is operated at open circuit, $I = 0$ and the voltage across the output terminals is defined as the *open-circuit voltage*. Assuming the shunt resistance is high enough to neglect the final term of the characteristic equation, the open-circuit voltage V_{OC} is:

$$V_{OC} \approx \frac{nkT}{q} \ln\left(\frac{I_L}{I_0} + 1\right). \qquad (2\text{-}7)$$

Similarly, when the cell is operated at short circuit, $V = 0$ and the current through the terminals is defined as the *short-circuit current*. It can be shown that for a high-quality solar cell (low R_S and I_0, and high R_{SH}). The short circuit current I_{SC} is:

$$I_{SC} \approx I_L. \qquad (2\text{-}8)$$

It should be noted that it is not possible to extract any power from the device when operating at either open circuit or short circuit conditions.

Solar cell efficiency

Solar cell efficiency is the ratio of the electrical output of a solar cell to the incident energy in the form of sunlight. The energy conversion efficiency (η) of a solar cell is the percentage of the solar energy to which the cell is exposed that is converted into electrical energy.[10]

$$\eta = \frac{P_m}{E \times A_c} \qquad (2\text{-}9)$$

2-7 Maximum power point

A solar cell may operate over a wide range of voltages (V) and currents (I). By increasing the resistive load on an irradiated cell continuously from zero (a *short circuit*) to a very high value (an *open circuit*) one can determine the maximum power point, the point that maximizes V×I; that is, the load for which the cell can deliver maximum electrical power at that level of irradiation. (The output power is zero in both the short circuit and open circuit extremes). [11]

2-8 Fill factor

Another defining term in the overall behavior of a solar cell is the *fill factor* (*FF*). This is the available *power* at the *maximum power point* (P_m) divided by the *open circuit voltage* (V_{OC}) and the *short circuit current* (I_{SC}):

$$FF = \frac{P_m}{V_{OC} \times I_{SC}} = \frac{\eta \times A_c \times E}{V_{OC} \times I_{SC}}. \qquad (2\text{-}10)$$

The fill factor is directly affected by the values of the cell's series and shunt resistances. Increasing the shunt resistance (R_{sh}) and decreasing the series resistance (R_s) lead to a higher fill factor, thus resulting in greater efficiency, and bringing the cell's output power closer to its theoretical maximum.[12]

Chapter three

Spectrum of Solar Radiation

3-1 Introduction:

The sun light spectrum consists of a wide range of law frequency, visible light and high frequency radiation. To increase solar cell efficiency it is important to see how can one gets the utmost penfit of this wide frequency range. All these topic are exhibited in this chapter.

3-2 Sunlight:

Sunlight is a portion of the Electromagnetic radiation given off by the Sun, in particular infrared visible and ultraviolet light. On Earth, sunlight is filtered through the Earth’s atmosphere, and is obvious as daylight when the Sun is above the horizon. When the direct solar radiation is not blocked by clouds, it is experienced as **sunshine**, a combination of bright light and radiant heat. When it is blocked by the clouds or reflected off other objects it is experienced as diffused light. The World Metrological Organization uses the term "sunshine duration" to mean the cumulative time during which an area receives direct irradiance from the Sun of at least 120 watts per square.[1]

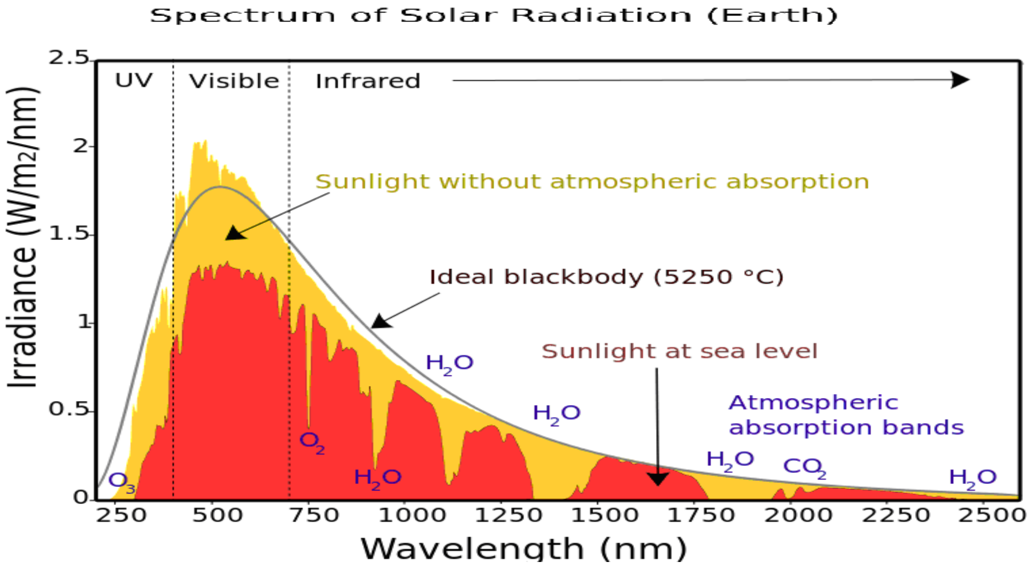


Figure (3-1): Spectrum of the solar radiation

Our eyes are sensitive to light which lies in a very small region of the electromagnetic spectrum labeled "visible light". This "visible light" corresponds to a wavelength range of 400 - 700 nanometers (nm) and a color range of violet through red. The human eye is not capable of "seeing" radiation with wavelengths outside the visible spectrum. The visible colors from shortest to longest wavelength are: violet, blue, green, yellow, orange, and red. Ultraviolet radiation has a shorter wavelength than the visible violet light. Infrared radiation has a longer wavelength than visible red light. The white light is a mixture of the colors of the visible spectrum. Black is a total absence of light.

Earth's most important energy source is the Sun. Sunlight consists of the entire electromagnetic spectrum.

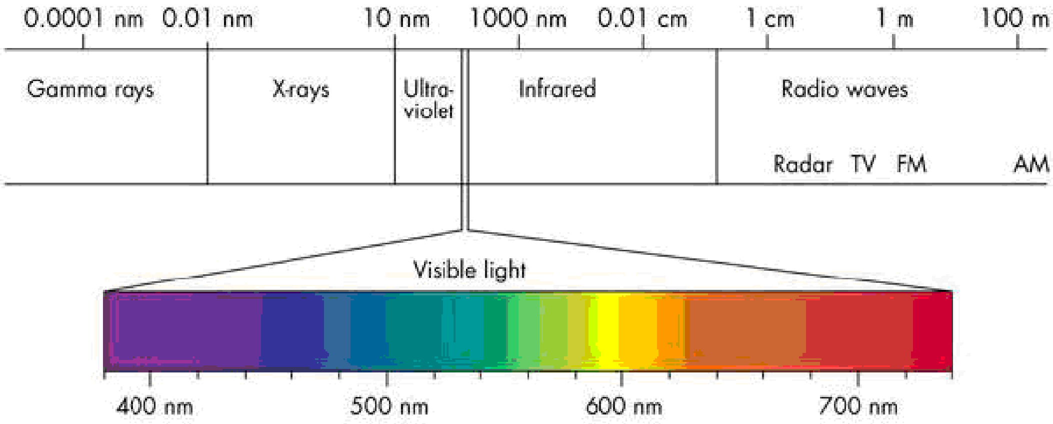


Figure (3-2): Sunlight consists of the entire electromagnetic spectrum.

3-3 Solar cell concepts

In a conventional solar cell, light is absorbed by a semiconductor, producing an electron-hole (e-h) pair; the pair may be bound and is referred to as an Exciton. This pair is separated by an internal electric field (present in p-n junctions or Schottky diodes) and the resulting flow of electrons and holes creates electric current. The internal electric field is created by doping one part of semiconductor interface with atoms that act as electron donors (n-type doping) and another with electron acceptors (p-type doping) that results in a p-n junction. Generation of an e-h pair requires that the photons have energy exceeding the band gap of the material. Effectively, photons with energies lower than the band gap do not get absorbed, while those that are higher can quickly (within about 10^{-13} s) thermalize to the band edges, reducing output. The unabsorbed limitation reduces the current, while the higher energy photons thermalization reduces the voltage. As a result, semiconductor cells suffer a trade-off between voltage and current (which can be in part alleviated by using multiple junction implementations). The detailed balance calculations show that this efficiency can not exceed 31% if one uses a single material for a solar cell.[3]

3-4 Loss mechanisms

The theoretical performance of a solar cell was first studied in depth in the 1960s, and is today known as the Shckley-queisser Limit. The limit describes several loss mechanisms that are inherent to any solar cell design.

The first are the losses due to blackbody radiation, a loss mechanism that affects any material object above absolute Zero. In the case of solar cells at standard temperature and pressure, this loss accounts for about 7% of the power. The second is an effect known as "recombination", where the electrons created by the photoelectric effect meet the electron holes left behind by previous excitations. In silicon, this accounts for another 10% of the power.

However, the dominant loss mechanism is the inability of a solar cell to extract all of the power in the photon, and the associated problem that it cannot extract any power at all from certain photons. This is due to the fact that the electrons must have enough energy to overcome the band gap of the material.

If the photon has less energy than the band gap, it is not collected at all. This is a major consideration for conventional solar cells, which are not sensitive to most of the infrared spectrum, although that represents almost half of the power coming from the sun. Conversely, photons with more energy than the band gap, say blue light, initially eject an electron to a state high above the band gap, but this extra energy is lost through collisions in a process known as "relaxation". This lost energy turns into heat in the cell, which has the side-effect of further increasing blackbody losses.[13]

Combining all of these factors, the maximum efficiency for a single-band gap material, like conventional silicon cells, is about 34%. That is, 66% of the energy in the sunlight hitting the cell will be lost. Practical concerns further reduce this, notably reflection off the front surface or the metal terminals, with modern high-quality cells at about 22%.

The efficiency of a single-junction solar cell, it is essentially impossible for a single-junction solar cell, under un-concentrated sunlight, to have more than 34% efficiency according to The Shockley – Queissar Limit. A multi-junction cell, however, can exceed that limit

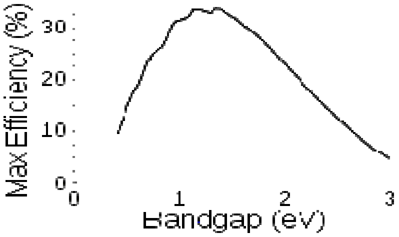


Figure (3-3): shows Queissar limit

Lower, also called narrower, band gap materials will convert longer wavelength, lower energy photons. Higher, or wider band gap materials will convert shorter wavelength, higher energy light An analysis of the AM1.5 spectrum ***(See appendix I)***, shows the best balance is reached at about 1.1 eV, in the near infrared, which happens to be very close to the natural band gap in silicon and a number of other useful semiconductors.

The maximum thermodynamic efficiency for the conversion of un-concentrated solar irradiance into Electrical energy in the radiative limit assuming detailed balance and a single threshold absorber was calculated by Shockley and Queisser in 1961 to be about 31%; Since Conversion efficiency is one of the most important parameters to optimize for implementing photovoltaic on a truly large scale, several schemes for exceeding the Shockley–Queissar limit have been proposed and are under active investigation. These approaches include tandem cells, hot carrier solar cells , solar cells producing multiple electron–hole pairs per photon through impact ionization , multi-band and impurity solar cells , and thermo photovoltaic (thermo photonic Cells). Here, we will only discuss the effects of size quantization. The solar spectrum contains photons with energies ranging from about 0.5 to 3:5 eV. Photons with energies below the semiconductor band gap are not absorbed, while those with energies above the band gap create electrons and holes with a total excess kinetic energy equal to the difference between the photon energy and the band gap. This excess kinetic energy creates an effective temperature for the carriers that is much higher than the lattice temperature; such carriers are called “hot electrons and hot holes”,

Numerical analysis shows that the 31% efficiency is achieved with a band gap of 1.3-1.4 eV, corresponding to light in the near infrared spectrum. This band gap is close to that of silicon (1.1 eV), one of the many reasons that it dominates the market. However, silicon's efficiency is limited to about 29%. It is possible to improve on a single-junction cell by vertically stacking cells with different band gaps – termed a "tandem" or "multi-junction" approach. The same analysis shows that a two layer cell should have one layer tuned to 1.64 eV and the other to 0.94 eV, providing a theoretical performance of 44%. A three-layer cell should be tuned to 1.83, 1.16 and 0.71 eV, with an efficiency of 48%. An "infinity-layer" cell would have a theoretical efficiency of 86%, with other thermodynamic loss mechanisms accounting for the rest.[4]

Most tandem-cell structures are based on higher performance semiconductors, notably indium gallium arsenide (InGaAs). Three-layer InGaAs/GaAs/InGaP cells (band gaps 1.89/1.42/0.94 eV) hold the efficiency record of 42.3% for experimental examples.[14]

Traditional (crystalline) silicon preparation methods do not lend themselves to this approach due to lack of band gap tunability. Thin-films of amorphous silicon, which due to a relaxed requirement in crystal momentum preservation can achieve direct band gaps and intermixing of carbon, can tune the band gap, but other issues have prevented these from matching the performance of traditional cells.[2]

The solution to this is by reducing the size of the crystal to few atoms to the size of a dot then to quantum dot .Behavior is different when low energy photon falls, an electron will be excited, the void of the electron acts like positive charge, and hops across the lattice and the hole gets attracted and unite like an atom lowering the energy, and the energy is not wasted. The smaller the quantum dot gets, changing the size which leads to changing the band gap. The smaller the quantum dots the larger the band gap, by tuning the band gap the whole solar spectrum produce electron in the conduction band.

3-5 Quantum dots

Quantum dots are semiconductor particles that have been reduced below the size of the Exciton Bohr radius and due to quantization considerations, the electron energies that can exist within them become finite, much alike energies in an atom. Quantum dots have been referred to as "artificial atoms". These energy levels can be tuned by changing their size, which in turn defines the band gap. The dots can be grown over a range of sizes, allowing them to express a variety of band gaps without changing the underlying material or construction techniques.[15]

In typical wet chemistry preparations, the tuning is accomplished by varying the synthesis duration or temperature. The ability to tune the band gap makes quantum dots desirable for solar cells. Single junction implementations using lead sulfide (PbS) QDs have band gaps that can be tuned into the far infrared, frequencies that are typically difficult to achieve with traditional.

Half of the solar energy reaching the Earth is in the infrared, most in the near infrared region. A quantum dot solar cell makes infrared energy as accessible as any other.[16]

Moreover, QDs offer easy synthesis and preparation. While suspended in a colloidal liquid form they can be easily handled throughout production, with fume hood as the most complex equipment needed. QDs are typically synthesized in small batches, but can be mass-produced. The dots can be distributed on a substrate by spin coating, either by hand or in an automated process. Large-scale production could use spray-on or roll-printing systems, dramatically reducing module construction costs.

It is quite important the next chapter will be devoted to quantum dots to talk about what are the quantum dots, how they can be used to impact the energy band scale, how the quantum dots can be used in solar energy conversion of solar cells to electricity, and how this technology can be used in solar energy conversion hope to take away what is required from these information to build a mathematical model of quantum dots solar cells.

Chapter four

Quantum dots

4-1 Introduction:

Quantum dots were discovered in solids (glass crystals) in 1980 by Russian physicist Alexei Ekimov, while working at the Vavilov State Optical Institute. In late 1982, American chemist Louis E.Brus, then working at Bell Laboratories (and now a professor at Columbia University), discovered the same phenomenon in colloidal solutions, colloidal is small particle in liquid (where small particles of one substance are dispersed throughout another). He discovered that the wavelength of light emitted or absorbed by a quantum dot changed over a period of days as the crystal grew, and concluded that the confinement of electrons was giving the particle quantum properties, that is to say the band gap experimentally is a function of size

American chemist Louis E.Brus started with a solvent to create a reaction that grows particles in liquids by injecting a reagent to nucleate and grow a solid phase, as the reaction goes on big particles germinate and fall at the bottom of the beaker. For the purpose to study very small quantum dots he stopped the reaction as quickly as he could at the point of nucleation where there might be hundred or thousand particles of atoms ,then he studied it ,he observed the band gap is basically related to the diameter , the smaller the particle the higher the energy of the band gap. Very small semiconductor particles absorb light in **blue**, intermediate in green and larger ones in red. This quantum dots mechanical effect shift the threshold all the way across the visible light from red to the green to the blue to the ultra violet.

Therefore Quantum dots are crystals a few nanometers wide, so they're typically a few dozen atoms across and contain anything from perhaps a hundred to a few thousand atoms. They're made from a semiconductor such as silicon, but can be chemically treated so it behaves like either). And although they're crystals, they behave more like individual atoms, hence the nickname artificial atoms.

Quantum dots are precise crystals, so you make them in much the same way you'd make any other precise semiconductors crystals. Typical methods include molecular beam epitaxy (MBE, in which beams of atoms are fired at a "base" or substrate so a single crystal slowly builds) ion implementation (where ions are accelerated electrically and fired at a substrate), and X-ray lithography (a kind of atomic-scale engraving process using x rays). ***(See appendix II)***

A quantum dot gets its name because it's a tiny speck of matter so small that it's effectively concentrated into a single point (in other words, it's zero-dimensional). As a result, the particles inside it that carry electricity (electrons and holes) are trapped ("constrained") and have well-defined energy levels according to the laws of quantum theory.

So far, quantum dots have attracted most interest, because of their interesting optical properties; they're being used for all sorts of applications. In this thesis an application to photovoltaic is investigated to create an (electron–hole) pair, but they should be separated, the electron has to jump off the particle and the hole has jump off the particle to go in the other direction, as a result current will flow in an external circuit.

Still quantum dots are being hailed as a breakthrough technology in the development of more efficient solar cells. In a traditional solar cell, photons of sunlight knock electrons out of a semiconductor into a circuit, making useful electric power, but the efficiency of the process is quite low. Quantum dots produce more electrons (or holes) for each photon that strikes them, potentially offering a boost in efficiency of perhaps 10 percent over conventional semiconductors.

4-2 Definition of quantum dots:

From the above mentioned information, a quantum dot can be defined as a semiconductor nano particle whose diameter is than twice the Bhor radius of Exciton in bulk material. They are very small and they have special properties according to their size .Quantum dots absorb light and converted it into different colors after being illuminated by light, hence boost electrons into conduction bands to produce electricity that flows to the positive terminal. An addition or removal of electrons changes its properties in some useful way, all atoms of course are quantum dots, but multi molecular combinations can also have these characteristics.

4-3 How do quantum dots work?

Quantum dots typically measured in nanometers (10^{-9}m), when they are illuminated by ultra violet light or any high frequency some electrons receive enough energy to break free from bonds of their atoms .This capability allow them to move around the nano-particles creating the conduction band in which electrons are free to move through the material and conduction of electricity will take place.

4-4 Quantum dots confinements:

Quantum dot has the property to confine their excited electrons (or Exciton) in all three spatial dimensions .When this Exciton drop back to its orbit around the atom to valance band , emits light with the same energy that the atom originally absorbed. The color (wavelength and frequency) of light an atom emits depends on what the atom is, or on the energy difference between conduction band and the valance band .The smaller the nano-particle the higher the energy difference between conduction band and the valance band, this resolve in deeper blue color .For larger particles the energy is lower which shift this glow to red part of the spectrum. Many semiconductors substances have been used for these quantum dots. Common quantum dots materials include Cdse, Cds, CaTe, PbSe, & PbS. Nano-particles of any semiconductor substance have the properties of the quantum dots. The gap between the valance band and the conduction band which present in semiconductors causes quantum dots to fill the rest.

Because quantum dots have a tendency to stick together if they get too near each other and when they do this, they lose their interesting and useful characteristics. To stop this happening, molecules are attached to the surface so the dots can no longer get as close.

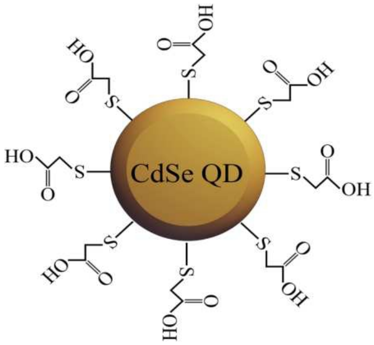


Figure (4-1):Shows CdSe Quantum dots

However, the presence of the molecules changes the energy levels of the quantum dot and it is hard to find out how. When quantum dots are used in solar cells, this may lead to the cell not working or not being very efficient. Gabriela Kissling at the University of Bristol is finding out exactly how the energy levels change when molecules are added to help other researchers build better solar cells.

4-5 Quantum dots nano crystal structure:

In the following figure there is a Transmission Electron Microscope image (TEM) of a series of quantum dots, resumed by one of them intentionally 5nm in diameter with lattice fringes associated with this material , therefore quantum dots can penetrate to each other and always there is a distance between them

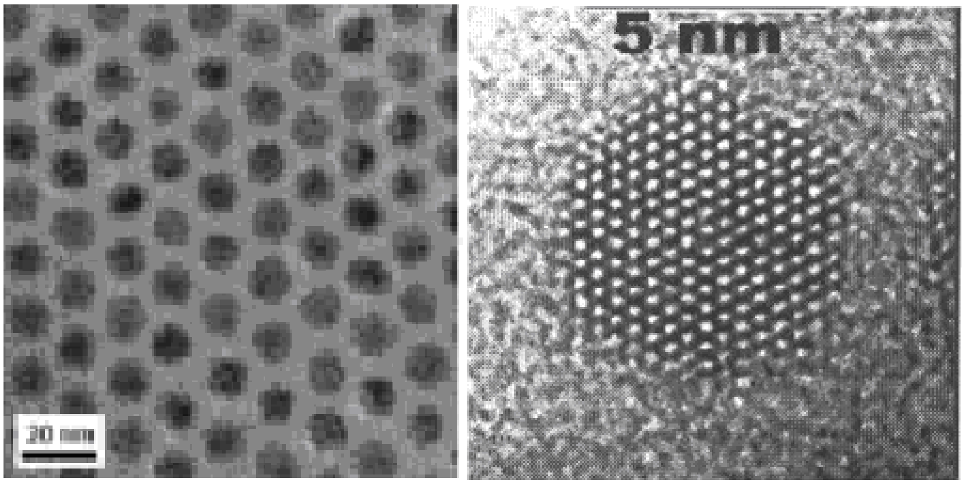


Figure (4-2): series of quantum dots, resumed by one of them intentionally 5nm in diameter with lattice fringes associated with this material.

Quantum dots have regular structures, each one of them has roughly the same shape, roughly the same size .In between them there are spaces, and these spaces are not pure vacuum, and actually they are organic ligand attached to the molecules.

These ligand allow the nano particle to be in stable suspension on the solution so they can be synthesized in a form of ink .ligand are almost carbon.

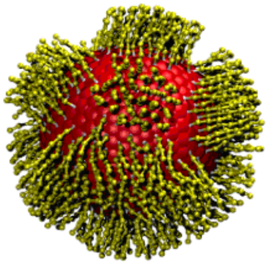


Figure (4-3): Shows quantum dot after attached to the molecules

4-6 Creating Energy from the sun light:

When quantum dots are used in solar cells, this may lead to cells not working or not being very efficient, therefore we should have to find out exactly how the energy level changes when the molecules are added. Our aim is to make solar cells more efficient by capturing the sun light and turn it to electricity; quantum dots are tiny particles to capture the sun light. If happen to be there are more than one quantum dot in the system, as have been mentioned before they can stick together, hence they loose their properties, to avoid that addition of molecules to the surface will not allow them to sit together any more, but they can come close enough .Unfortunately the molecules take some energy levels in the quantum dots. It is very important to show why this happen. In the following energy diagram, quantum dots are represented:

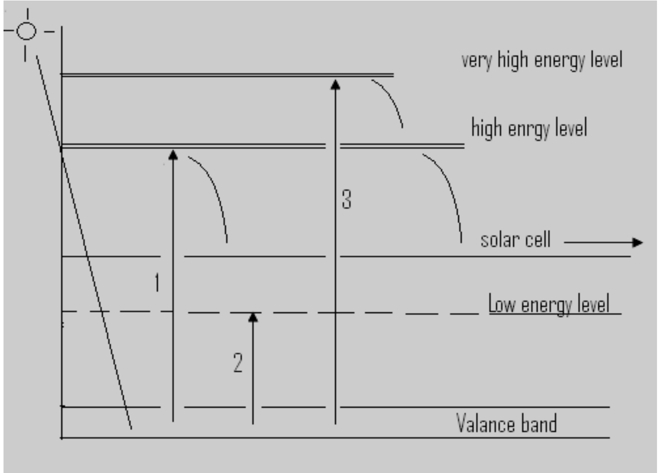


Figure (4-4): Energy diagram quantum dot

Sun shine the light ,hits the quantum dot electrons in the valance band ,an electron will be excited up to the higher energy level ,it reaches the solar cell by following energy levels in the solar cell like stair case ,then gets energy to broadcast for something else.

If the energy level tuned to the dotted line level by shrinking the gap, the electron doesn’t reach the surface of the cell and gives no power.

Molecules can move the energy band to a very high level. The electron at high energy band gap can have higher energy to reach the solar surface; to reach the surface it should loose energy.

Gabriela Kissling at the University of Bristol is trying to find out where exactly quantum dot molecules move the energy level in a big crystal to, and help as well with staircase higher or lower down. She is going to have the measure of energy level in a big crystal without any molecules to the surface present, then attach molecules to the surface & measure the energy level again to find out the difference, this information with other information will help the researchers to make the solar cell more efficient.

One of our aims in this thesis is the study of how quantum dots absorb sun light, & what energy gap will be selected for this purpose. Laurie King at Imperial College London in her PHD research in quantum dots presented special nano crystals, under the title: quantum dots absorb UV light and emit the energy as visible light in the form of a colour. The colour depends on the size of the quantum dot. Smaller dots are green and larger dots are red. Quantum dots can be used in solar cells as they absorb light from the sun and can also emit the energy as electrical energy.

In conclusion to this chapter, the efficiency of semiconductor photovoltaic is found to be related to the energy gap, silicon is found to be the most ideal to energy gap, therefore in the next chapter energy bands are disused

Chapter five

Energy Bands

5-1 Introduction:

In last chapter, the basics of what quantum dots are described. In particular, the unique properties of quantum dot materials are examined, and how these properties can be exploited by scientists and engineers to yield low-cost, light-weight solar modules capable of converting sunlight into electricity in a direct fashion. Additionally, the basics of solar cell characterization and light absorption are detailed and related to the band gap of quantum dot materials. Finally, the potential impact of solar technologies on the energy landscape is being discussed.

Regular solar cell, each photon collision generates a particle pair consisting of one free hole and one free electron. Quantum Dots are extremely small "nano crystals” interspersed in a larger semi conducting material. Quantum Dots (QDs) range between 1 and 20 nanometers in size. Semiconductors at this size have different physical properties than their big brothers. When photons with energy greater than the band gap energy collide with a Quantum Dot several "hot" hole/electron pairs can be created as opposed to one pair and heat. Although silicon can be used as a nano crystal, lead selenide (PbSE) also a semiconductor, is being used more frequently as the material of choice. It is quite obvious the band gap in bulk material is fixed by the choice of the material, in quantum dots band gaps are tunable across a wide range of energy levels by changing the dot size .This property makes the quantum dots attractive for multi junction solar cells where variety of materials are used to improve the efficiency by harvesting multiple portion of solar spectrum .Therefore a quantum dot solar cell is to be designed to replace bulk materials.

Another characteristic of a Quantum Dot is that different sizes capture different wavelengths of light. Small Dots capture small wavelengths and larger dots bigger wavelengths. Some researchers have figured out how to stack the dots from small to large to capture more photon energy similar to how tandem cells do. Once a hot electron is created inside a Quantum Dot, it stretches its lifetime

5-2 Formation of an energy band:

Energy bands consisting of a large number of closely spaced energy levels exist in crystalline materials. The bands can be thought of as the collection of the individual energy levels of electrons surrounding each atom. The wave functions of the individual electrons, however, overlap with those of electrons confined to neighboring atoms. The Pauli Exclusion Principle does not allow the electron energy levels to be the same so that one obtains a set of closely spaced energy levels, forming an energy band. The energy band model is crucial to any detailed treatment of semiconductor devices. It provides the framework needed to understand the concept of an energy band gap and that of conduction in an almost filled band as described by the empty states.

In this section, we present the free electron model and the Kronig-Penney model. Then we discuss the energy bands of semiconductors and present a simplified band diagram.

To discuss this important phenomena , in case of , energy band diagram in solids lattice structures, that is, the energy bands, how the energy bands are formed ,it is an important concept to understand ,for this, we can take a hydrogen atom as our model to see in a single atom how electron can occupy energy levels ,then in the case of solids an electron of one atom is also in the influence of other atoms in the surrounding ,due to this ,energy levels are modified

5-3 The Hydrogen Atom

The study of the hydrogen atom is more complicated than an electron confined to move on a line. Not only does the motion of the electron occur in three dimensions but there is also force acting on the electron. This force, the electrostatic force of attraction, is responsible for holding the atom together. The magnitude of this force is given by the product of the nuclear and electronic charges divided by the square of the distance between them. If an electron confined to move on a line, the total energy was entirely kinetic in origin since there were no forces acting on the electron. In the hydrogen atom however, the energy of the electron, because of the force exerted on it by the nucleus, will consist of a potential energy (one which depends on the position of the electron relative to the nucleus) as well as a kinetic energy. The potential energy arising from the force of attraction between the nucleus and the electron is:

$$PE = -e^2/r \qquad (5\text{-}1)$$

Let us imagine for the moment that the proton and the electron behave classically. Then, if the nucleus is held fixed at the origin and the electron allowed moving relative to it, the potential energy would vary in the manner indicated in Fig 5-1. The potential energy is independent of the direction in space and depends only on the distance *r* between the electron and the nucleus. Thus Fig. 5-1 refers to any line directed from the nucleus to the electron. The *r*-axis in the figure may be taken literally as a line through the nucleus. Whether the electron moves to the right or to the left the potential energy varies in the same manner.

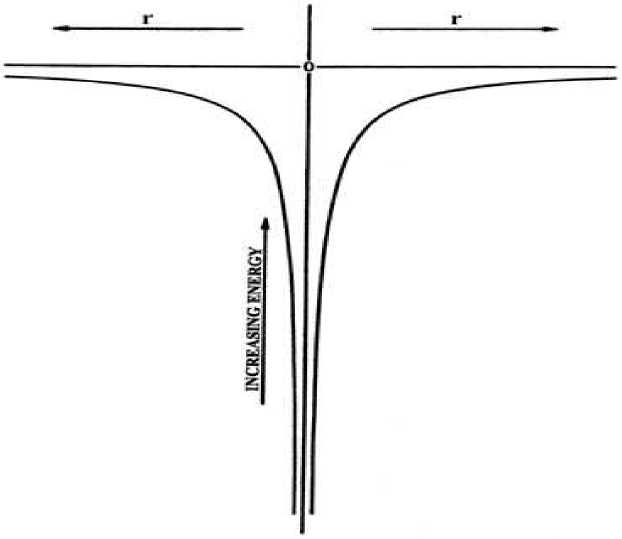


Figure (5-1): The potential energy of interaction, as a function of the distance *r* between a nucleus (at the origin) and an electron

The potential energy is zero when the two particles are very far apart ($r = \infty$), and equals minus infinity when *r* equals zero. We shall take the energy for $r = \infty$ as our zero of energy. Energy at any value of r will be measured relative to its value. When a stable atom is formed, the electron is attracted to the nucleus, *r* is less than infinity, and the energy will be negative. A negative value for the energy implies that energy must be supplied to the system if the electron is to overcome the attractive force of the nucleus and escape from the atom. The electron has again "fallen into a potential well." However, the shape of the well is no longer a simple square one as previously considered for an electron confined to move on a line, but has the shape shown in Fig. 5-1. This shape is a consequence of there being a force acting on the electron and hence a potential energy contribution which depends on the distance between the two particles (An electron and a proton). This is the nature of the problem

5-4 Energy band diagram of two closely spaced atoms:

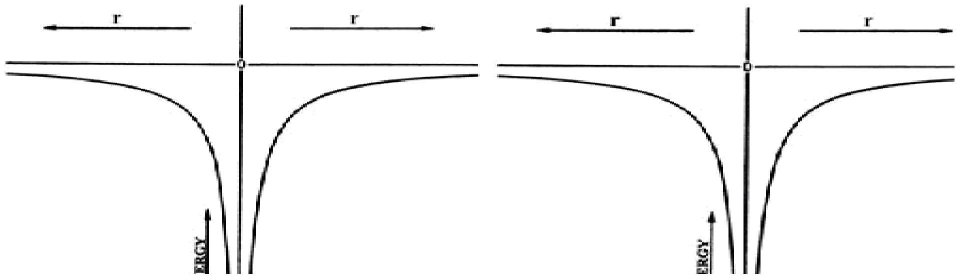


Figure (5-2): Energy band diagram of two closely spaced atoms

We would like to discuss the energy band diagram of two closely spaced atoms , there are two energy band diagrams for two different atoms which are closely spaced .in this situation the separation between the two atoms is so large ,that the energy of ,one electron in one atom, is not affected by the other. Both of these curves are rectangular hyperbola, because these are almost in the influence of their individual nuclei which are located at the centre, y-axis represents the potential. When these atoms are getting close together after the separation decreases below specific value, overlapping of orbital between the two atoms starts to take place.

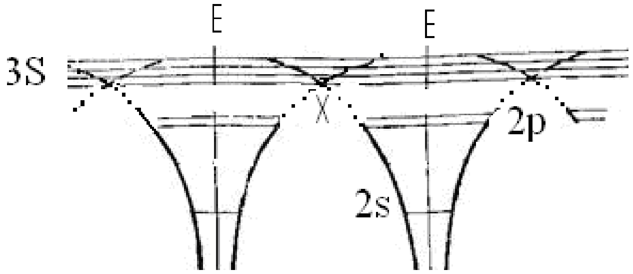


Figure (5-3): Energy band diagram when these atoms are getting close together

As separation decreases overlapping increases till we reach a situation where the 3S orbital overlap, the zones 2p ,2s remain under the influence of their individual nuclei

In this situation the electron in the 3S orbital or in any orbital above , is free to move in the whole combined 3S orbital (called molecular orbital), the other electrons in 2p, 2s remains moving under the influence of their nuclei of their individual atoms, and they are not allowed to move in the atom zone. At the point x ,potential energies of both atoms are equal and it lies in midway between the two, electrons above are free ,those below are bounded. If we continue to bring them more closer an electron cloud is formed .some of them are associated with their individual atoms others in the outer zone start getting to overlap ie 3S and above .

Because of the **Pauli Exclusion Principle**, which states that; no two fermions can have the exact same set of quantum numbers. For this reason only two electrons can occupy each electron energy level – one electron can have spin up and the other can have spin down, so that they have different spin quantum numbers, even though the electrons have the same energy. So intersection between two states at point X will not be allowed.

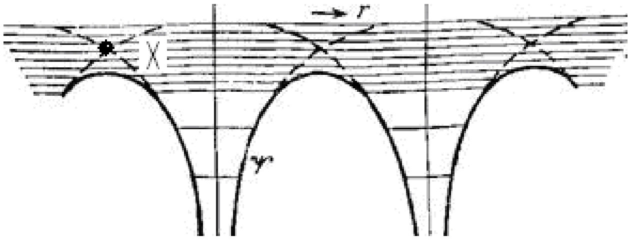


Figure (5-4): Energy band diagram when these atoms are getting close together without point x

In quantum statistics, **Fermi–Dirac statistics** describes a distribution of particles over energy states in systems consisting of many identical particles that obey the Pauli Exclusion Principle. Fermi–Dirac (F–D) statistics applies to identical particles with half-integer spin in a system

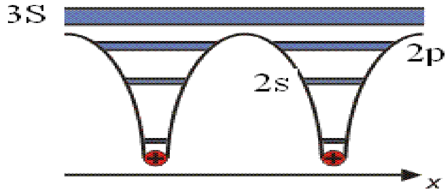


Figure (5-5): The Energy band diagram when these atoms are getting close together without point x

These constraints on the behavior of a system of many fermions can be treated statistically. The result is that electrons will be distributed into the available energy levels according to the Fermi Dirac Distribution:

$$f(\varepsilon) = \frac{1}{\exp\left(\frac{(E-\mu)}{k_B T}\right)+1} \qquad (5\text{-}2)$$

Where f (ε) is the occupation probability of a state of energy ε, k_B is Boltzmann's constant, μ is the chemical potential, and T is the temperature in Kelvin.

At absolute zero the value of the chemical potential, μ, is defined as the Fermi energy. At room temperature the chemical potential for metals is virtually the same as the Fermi energy – typically the difference is only of the order of 0.01%.

In order to understand the behavior of electrons at finite temperature qualitatively in metals and pure un-doped semiconductors, it is clearly sufficient to treat μ as a constant to a first approximation. With this approximation, the Fermi-Dirac distribution can be plotted at several different temperatures. In the figure below, μ was set at 5 eV.

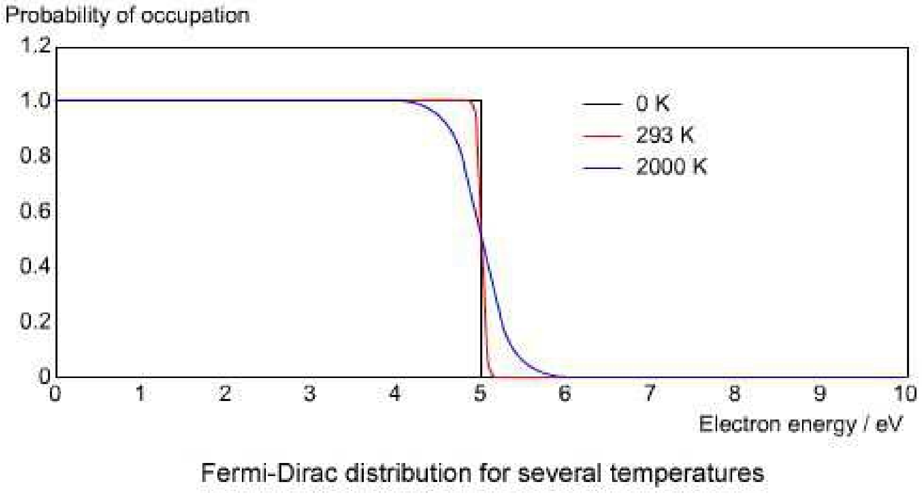


Figure (5-6): Fermi distribution for several temperatures

From this figure it is clear that at absolute zero the distribution is a step function. It has the value of 1 for energies below the Fermi energy, and a value of 0 for energies above. For finite temperatures the distribution gets smeared out, as some electrons begin to be thermally excited to energy levels above the chemical potential, μ. The figure shows that at room temperature the distribution function is still not very far from being a step function.

In solids atoms are arranged in a fixed lattice structure, all electrons in the overlapping region or orbital in the lattice structure are free to move in the whole lattice and they are called free electrons and those below are called bounded electrons.

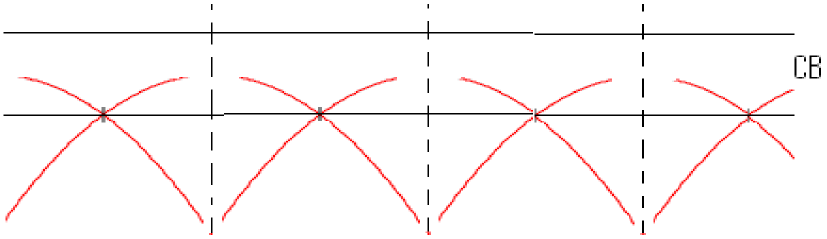


Figure (5-7): Energy band diagrams

We are trying to figure out why we get that band diagram in semi conductor, we have a set of energy levels which have a continuous density of states. Also we have a forbidden region E_g where we have no carriers there, called the band gap .we can use some quantum mechanics in particular to formalize a model to explain where the band structure comes from. Start from De Broglie equation for any particle that can be described as wave as well as a particle;

$$p = \frac{h}{\lambda} \qquad (5\text{-}3)$$

The equations can also be written as;

$$\mathbf{p} = \hbar\mathbf{k} \qquad (5\text{-}4)$$

For a free particle Energy is all kinetic;

$$E = \frac{p^2}{2m} = \frac{\hbar^2 \mathbf{k}^2}{2m} \qquad (5\text{-}5)$$

$$\frac{\hbar^2}{2m} = \text{constant} \qquad (5\text{-}6)$$

Therefore parabolic relationship between E & K

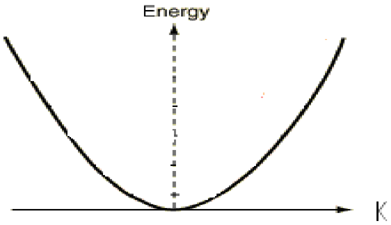


Figure (5-8): relationship between E & K of electron

Energy, $E_h = -E_e$: The electron previously in the valence band had an energy *Ee* so removing it leaves a hole with energy *–Ee (energy loss of an atom).*So the hole has the opposite momentum and energy to the electron that was previously there.

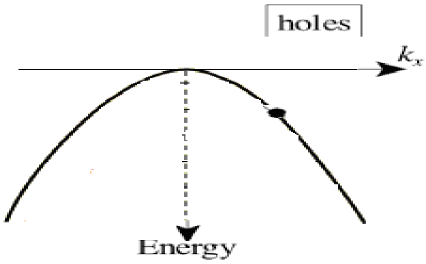


Figure (5-9): relationship between E & K of hole

5-5 Kronig-Penney Model

We are interested in the potential seen in the lattice arranged in a periodic manner, each atom looks to have infinitely large negative potential near the nuclei periodic set of atoms.

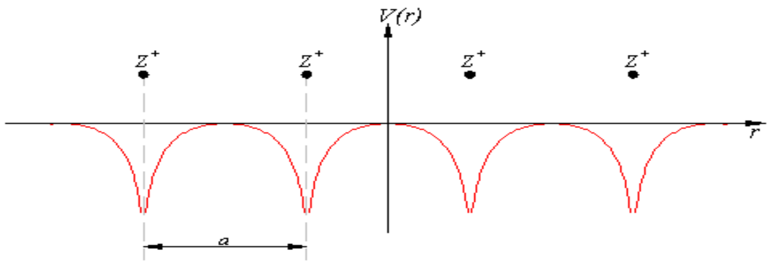


Figure (5-10): Kronig-Penney Model

The Kronig-Penney model [1] is a simplified model for an electron in a one-dimensional periodic potential. He treated potential as a series of steps (series of potential wells)

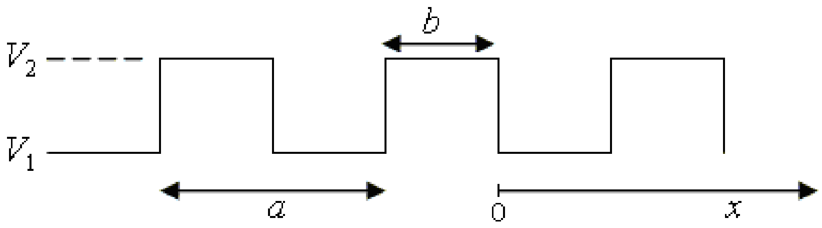
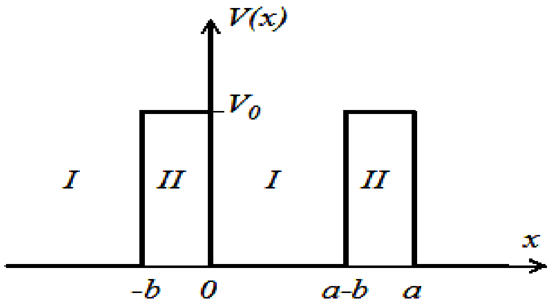


Figure (5-11): Kronig-Penney Model

Then he made an approximation to treat it as a set of delta functions. This is an instructive tool to demonstrate how the band structure can be calculated for a period potential, and how allowed and forbidden energies are obtained when solving the corresponding Schrödinger equation. The potential assumed in the model is shown in the following figure;



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Figure(5-12) The periodic potential assumed in the Kronig-Penney model. The potential barriers (region II) with width, *b*, are spaced by a distance (region I), *a-b*, and repeated with a period, *a*.

The Kronig-Penney consists of an infinite series of rectangular barriers with potential height, V_0, and width, *b*, separated by a distance, *a-b*, resulting in a periodic potential with period, *a*. The analysis requires the use of Bloch functions, traveling wave solutions multiplied with a periodic function, which has the same periodicity as the potential.

$$u(x+a)=u(x) \qquad (5\text{-}7)$$

The solution to Schrödinger's equation for the Kronig-Penney potential is obtained by assuming that the solution is a Bloch function, namely a traveling wave solution of the form, e^{ikx}, multiplied with a periodic solution, *u(x)*, which has the same periodicity as the periodic potential.

The total wave function is therefore of the form:

$$\Psi(x)=u(x)e^{ikx} \qquad (5\text{-}8)$$

where *u(x)* is the periodic function as defined by *u(x)* = *u(x + a)*, and *k(x)* is the wave number.

Rewrite Schrödinger equation using this wave function considering first region I, between the barriers where *V(x)* = 0 and then region II, the barrier region where $V(x) = V_0$:

In region I, Schrödinger's equation becomes:

$$\frac{d^2u_I(x)}{dx^2}+2ik\frac{du_I(x)}{dx}+(\beta^2-k^2)u_I(x)=0 \text{ for } 0<x<a\text{-}b \qquad (5\text{-}9)$$

With

$$\beta=\frac{\sqrt{2mE}}{\hbar} \qquad (5\text{-}10)$$

While in region II, it becomes:

$$\frac{d^2u_{II}(x)}{dx^2}+2ik\frac{du_{II}(x)}{dx}-(k^2+\alpha^2)u_{II}(x)=0 \text{ for } a\text{-}b<x<a \qquad (5\text{-}11)$$

With

$$\alpha=\frac{\sqrt{2m(V_0-E)}}{\hbar} \qquad (5\text{-}12)$$

A virtue of this model is that it is possible analytically determine the Energy Eigen values and Eigen functions. It is also possible to find analytic expressions for the dispersion relations (*E* vs. *k*) and the electron density of states. Derivations are given in appendix)

The possible states that the electron can occupy are determined by the Schrödinger equation,

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi=E\psi. \qquad (5\text{-}13)$$

In the case of the Kronig-Penney model, the potential *V*(*x*) is a periodic square wave.

From the appendix it can be seen that the Solutions for *k* and *E* are obtained when the following equation is satisfied:

$$\cos ka=F=\frac{\alpha^2-\beta^2}{2\alpha\beta}\sinh \alpha b\sin \beta(a-b)+\cosh \alpha b\cos \beta(a-b) \qquad (5\text{-}14)$$

Where

$$\alpha=\frac{\sqrt{2m(V_0-E)}}{\hbar} \text{ and } \beta=\frac{\sqrt{2mE}}{\hbar} \qquad (5\text{-}15)$$

This transcendental equation can be further simplified for the case where the barrier is a delta function

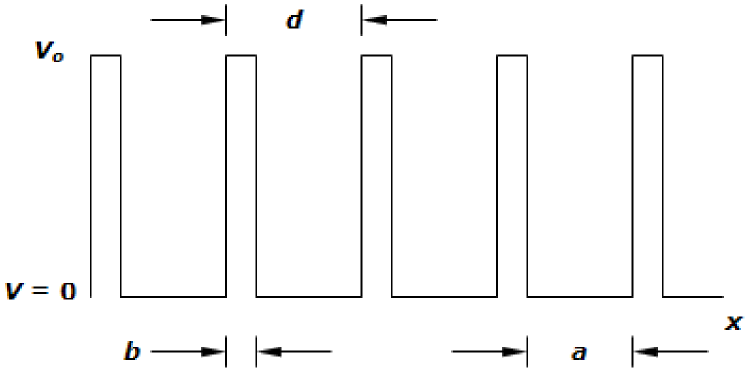


Figure (5-13):Kronig penny model, the optional barriers b very small, and higher V very large, with area, $V_0 b$,

F Bloch in 1928 proposed the trial wave function for the solution as

$$\psi(x) = u_k(x)e^{-ikx}. \qquad (5\text{-}16)$$

he dispersion model for Kronig-Penny model can be simplified if the potential arriers are assumed to be delta functions. This relation takes the form

$$\cos ka = F = P\frac{\sin \beta a}{\beta a} + \cos \beta a \qquad (5\text{-}17)$$

With

$$\beta = \frac{\sqrt{2mE}}{\hbar} \text{ and } P = \frac{mV_0 ba}{\hbar^2} \qquad (5\text{-}18)$$

K is the wave number of the electron, b is the width of original potential well of depth V0 and a spacing between potential wells.

This is a plane wave solution with a modulating function. The modulating function will have the lattice periodicity.

$$u_k(x + L) = u_k(x) \qquad (5\text{-}19)$$

plotting the left-hand-side of the equation given in the question against (Ka) will result in this graph:

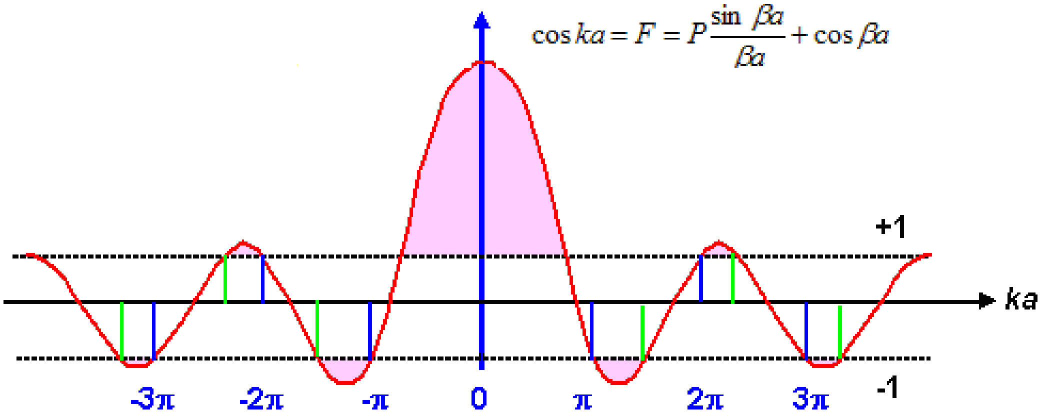
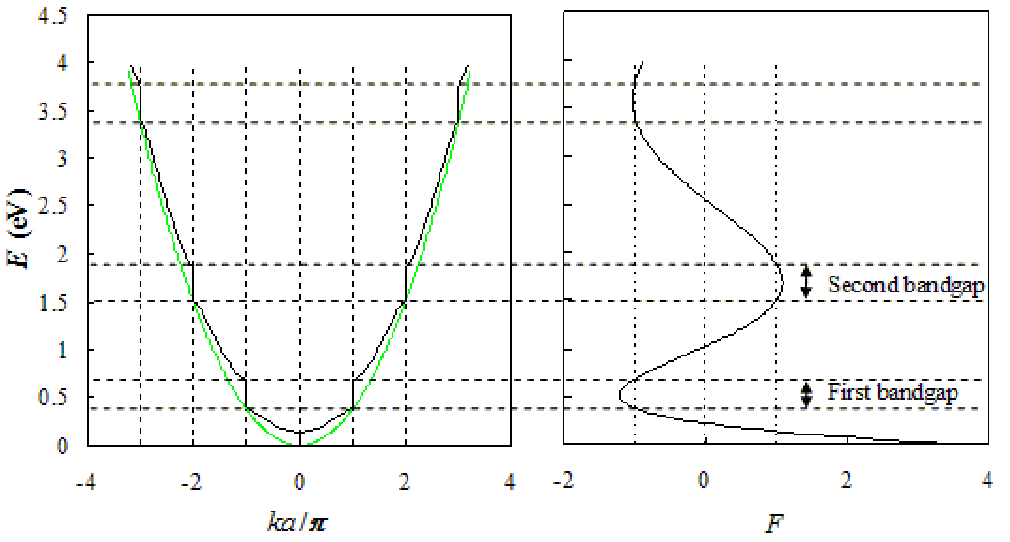


Figure (5-14): The emergence of energy bands and forbidden gaps in the spectrum of electron energies in a periodic crystal.

A intuitive picture of how these bands arise is clear if we note that :

This equation can only be solved numerically. Solutions are only obtained if the function, *F*, is between -1 and 1 since it has to equal cos (*ka*). The energy, *E*, is plotted as function of *ka*/□ and the function *F* in the following Figure



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Figure(4-15) : Graphical solution to the Kronig-Penney model for a = 1nm and V_0b = 0.2 nm-eV. Shown is the energy, E, versus ka/π and F, which has to equal cos (ka), from which one can identify the allowed energies.

The corresponding band structure is shown below (black curve) as well as the energy for a free electron (gray curve). Three different forms are presented, namely the $E(k)$ diagram, the $E(k$ diagram combined with the reduced-zone diagram as well as the reduced-zone diagram only.

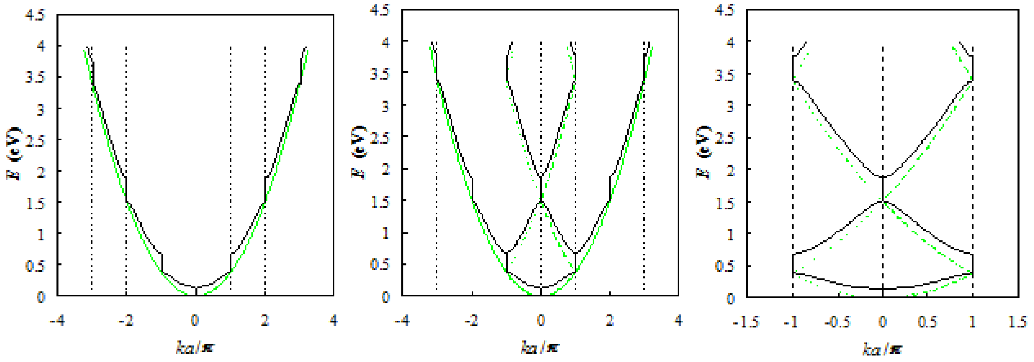

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Figure (5-16).: Energy versus ka/π as presented in Figure (4-16) (black curves) compared to that of a free electron (gray curves). Shown are: a) the $E(k)$ diagram, b) the $E(k)$ diagram combined with the reduced-zone diagram and c) the reduced-zone diagram only.

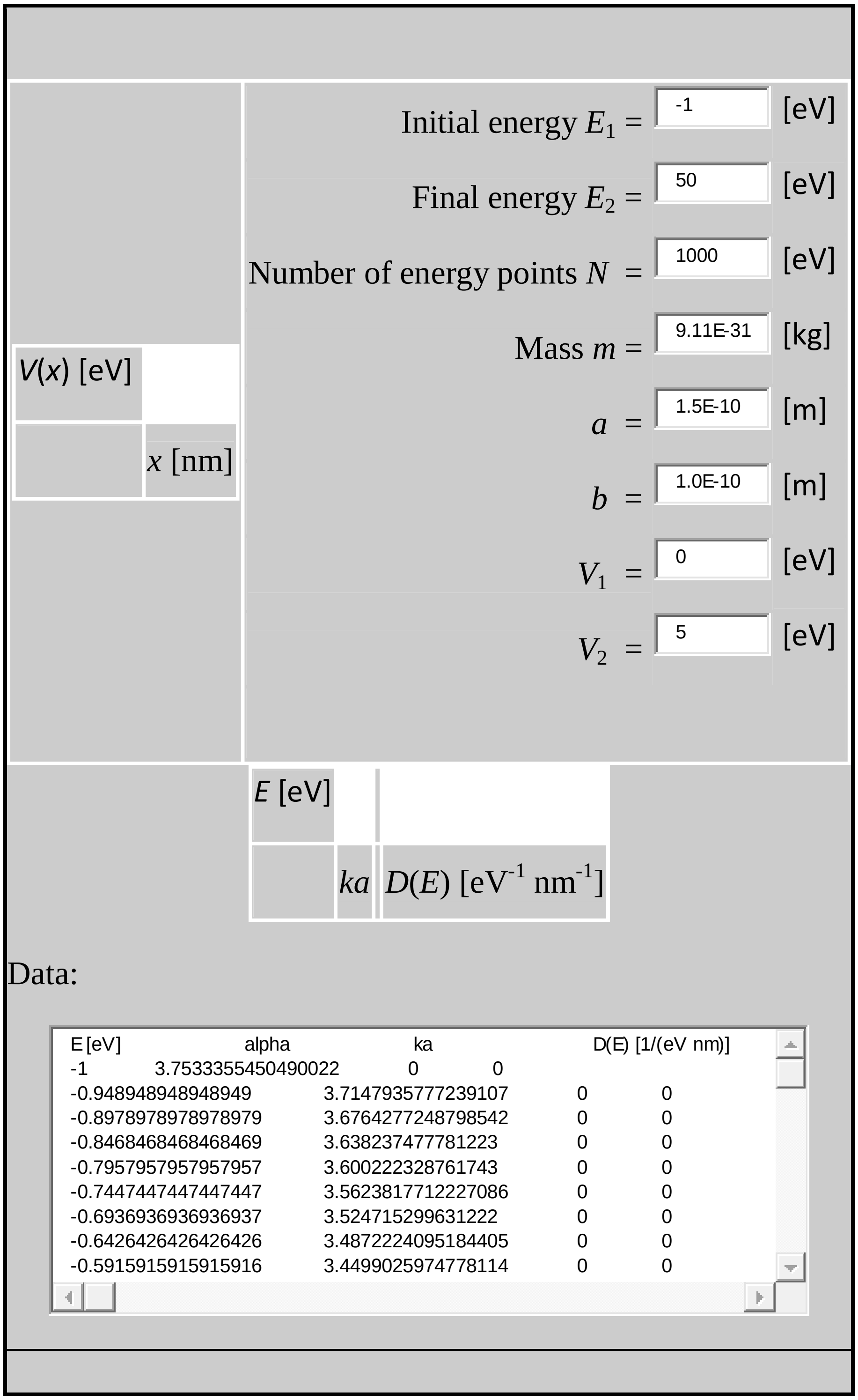
From Figure (5-16).a we observe the following: The *E*(*k*) relation resembles a parabola except that only specific ranges of energies are valid solutions to Schrödinger's equation and therefore are allowed, while others are not. The range of energies for which there is no solution is referred to as an energy band gap. The transitions between allowed and forbidden energies occur at non-zero integer multiples of *ka*/□. These correspond to local minima and maxima of the *E*(*k*) relation. The reduced-zone diagram shown in Figure (5-16).c contains the first three bands and energy band gaps. For instance the second energy band gap occurs between 1.5 and 2 eV, between the band maximum of the second band and the band minimum of the third band.

Complete energy band diagrams of semiconductors are very complex. However, most have features similar to that of the diamond crystal. In this section, we first take a closer look at the energy band diagrams of common semiconductors. We then present a simple diagram containing only the most important features.

5-6 Below is another solution to the problem.

Please find here below another solution to the problem, which can be computerized to find analytic expressions for the dispersion relation (*E* vs. *k*) and the electron density of states. The program is found in in appendix (III)

This form can be used to plot the dispersion relation and the density of states for the Kronig Penney model.



Initial energy E_1 = -1 [eV]

Final energy E_2 = 50 [eV]

Number of energy points N = 1000 [eV]

Mass m = 9.11E-31 [kg]

a = 1.5E-10 [m]

b = 1.0E-10 [m]

V_1 = 0 [eV]

V_2 = 5 [eV]

Data:

```
E [eV]                alpha                ka                D(E) [1/(eV nm)]
-1           3.7533355450490022          0            0
-0.948948948948949            3.7147935777239107          0            0
-0.8978978978978979           3.6764277248798542          0            0
-0.8468468468468469           3.638237477781223           0            0
-0.7957957957957957           3.600222328761743           0            0
-0.7447447447447447           3.5623817712227086          0            0
-0.6936936936936937           3.524715299631222           0            0
-0.6426426426426426           3.4872224095184405          0            0
-0.5915915915915916           3.4499025974778114          0            0
```

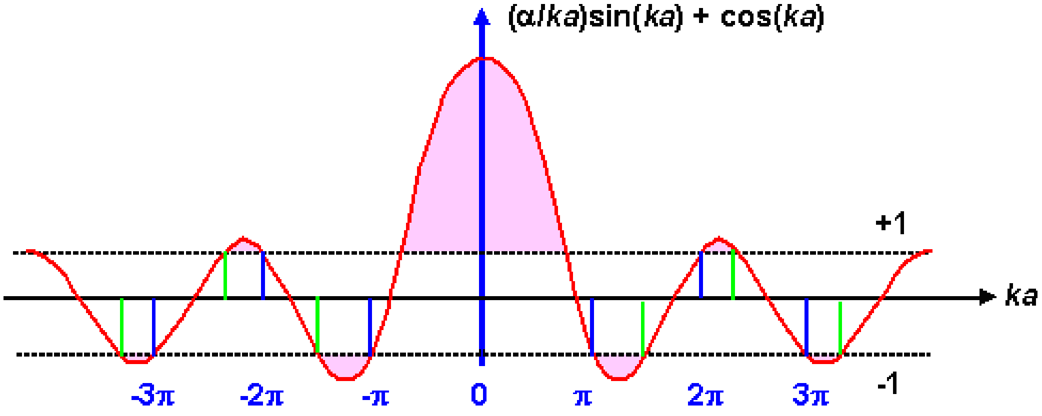


Figure (5-17): And I understand that for the equation to hold true, the left-hand-side cannot go above 1 or below -1, hence the regions shaded pink in the above plot are invalid solutions of the equation in the question.

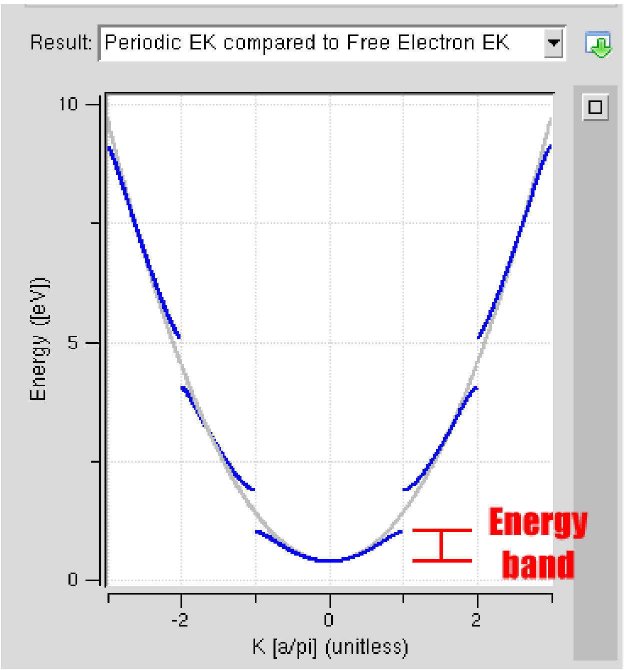


Figure (5-18): E & K diagram

5-7**Direct and indirect band gap semi-conductors**:

The band gap represents the minimum energy difference between the top of the valence band and the bottom of the conduction band, however, the top of the valence band and the bottom of the conduction band are not generally at the same value of the electron momentum. In a **direct band gap semiconductor**, the top of the valence band and the bottom of the conduction band occur at the same value of momentum, as in the schematic below.

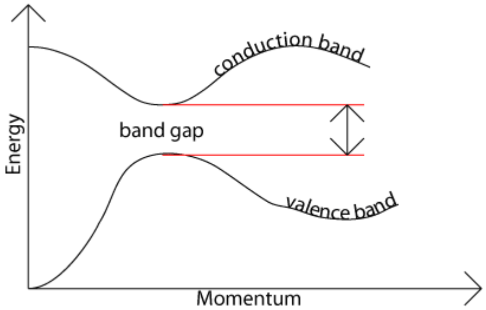


Figure (5-19): direct band gap semiconductor,

In an **indirect band gap semiconductor**, the maximum energy of the valence band occurs at a different value of momentum to the minimum in the conduction band energy:

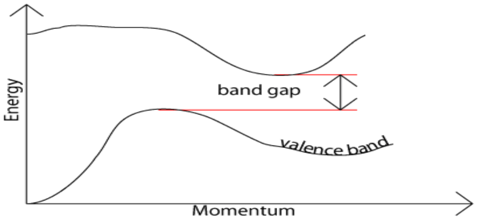


Figure (5-20): Indirect band gap semiconductor

The difference between the two is most important in optical devices. As the photon provides the energy, to produce an electron-hole pair, each photon of energy *E* has momentum;

$$p = \frac{E}{c} \qquad (5\text{-}20)$$

Where, *c* is the velocity of light.

An optical photon has energy of the order of 10^{-19} J and, since $c = 3 \times 10^{8}$ ms$^{-1.}$ A typical photon has a very small amount of momentum.

A photon of energy E_g, where E_g is the band gap energy, can produce an electron-hole pair in a direct band gap semiconductor quite easily, because the electron does not need to be given very much momentum. This is possible, because such an electron requires interacting only with the photon in order to either gain or lose momentum..

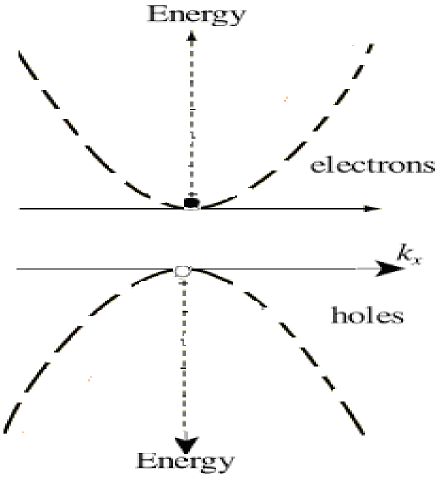


Figure (5-21): E&K diagram of direct band gap semiconductor

However, an electron must also undergo a significant change in its momentum for a photon of energy E_g to produce an electron-hole pair in an indirect band gap semiconductor. This is possible, but it requires such an electron to interact not only with the photon to gain energy, but also with a lattice vibration called a phonon in order to either gain or lose momentum.

The indirect process proceeds at a much slower rate, as it requires three entities to intersect in order to proceed: an electron, a photon and a phonon. This is analogous to chemical reactions, where, in a particular reaction step, a reaction between two molecules will proceed at a much greater rate than a process which involves three molecules.

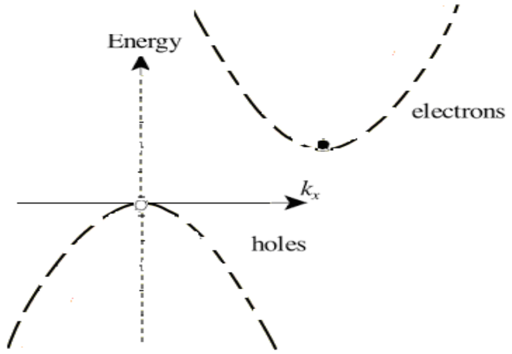


Figure (5-22): E&K diagram of indirect band gap semiconductor

The same principle applies to recombination of electrons and holes to produce photons. The recombination process is much more efficient for a direct band gap semiconductor than for an indirect band gap semiconductor, where the process must be mediated by a photon.

5-8 Band gap of germanium (Ge) Measurement

.There are no available facilities for practical work in most of Sudan universities, the only available experiment found at Shendi University is band gap measurement of germanium semiconductor .This experiment has been carried at Shendi University to measure the band gap of Ge.

5-8-1 Aim of the experiment:

The conductivity of a germanium test piece is measured as a function of temperature. The energy gap is determined from the measured values.

5-8-2 Tasks:

The current and voltage are to be measured across a germanium test piece as a function of temperature.

From the measurement, the conductivity σ is to be calculated and plotted against the reciprocal of the temperature T. A linear plot is obtained, from whose slope the energy gap of germanium can be determined.

5-8-3 Equipments needed:

Equipment	No.
Hall effect module 11801.00	1
Intrinsic conductor, Ge, carrier board 11807.01	1
Power supply 0-12 V DC/ 6 V, 12 V AC 13505.93	1
Tripod base -PASS- 02002.55	1
Support rod -PASS-, square, l = 250 mm 02025.55	1
Right angle clamp -PASS- 02040.55	1
Digital multi meter 2010 07128.00	2
Connecting cable, 4 mm plug, 32 A, black, l = 50 cm 07361.05	2
Connecting cable, 4 mm plug, 32 A, red, l = 10 cm 07359.01	1
Connecting cable, 4 mm plug, 32 A, blue, l = 10 cm 07359.04	1

What you need: Complete Equipment Set, Manual on CD-ROM included

Band gap of germanium P2530401/11

5-8-4 Theory:

The test piece is connected via a series resistor to the direct voltage out put of the power unit. The current should not exceed 30mA. The voltage across the test piece is measured with a multi meter. The conductivity is defined as following:

$$\sigma = \frac{1}{\text{p}} = \frac{LI}{AU} \qquad (5\text{-}21)$$

Where: ρ = Specific resistivity

L=length of test specimen

A =cross section

I =current

U =voltage

Dimensions of Ge plate (20*10*1 mm^3)

On the back of the board is the heating coil, supplied by the alternating voltage output of the unit. It is recommended that the test piece be warmed up slowly for the measurement, applying firstly 2v, then, 4v and finally 6v.

The maximum permissible temperature of 175^{o}C must not be exceeded. It is also possible to warm up to the maximum temperature first of all, and then take measurement during the cooling down period.

The test piece temperature is determined using the cu/cuNi thermocouple and the mV meter.

The conductivity of semiconductor is characteristically a function of temperature. The temperature dependence is in this case essentially described by an exponential function.

$$\sigma = \sigma.\ \text{Exp} - \frac{E_g}{2KT} \qquad (5\text{-}22)$$

$$E_g = Energy\ gap$$

K=Boltzmann's constant

T = Absolute temperature

The logarithm of this equation

Ln$\sigma = Ln\sigma. - \frac{E_G}{2KT}$ (5-23)

Is with y = Lnσ and x = $\frac{1}{T}$

A linear equation on the type

Y = a + mx (5-24)

Where: m = - $\frac{E_g}{2K}$

$E_g = 2Km$ (5-25)

Set up and procedure:

Units of the experiment is set up as shown in the following picture

Figure (5-23**):** Band gap of germanium (Ge) Measurement

5-8-5 Procedure:

Electrical circuit as in the figure below:

Fig. 2

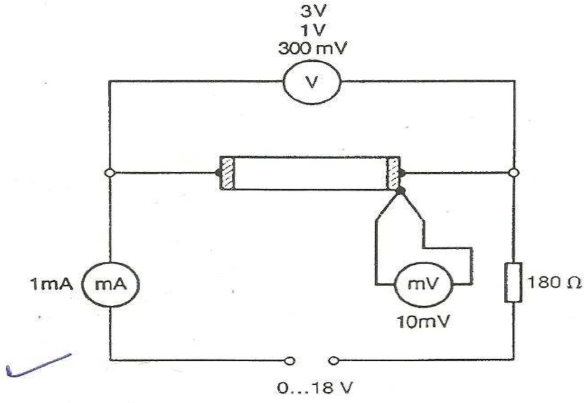


Figure (5-24): Shown electrical circuit

Heated the test piece germanium using a heating coil, even the maximum permissible temperature of 175C, and then gradually cooled.

The take measurement current and voltage during the cooling down period.

5-8-6 Results:

L=20mm=0.02m , A=(1x10)mm=0.01m

I/mA	U/mv	T/K	$\frac{1}{T}$ K^{-1}	$\frac{I}{U}\frac{1}{\Omega}$	$\frac{IL}{UA}$ $1/m\Omega$	Lnσ
10	0.35	393	2.55* 10^{-3}	28.57	57.14	4.05
15	0.69	383	2.61* 10^{-3}	21.74	43.48	3.77
20	1.23	373	2.68* 10^{-3}	16.26	35.52	3.57
25	2.10	363	2.74* 10^{-3}	11.90	23.80	3.17
30	3.55	353	2.83* 10^{-3}	8.45	16.90	2.83
35	5.91	343	2.91* 10^{-3}	5.92	11.84	2.47
40	9.58	333	3* 10^{-3}	4.18	8.36	2.12

5-8-7 Calculation

X ≡ 1cm ≡ 0.2 x 10^{-3} K^{-1}

Y ≡ 1cm ≡ 0.2 x Ω^{-1} m^{-1}

Figure (5-25): Lnσ & $\frac{1}{T}$

Lnσ= Lnσ. - $\frac{E_g}{2kT}$ (5-26)

σ=1.58 $\frac{1}{m\Omega}$

$\frac{1}{T}$=0.42*10^{-3}K

m = $\frac{\sigma}{1/T}$ m=$\frac{1.58}{0.42*10^{-3}}$ =3.8$*\ 10^3$

$$E_g = 2km = 2 * 8.625 * 10^{-5} * 3.8 * 10^3 = 65.5 * 10^{-2} = 0.66ev$$

5-8-8Conclusion

It was found that the energy gap of test piece of germanium is (0.66.ev)

Chapter six

Density of States

6-1 **Confinement:**

The reduction of carrier degree of freedom is called quantum confinement, and it occurs when one or more of the dimensions of nanoparticle are sufficiently small, typically (10 nm).By confinement an interesting properties can be attained. The confinement can take place in 0D, 1D, 2D, and 3D confinement, known as a bulk, quantum well, quantum wire& quantum dot respectively. Although the research is interested in quantum dots, quantum dots are semiconductors have the properties to confine their excited electrons or excitons in all three spatial dimensions. When these excitons drop back in their orbits around the atom in the valance band they emit light, the color of the light depends on the energy difference E between the conduction band and the valence band. The smaller the nanoparticle, the higher the energy difference between the valence band and the conduction band , which resolve into deeper blue color. For larger particles the energy difference between valance band and conduction band is lower which shift s this glow to the red part of the spectrum.

For bulk material the resulting energy levels are quantized and they are no longer continuous, but as discrete. If the confinement can take place in one dimension the valance band and conduction band split into overlapping sub bands that get successively narrower as electron motion is restricted into more dimensions. However, these structures give the electron at least one degree of freedom (direction of propagation).

Confinement of the electrons results in the appearance of energy states shown in figure below;

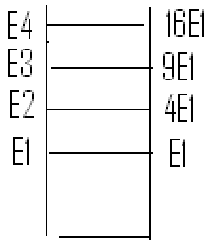


Figure (6-1): Energy level of electron

The energy of the lowest state is given by

$$E_1 = \frac{h^2 \pi^2}{2 m L^2} \qquad (6\text{-}1)$$

Energy of other states is;

$$E_g = \frac{h^2 \pi^2}{2 m L^2} n^2 = E_1 n^2 \qquad (6\text{-}2)$$

The confinement of the nano- crystal electrons results in an increase of the band gap according to the equation;

$$E_{QD} = E_g^{bulk} + \frac{\hbar^2 \pi^2}{2R^2} \left(\frac{1}{m_e} + \frac{1}{m_h} \right) \qquad (6\text{-}3)$$

Note that the smaller the radius of the quantum dot the larger the band gap, this implies the possibility of controlling the color of light emitted or absorbed by the quantum dot by changing their size

Incident photon Ep excites an electron from the filled valance band and promotes it to the next empty band known as conduction band leaving a hole behind. Electron and hole relax to the bottom of the conduction band and top of the valance band respectively .they recombine emitting light photon whose energy equal to the band gap of the quantum dot .

6-2 Density of states:

Determination of density of state (DOS) has two important usages ;

1- To derive the carrier (electron/hole) in the semiconductor.
2- To determine the most important state close to the minimum of the conduction band and hence the Fermi level.

How to do that could be seen at the end of this chapter .first to begin with the derivation of DOS (E) in 3D bulk material as a function of energy

Before we can calculate the density of carriers in a semiconductor, we have to find the number of available states at each energy level. The number of electrons at each energy level is then obtained by multiplying the number of states with the probability that a state is occupied by an electron. Since the number of energy levels is very large and dependent on the size of the semiconductor, we will calculate the number of states per unit energy and per unit volume

To calculate various optical properties such as the rate of absorption or emission and how electrons and holes distribute themselves within a solid, the number of available states per unit volume per unit energy should be known. We first calculate the available states in k-space and then use the energy-momentum relation in parabolic bands to give the density of states in terms of energy.

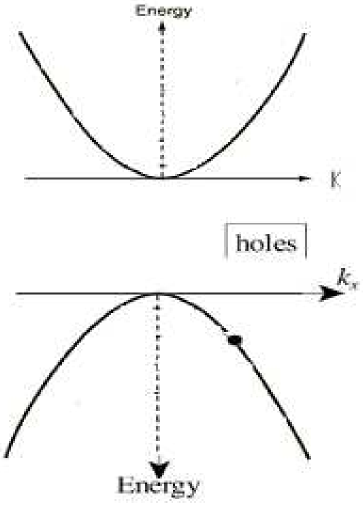


Figure (6-2): E&K diagram of electron and hole

The density of states in a semiconductor equals the density per unit volume and energy of the number of solutions to Schrödinger's equation. We will assume that the semiconductor can be modeled as an slab of bulk material the wave function can be drawn in particular direction let be x. The semiconductor is assumed a cube with side *L*. This assumption does not affect the result since the density of states per unit volume should not depend on the actual size or shape of the semiconductor.

Classically, all values of energy would be allowed and there would be no restriction on the number of electrons with the same value of **k.** However, at atomic scales, the effects of quantum mechanics dominate and two further famous principles come into play. These are the Heisenberg uncertainty principle and the Pauli exclusion principle. Together, these two rules mean that the wave function for the electron must satisfy the Schrödinger equation, subject to boundary conditions. The solution of the Schrödinger equation leads to wave functions of the form:

$$\Psi = A \sin(k_x x) - B \cos(k_x x) \qquad (6\text{-}4)$$

The solutions to the wave equation (equation Appendix IV (6-4) where *V*(*x*) =

0 are sine and cosine functions:

6-3 Calculation of the density of states in 3D semiconductor:

The density of states in a semiconductor equals the density per unit volume and energy of the number of solutions to Schrödinger's equation. We will assume that the semiconductor can be modeled as an slab of bulk material the wave function can be drawn in particular direction let be x. The semiconductor is assumed a cube with side *L*. This assumption does not affect the result since the density of states per unit volume should not depend on the actual size or shape of the semiconductor.

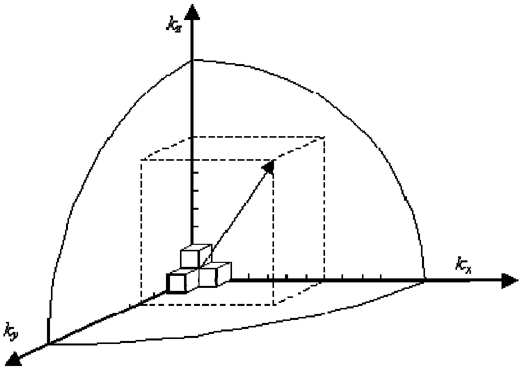
The solutions to the wave equation ,where $V(x) = 0$ are sine and cosine functions:

$$\Psi = A\sin(k_x x) + B\cos(k_x x) \qquad (6\text{-}5)$$

Where *A* and *B* are constants to be determined from the boundary conditions. The wave function must be zero at the infinite barriers of the well. At $x = 0$ the wave function must be zero so that only sine functions can be valid solutions or *B* must equal zero. At $x = L$, the wave function must also be zero yielding the following possible values for the wave number, k_x.

$$k_x = \frac{n\pi}{L}, \qquad \text{Where} \quad n = 1,2,3\ldots \qquad (6\text{-}6)$$

This analysis can now be repeated in the *y* and *z* direction. Each possible solution then corresponds to a cube in *k*-space with size $n\pi/L$ as indicated on Figure Below;



Figure(6- Calculation of the number of states with wave number less than *k*.
3):

The total number of solutions with a different value for k_x, k_y and k_z and with a magnitude of the wave vector less than k is obtained by calculating the volume of one eighth of a sphere with radius k and dividing it by the volume corresponding to a single solution, $(\frac{\pi}{L})^3$, yielding:

$$N = 2\times\frac{1}{8}\times(\frac{L}{\pi})^3\times\frac{4}{3}\times\pi\times k^3 \qquad (6\text{-}7)$$

A factor of two is added to account for the two possible spins of each solution. The density per unit energy is then obtained using the chain rule:

$$\frac{dN}{dE} = \frac{dN}{dk}\frac{dk}{dE} = (\frac{L}{\pi})^3 \pi k^2 \frac{dk}{dE} \qquad (6\text{-}8)$$

By considering the electrons in a solid as a free electron gas, that is, the electrons are free to wander around the crystal without being influenced by the potential of the atomic nuclei; we can obtain a relationship for the number of available states in a solid. A free electron has a velocity v and a momentum **p** = m **v.** Its energy consists entirely of kinetic energy (V=0) therefore,

$$E = \frac{1}{2}m\mathbf{v}^2 = \frac{|\mathbf{p}|^2}{2m} \qquad (6\text{-}9)$$

Prince Louis De-Broglie, hypothesized that if waves could exhibit particle-like properties, then might particles also exhibit wave-like properties? This idea is expressed as particle-wave duality and allows us to give the electron a wave number **k.**

$$\mathbf{k} = \frac{\mathbf{p}}{\hbar} \tag{6-10}$$

In this way, the electron can be represented by a vector in velocity, momentum or k-space. If we choose to represent the electron state as a vector, it points in a direction given by the components magnitude of the basis vectors in k-space. It should be apparent that vectors of the same magnitude have the same energy forming spherical shells. This can be understood better, if we consider the equation for the energy of the electron in terms of **k.**

$$E = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2) = \frac{\hbar^2 k^2}{2m} \tag{6-11}$$

The kinetic energy *E* of a particle with mass m^* is related to the wave number, *k*, by:

$$E(k) = \frac{\hbar^2 k^2}{2m^*}, \text{ providing } \frac{dk}{dE} = \frac{m^*}{\hbar^2 k} \text{ and } k = \frac{\sqrt{2m^* E}}{\hbar} \tag{6-12}$$

And the density of states per unit volume and per unit energy, *g*(*E*), becomes:

$$g(E) = \frac{1}{L^3}\frac{dN}{dE} = \frac{8\pi\sqrt{2}}{h^3} m^{*3/2} \sqrt{E}, \text{for } E \geq 0 \tag{6-13}$$

The density of states is zero at the bottom of the well as well as for negative energies.

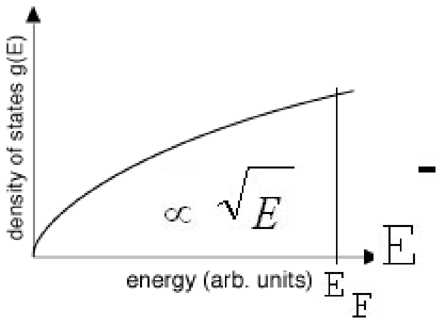


Figure (6-4): Density of states in 3D semiconductor (bulk semiconductor)

The same analysis also applies to electrons in a semiconductor. The effective mass takes into account the effect of the periodic potential on the electron. The minimum energy of the electron is the energy at the bottom of the conduction band, E_c, so that the density of states for electrons in the conduction band is given by:

$$g_c(E) = \frac{8\pi\sqrt{2}}{h^3} m^{*3/2} \sqrt{E - E_c}\text{, for } E \geq E_c \qquad (6\text{-}14)$$

$$g_c(E) = 0\text{, for } E < E_c$$

6-4 2-D Density of States

In two dimensional structures such as the quantum well, the procedure is much the same but this time one of the k-space components is fixed. Instead of a finding the number of k-states enclosed within a sphere. The problem is to calculate the number of k-states lying in an area of

$$V_{2D} = \left(\frac{\pi}{L}\right)^2 \qquad (6\text{-}15)$$

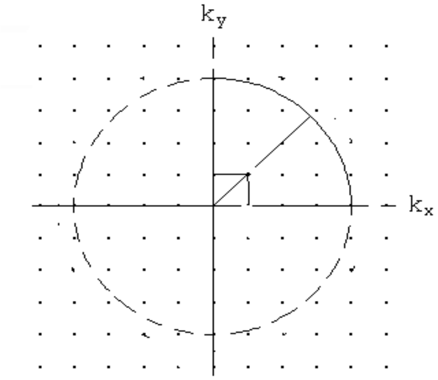


Figure (6-5): 2 k-space in 2D. The density of states at an energy E is the number of k-states per unit volume contained within an area

$$N = 2 \times \frac{1}{4} \times \left(\frac{L}{\pi}\right)^2 \times \pi \times k^2 \qquad (6\text{-}16)$$

Dividing the 'volume' of the k-state by the area and remembering to multiply by 2 to account for the electron spin states we get:

$$g_{c,2D} = \frac{dN_{2D}}{dE} = \frac{4\pi m^*}{h^2}, \text{for } E \geq E_{min} \qquad (6\text{-}17)$$

It is significant that the 2-d density of states does not depend on energy. Immediately, as the top of the energy-gap is reached, there is a significant number of available states. Taking into account the other energy levels in the quantum well, the density of states takes on a staircase like function given by:

$$g(E)_{2D}\,\mathrm{d}E = \frac{m}{\pi\hbar^2}\sum_i H(E-E_i)\,\mathrm{d}E \qquad (6\text{-}18)$$

Where $H\,(E\text{-}E_i)$ is the Heaviside function. It takes the value of zero when E is less than E_i and 1, when E is equal to or greater than E_i. E_i is the i-th energy level within the quantum well.

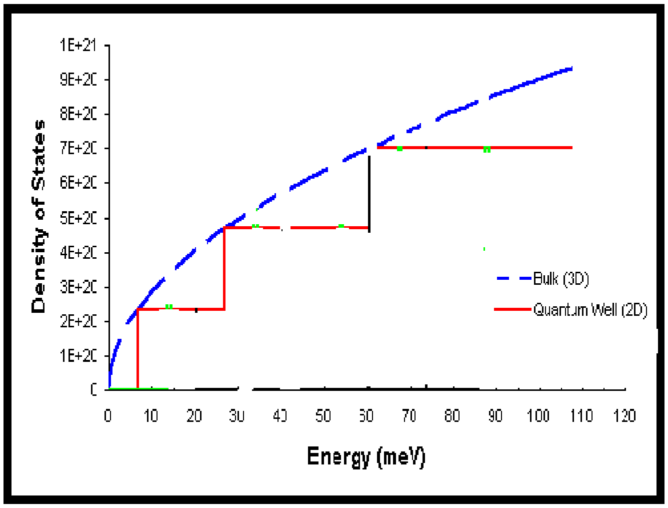


Figure (6-6): Density of states in 3D and 2D semiconductor (quantum well)

6-5 1-D Density of States

In one dimension two of the k-components are fixed, therefore the area of k-space becomes a length of a line.

$$V_{1D} = \frac{\pi}{L} \qquad (6\text{-}19)$$

$$N = 2\ \left(\frac{L}{\pi}\right)\ \times \pi \qquad (6\text{-}20)$$

Therefore the density of states per unit length in 1-d and multiplying by 2 for spin

For a one-dimensional semiconductor such as a quantum wire in which particles are confined along a line.

$$g_{c,1D} = \frac{dN_{1D}}{dE} = \sqrt{\frac{2\pi m^*}{h^2}}\,\frac{1}{\sqrt{E - E_{\min}}}, \text{for } E \geq E_{\text{mir.}} \qquad (6\text{-}21)$$

An example of the density of states 1 dimension is shown in the figure below:

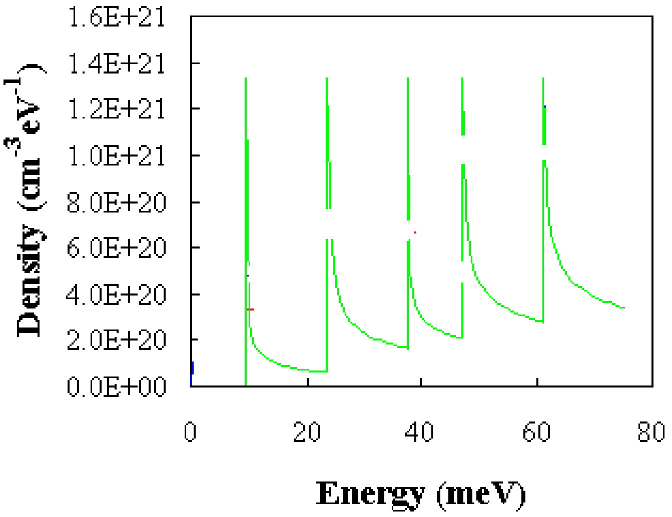


Figure (6-7): Density of states in 1D semiconductor (quantum wire)

For one dimension, the density of states per unit volume at energy *E* is given by

$$g(E)_{1D}\,\mathrm{d}E = \frac{2}{\pi}\,\mathrm{d}k = \frac{2}{\pi}\left(\frac{2mE}{\hbar^2}\right)^{-1/2}\frac{m}{\hbar^2}\,\mathrm{d}E = \frac{1}{\pi}\left(\frac{m}{\hbar^2}\right)^{1/2}\frac{1}{E^{1/2}}\,\mathrm{d}E \qquad (6\text{-}22)$$

Using more than the first energy level, the density of states function becomes

$$g(E)_{1D}\,\mathrm{d}E = \frac{1}{\pi}\left(\frac{2m}{\hbar^2}\right)^{1/2} \sum_i \left(\frac{n_i H(E-E_i)}{(E-E_i)^{1/2}}\right)\mathrm{d}E \qquad (6\text{-}23)$$

Where once again, $H(E-E_i)$ is the Heaviside function and n_i is the degeneracy factor. For quantum structures with dimensions lower than 2, it is possible for the same energy level to occur for more than one arrangement of confined states. To account for this, a second factor $n_i(E)$ is introduced.

6-6 0-D Density of States

In a 0-D structure, the values of k are quantized in all directions. All the available states exist only at discrete energies described and can be represented by a delta function. In real quantum dots, however, the size distribution leads to a broadening of this line function.

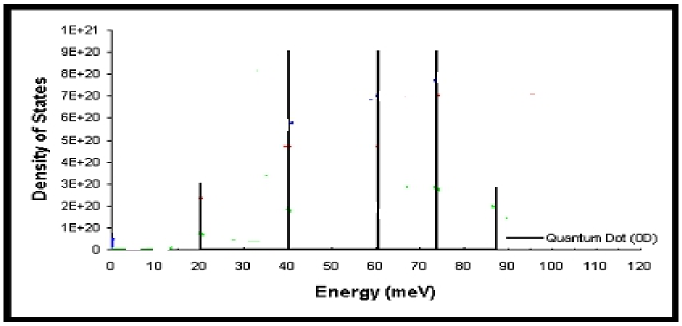


Figure (6-8): Density of states in 0D (quantum dot)

The four together for comparison;

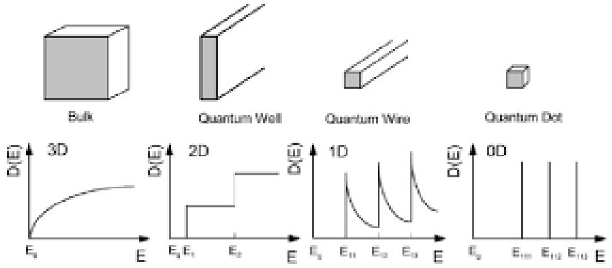


Figure (6-9): shows bulk & quantum well & quantum wire and quantum dot

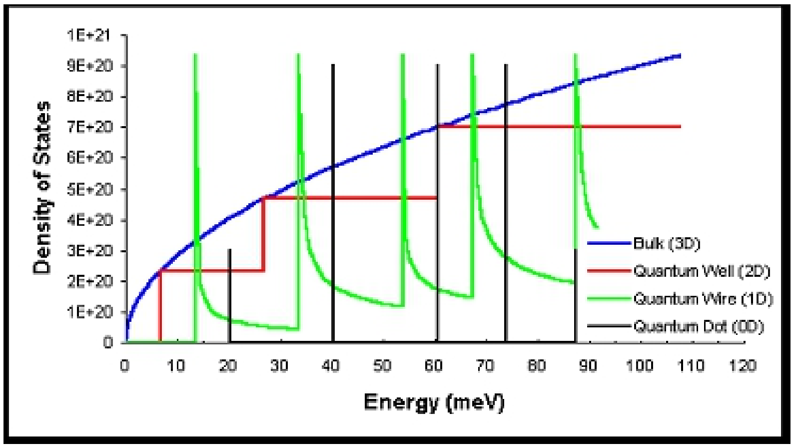


Figure (6-10): Density of states of bulk & quantum well & quantum wire and quantum dot

6-7 Density of occupied states (Carrier density):

6-7-1 Density of states:

Mathematical function that gives the possible energy quantum states per unit volume per unit energy of electrons inside a solid metal.

$$\rho(E) = \frac{8\sqrt{2}m^{3/2}\ \sqrt{E}}{h^3} \qquad \text{(6-23-1)}$$

6-7-2 Fermi Dirac probability function:

A function that describe the probability distribution energy quantum state being occupied by an electron in a metal solid of some temperature T

$$F\ (E) = \frac{1}{e^{\frac{E-E_f}{kt}} + 1} \qquad \textbf{(6-23-2)}$$

Where: E $\equiv$ is the energy of electron

$E_F\ \equiv energy\ of\ fermi\ level$

Combine (6-23-1), (6-23-2):

$$n(E) = \rho(E)F(E) = \frac{8\sqrt{2}m^{3/2}\ \sqrt{E}}{h^3} \text{ x } \frac{1}{e^{\frac{E-E_f}{kt}} + 1} \qquad \text{(6-24)}$$

This equation is known as density of occupied states. If we plot this equation on (xy) plane, then it gives the number of electron per unit volume which is the quantum states between some ranges of energy of some particular temperature T.

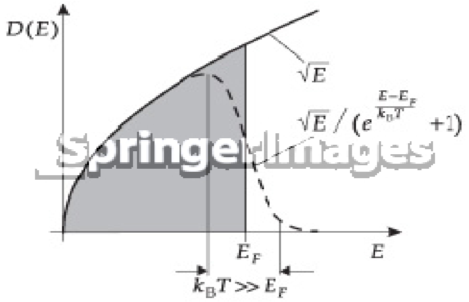


Figure (6-11): The curve represents the density of occupied state for a metal solid of same temperature T.

The curve represents the density of states at absolute zero.

Carve (2) tell us what happen to electrons in the metal solid, so we measure the temperature by increasing the temperature by (1,000 K), we increase the energy of electrons by only (0.1 Iev). Since this a very small amount, only the electronics very close to Fermi level can actually jump to higher quantum states

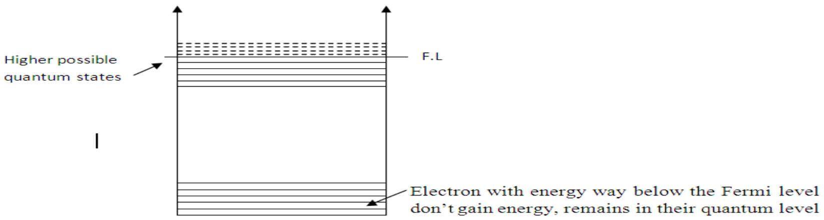


Figure (6-12); Fermi level

6-8 Fermi Dirac probability function:

Up to this point we discussed what happen to electrons in solid metal that are at absolute temperature zero. We saw at absolute zero, the electrons occupy all quantum states that have energies below the Fermi levels. But what happen when temperature is increased

We might expect that with increase in temperature, the motion of electrons increases; there by increasing the energy of electrons, this means that electrons begin filling quantum states of energies above Fermi level.

But regardless of energy increase, quantum mechanism dicates that a minimum of electrons can be found in quantum states with equal energies. The mathematical function that describes the probability distribution of energies of electrons at some temperature T is given by:

$$F(E) = \frac{1}{e^{(E-E_f)/kt}+1} \qquad (6\text{-}25)$$

Known on Fermi- Dirac probability function

Notice that if T $\longrightarrow 0$ $e^{(E-E_f)/kt} \longrightarrow 0$

If (E-E_f) $\longrightarrow 0$ if E $>$ E_f

For T=0

$$F(E) = \begin{cases} 0 & if \;\; E \;\; > E_f \\ 1 & if \;\; E \;\; = E_f \end{cases}$$

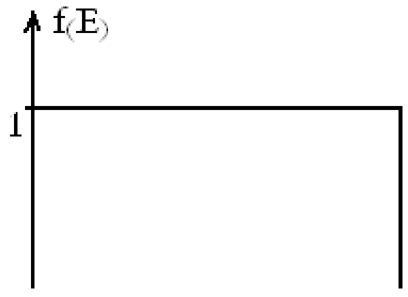


Figure (6-13): The graph tell us that all the quantum states below E_f are occupied with 100% certainty [F (E) = 1]

Now let us combine what curve look like at higher temperature. Let's suppose T=400k

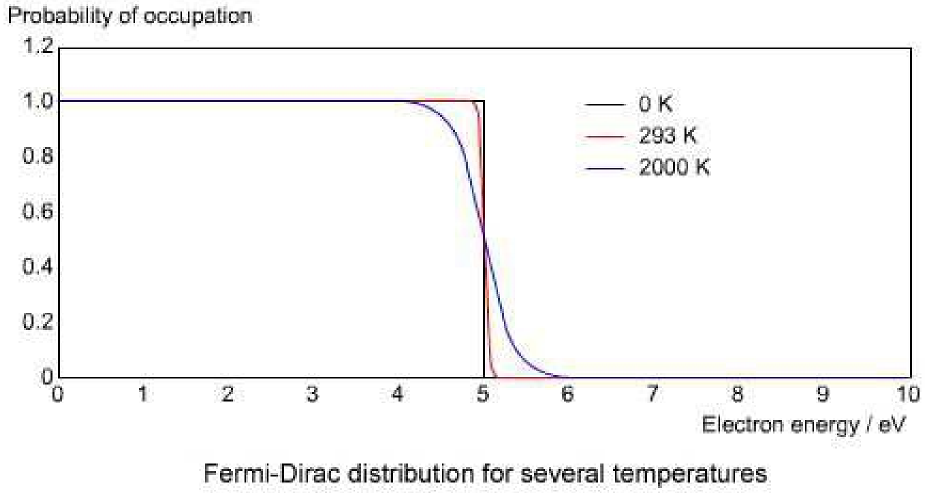


Figure (6-14): Fermi distribution for several temperatures

One interesting fact that comes from this equation (and curve) is that no matter what the temperature is, if E=E_f the exponential term particular quantum states 50% probability

Chapter seven

7-1 Pinch Top Nanotechnology Guide to Quantum Dot Fabrication:

Solar cell convert light energy into electricity energy, to collect a liquid junction solar cell step by step is going to be shown.

7-1-1 Step (1): Preparing the optically transparent electrode:

Cut off optically transparent electrode to appropriate size.

Test the electrode for conductivity, the back side is an insulating surface, used is a multi meters.

Wash the electrode in surfactant solution (soap, water) using an ultra sonic indicator.

Rinse with deionizer water and ethanol.

Immersion is electrode in ethanol bath for the second round of sonication.

7-1-2 Step (2): Depositing the compact layer:

The compact layer (Tio_2 layer) is a thin back layer just on the surface of electrode. This layer prevents short circuiting on the liquid junction solar cells.

Developed this layer an aqueous solution of ($Ticl_4$) is used .Titanium tetra chloride (a-k-a $Tickle_4$) all over the surface of the electrode.

Heated to 70° C to titanium dioxide

After heating rinse with deionizer water and ethanol

7-1-3 Step (3): Casting the active layer:

This layer is called Tio_2 active layer it a mesa pore support to provide a framework for depositing our quantum dots light absorbers. Active Tio_2 areas are marked out by using a take template and $Ti\ o_2$is caste by doctor blade technique. Using this simple technique we can simultaneously prepare multiple active areas

Heat electrode to 80°C - 500°C

7-1-4 Step (4): Appling the scattering layer:

The final tier in our photo anode is the scattering Tio_2 layer. This layer provides back scatter photons for quantum dot light absorbers in the active area.

Heat electrode to 80°C - 500°C

7-1-5 Step (5): Preparing the photo anode for sensitization:

Just before depositing solar cell sensitizer the photo anode is treated for the second time with $Ticl_4$ to increase the surface and to improve the quantum dot deposition.

Cut off individual solar cells for the optically transparent electrode.

7-1-6 Step (6): Sensitizing the photo anode:

There two methods to do this:

Method (1): Electro-phonetic deposition [E.P.D]:-

Allow the deposition of free sensitized colloidal quantum dot into photo anode after the electrode into quantum dot solution. High voltage is used to drive the particles into Tio_2 network. Looking to the front side of solar cell, we can see the brighter colored active area, this is because the majority of particles have been driven through the scattering layer, and now resides in the Mesa pore Tio_2 support using EPD we can deposit various sizes of quantum dot to tune the visible absorption of the solar cell making what is called rainbow solar cell.

Method (2): Successive ionic layer absorption and reaction [SILAR]:

To perform (SILAR), we can submerge a Tio_2 into action ($_{Cd}+2$) solution followed by rinse; submerge into anion solution ($_{S}-2$, $_{Se}-2$).

Used custom built instrument and software developed in the lab to automate the process to increase solar.

Cell throughput. During the first cycle of (SELAR) we can see white unsenitized electrode and after five cycles we can see the characteristic yellow color of cadmium sulphide.

7-1-7 Step 7: Depositing blocking layer:

After sensitizing Tio_2 film deposit zinc sulphide blocking layer used (SELAR). Thus layer back (SELAR) transform the sensitized and Tio_2 particles into liquid electrolyte then we use RGO for preparing counter electrode.

7-1-8 Step 8: Preparing the counter electrode:

Use a copper (RGO) (Reduced graphene oxide) composite material cast on a (fluorine dote tin oxide) electrode.

Placed the counter electrodes in oven at 110C over night. A part film spacer is melted on the surface of the electrode of the copper RGO composite material is allowed to the react with poly sulphide electrolyte to from copper sulphide RGO.

7-1-9 Step 9: Assembling the solar cell:

First several drops electrolyte are placed in the counter electrode.

7-2 Conclusion:

Nanotechnology is a field of applied science and technology covering a broad range of topics. Nanotechnology is extremely diverse ranging from novel extensions of conventional device physics, to completely new approaches based upon molecular self assembly, to develop new materials in nan scale dimensions, even to the speculation on whether we can directly control matter on the atomic scale. The main unifying theme is the control of matter on a scale smaller than one micrometer, as well as *the fabrication of devices on this same length scale and the development of new materials.*

Quantum dot solar cells, on the other hand, are cheaper to produce than conventional ones, and can be processed at relatively low temperatures. Furthermore, quantum dot solar cells can be fabricated on surfaces of arbitrary shape and flexibility, paving the way to a range of novel applications. Therefore, quantum dot solar cells are likely to play an important role in addressing, at least in some small part, man's future energy needs. Here, the physics of quantum dot photovoltaic are reviewed, with particular emphasis on the computational tools which can be used to investigate these systems. In particular, the authors discuss the application of nanotechnology in self-assembling complex nan scale structures which can be tailored to optimize photovoltaic performance.

Although the role of computer simulations, in correlating these intricate structures, with their performance, can not only reveal interesting new insights into current devices, but also elucidate potentially new systems with more optimized nanostructures, but unfortunately it is not included in this thesis and it can be left for future work.

Hope for nanotechnology even encompass four years of development, researchers still need to determine why these films are so stable but we have to go along way before they are commercially reliable

7-3 Future work:

With the urgent need to harvest and store solar energy, especially with the *dramatic unexpected changes in oil prices, the design of new generation of solar energy storage systems has grown in importance. Besides diminishing the role of the oil, these systems provide green energy which would help reducing air pollution. Solar energy would be stored in different forms of energy; thermal, electric, hybrid thermal/electric, thermo chemical, photochemical, and photo capacitors. The nature of solar energy, radiant thermal energy, magnifies the role and usage of thermal energy storage (TES) techniques. The future work can be carried to study different techniques/technologies for solar thermal energy storage can be introduced for both terrestrial and space applications. Enhancing the performance of these techniques using nanotechnology could be introduced as well as using of advanced materials and structures. The study should also introduce the main features of the other techniques for solar energy storage along with recent conducted research work. Economic and environment feasibility studies can be also introduced.*

At last and not the least it has been mentioned that nanotechnology is extremely diverse, so it could be extended to include the photo electronics as well.

Appendix 1

However, the dominant loss mechanism is the inability of a solar cell to extract all of the power in the photon, and the associated problem that it cannot extract any power at all from certain photons. This is due to the fact that the electrons must have enough energy to overcome the bandgap of the material.

If the photon has less energy than the bandgap, it is not collected at all. This is a major consideration for conventional solar cells, which are not sensitive to most of the infrared spectrum, although that represents almost half of the power coming from the sun. Conversely, photons with more energy than the bandgap, say blue light, initially eject an electron to a state high above the bandgap, but this extra energy is lost through collisions in a process known as "relaxation". This lost energy turns into heat in the cell, which has the side-effect of further increasing blackbody losses.[13]

Combining all of these factors, the maximum efficiency for a single-bandgap material, like conventional silicon cells, is about 34%. That is, 66% of the energy in the sunlight hitting the cell will be lost. Practical concerns further reduce this, notably reflection off the front surface or the metal terminals, with modern high-quality cells at about 22%.

Lower, also called narrower, bandgap materials will convert longer wavelength, lower energy photons. Higher, or wider bandgap materials will convert shorter wavelength, higher energy light An analysis of the AM1.5 spectrum, shows the best balance is reached at about 1.1 eV, in the near infrared, which happens to be very close to the natural bandgap in silicon and a number of other useful semiconductors.

- **AM2~3**

AM2 (z=60°) to AM3 (z=70°) is a useful range for estimating the overall average performance of solar cells installed at high latitudes such as in northern Europe. Similarly AM2 to AM3 is useful to estimate wintertime performance in temperate latitudes, e.g. airmass coefficient is greater than 2 at all hours of the day in winter at latitudes as low as 37°.

- **AM38**

- AM38 is generally regarded as being the airmass in the horizontal **AM0**

The spectrum outside the atmosphere, approximated by the 5,800 K black body, is referred to as "AM0", meaning "zero atmospheres". Solar cells used for space power applications, like those on communications satellites are generally characterized using AM0.

- **AM1**

The spectrum after travelling through the atmosphere to sea level with the sun directly overhead is referred to, by definition, as "AM1". This means "one atmosphere". AM1 (z=0°) to AM1.1 (z=25°) is a useful range for estimating performance of solar cells in equatorial and tropical regions.

- **AM1.5**

Solar panels do not generally operate under exactly one atmosphere's thickness: if the sun is at an angle to the Earth's surface the effective thickness will be greater. Many of the world's major population centres, and hence solar installations and industry, across Europe, China, Japan, the United States of America and elsewhere (including northern India, southern Africa and Australia) lie in temperate latitudes. An AM number representing the spectrum at mid-latitudes is therefore much more common.

"AM1.5", 1.5 atmosphere thickness, corresponds to a solar zenith angle of z=48.2°. While the summertime AM number for mid-latitudes during the middle parts of the day is less than 1.5, higher figures apply in the morning and evening and at other times of the year. Therefore AM1.5 is useful to represent the overall yearly average for mid-latitudes. The specific value of 1.5 has been selected in the 1970s for standardization purposes, based on an analysis of solar irradiance data in the conterminous United States.[9] Since then, the solar industry has been using AM1.5 for all standardized testing or rating of terrestrial solar cells or modules, including those used in concentrating systems. The latest AM1.5 standards pertaining to photovoltaic applications are the ASTM G-173[10][11] and IEC 60904, all derived from simulations obtained with the SMARTScode

direction (z=90°) at sea level.[6] However, in practice there is a high degree of variability in the solar intensity received at angles close to the horizon as described in the next section Solar intensity.

- **At higher altitudes**

The *relative* air mass is only a function of the sun's zenith angle, and therefore does not change with local elevation. Conversely, the *absolute* air mass, equal to the relative air mass multiplied by the local atmospheric pressure and divided by the standard (sea-level) pressure, decreases with elevation above sea level. For solar panels installed at high altitudes, e.g. in an Altiplano region, it is possible to use a lower absolute AM numbers than for the corresponding latitude at sea level: AM numbers less than 1 towards the equator, and correspondingly lower numbers than listed above for other latitudes. However, this approach is approximate and not recommended. It is best to simulate the actual spectrum based on the relative air mass (e.g., 1.5) and the *actual* atmospheric conditions for the specific elevation of the site under scrutiny.

Multi-junction cells

Cells made from multiple materials have multiple bandgaps. So, it will respond to multiple light wavelengths and some of the energy that would otherwise be lost to relaxation as described above, can be captured and converted.

For instance, if one had a cell with two bandgaps in it, one tuned to red light and the other to green, then the extra energy in green, cyan and blue light would be lost only to the bandgap of the green-sensitive material, while the energy of the red, yellow and orange would be lost only to the bandgap of the red-sensitive material. Following analysis similar to those performed for single-bandgap devices, it can be demonstrated that the perfect bandgaps for a two-gap device are at 1.1 eV and 1.8 eV.[14]

Conveniently, light of a particular wavelength does not interact strongly with materials that are not a multiple of that wavelength. This means that you can make a multijunction cell by layering the different materials on top of each other, shortest wavelengths on the "top" and increasing through the body of the cell. As the photons have to pass through the cell to reach the proper layer to be absorbed, transparent conductors need to be used to collect the electrons being generated at each layer.

Appendix II

What is molecular beam epitaxy?

To make an interesting new crystal using MBE, you start off with a base material called a **substrate**, which could be a familiar semiconductor material such as silicon, germanium, or gallium arsenide. Then you fire relatively precise beams of molecules (heated up so they're in gas form) at the substrate from "guns" called **effusion cells**. You need one "gun" for each different beam, shooting a different kind of molecule at the substrate, depending on the nature of the crystal you're trying to create. The molecules land on the surface of the substrate, condense, and build up very slowly and systematically in ultra-thin layers, so the complex, single crystal you're after grows one atomic layer at a time. That's why MBE is an example of what's called **thin-film deposition**. Since it involves building up materials by manipulating atoms and molecules, it's also a perfect example of what we mean by nanotechnology .

Photo: Molecular beam epitaxy (MBE) in action. MBE takes place in ultrahigh vacuum chambers like this, at temperatures of around 500°C (932°F), to ensure a totally clean, dust-free environment; the slightest contamination could ruin the crystal. Photo by Jim Yost courtesy of US DOE/NREL (U.S. Department of Energy/National Renewable Energy Laboratory).

That's pretty much MBE in a nutshell. If you want a really simply analogy, it's a little bit like the way an inkjet printer makes layers of colored print on a page by firing jets of ink from hot guns. In an inkjet printer, you have four separate guns firing different colored inks (one for cyan ink, one for magenta, one for yellow, and one for black), which slowly build up a complex colored image on the paper. In MBE, separate beams fire different molecules and they build up on the surface of the substrate, albeit more slowly than in inkjet printing—MBE can take hours! Epitaxially simply means "arranged on top of," so all molecular beam epitaxy really means is using beams of molecules to build up layers on top of a substrate.

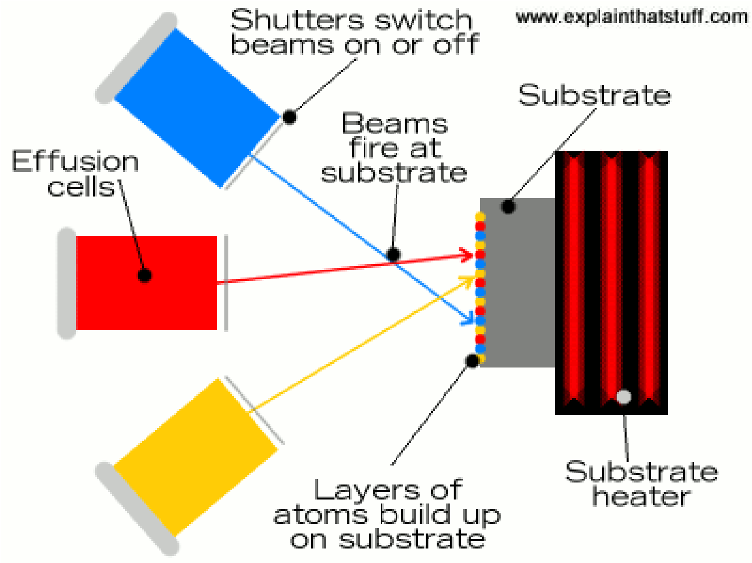


Photo: Molecular beam epitaxy (MBE) means creating a single crystal by building up orderly layers of molecules on top of a substrate (base layer).

Quantum dots are extremely small semiconductor structures, usually ranging from 2-10 nanometers (10-50 atoms) in diameter. At these small sizes materials behave differently, giving quantum dots unprecedented tunability and enabling never before seen applications to science and technology.

Appendix III

Kronig-Penney model

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[Problem 13] Kronig-Penney model: Plot the energy vs. wave vector for repulsive delta-function potentials. V(x) =h^2/ ($8p^2a$) lSd(x-na) where a is the distance between adjacent delta functions. Using boundary conditions, one obtains the equation:

Cos (qa) = cos (ka) +λ/2 sin (ka)/(ka). We use 3π for λ. Obtain k^2 as a function of q.

See "Physics and Mathematics", Patrick Tam, Computers in physics, p.342, May/June, 1991. The solution 1 below is based on his article. He used Mathematica.

[Solution] solution 1 (ver. 6.01)

Reset parameters

```
> restart:
```

```
> with(plots):
```

band: number of bands (you can change the number of bands here),

div: number of mesh points in a band

q: wave vector

a: distance between adjacent repulsive delta functions

```
> div:=30:band:=3:
```

```
> div1:=div+1:
```

Dimensioning of q, k, and energy

```
> q:=array(1..band,1..div1):
```

```
> k:=array(1..band,1..div1):
```

```
> energy:=array(1..band,1..div1):
```

The eigenvalue equation to be solved (See p.344, Computers in Physics, May/June 1991)

```
> eq:=cos(qa)=cos(ka)+3*Pi/2*sin(ka)/ka:
```

Solve the equation for each q in each band

```
> for n from 1 to band do
> for i from 1 to div1 do
> q[n,i]:=(i-1)*Pi/div+(n-1)*Pi:
> # q value
> qa:=q[n,i]:
> # solution k
> k[n,i]:=fsolve(eq,ka,(n-1)*Pi..n*Pi):
> # energy=k^2
> energy[n,i]:=k[n,i]^2:
> od:
> od:
> listqp:=array(1..2*(div+1)):
```

(q,energy) of the right branches

```
> for n from 1 to band do
> for i from 1 to div1 do
> listqp[2*i-1]:=q[n,i]:
> listqp[2*i]:=energy[n,i]:
> od:
> # plotlist[n] contains (q1,E1,q2,E2,...) for n-th band on the right branches
> plotlist[n]:=convert(listqp,list):
> od:
```

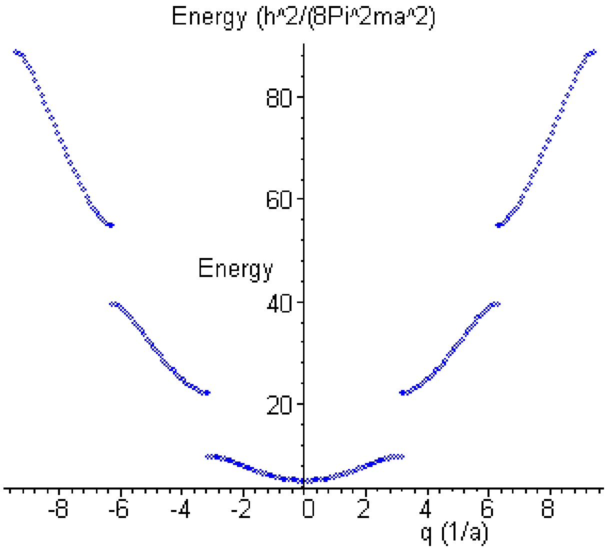
```
>
> # (-q, energy) of the left branches
> for n from band+1 to 2*band do
> for i from 1 to div1 do
> listqp[2*i-1]:=-q[n-band,i]:
> listqp[2*i]:=energy[n-band,i]:
> od:
> plotlist[n]:=convert(listqp,list):
> od:
```

qelist contains the list of (q,energy) for all bands

```
> qelist:=[seq(op(plotlist[i]),i=1..2*band)]:
```

Plot the qelist.

```
> pointplot(qelist,title="Energy (h^2/(8Pi^2ma^2)",style=point,symbol=circle,symbolsize=4,color=blue,labels=[" q (1/a)","Energy"]);
```



Below is another solution to the problem.

```
> # Kronig-Penney model solution 2
```

Reset parameters

```
restart:
```

Number of bands

```
> band:=3:

> y:=proc(qa)

> local i,n,ka,eq;
```

Loop to determine to which band q belongs

```
> for i to band+1 do

> if abs(qa)-(i-1)*evalf(Pi)>=0 \

> and abs(qa)-i*evalf(Pi)<0

> then

> n:=i;

> break;

> fi;

> od:

>
```

The eigenvalue equation

```
> eq:=cos(qa)=cos(yy)+3*Pi/2*sin(yy)/yy;
```

Solution k

```
> ka:=fsolve(eq,yy,(n-1)*Pi..n*Pi);
```

Energy = k^2

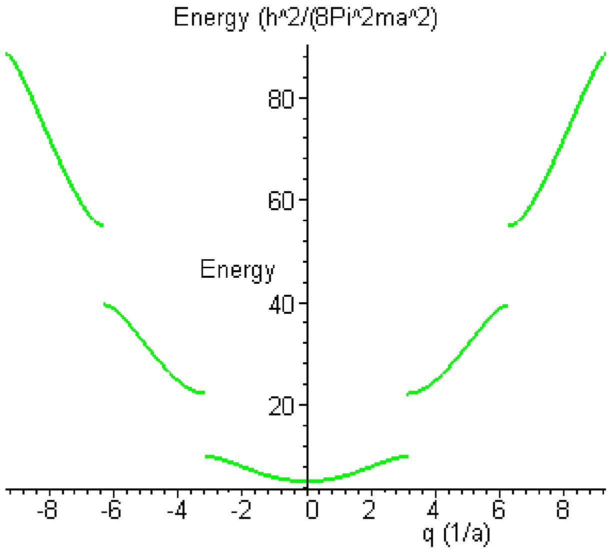
```
> ka^2;

> end:
```

0.99 below is used to avoid fictitious vertical line at the two extreme discontinuous boudaries.

```
> plot(y,-band*Pi*0.99..band*Pi*0.99,title=`Energy
(h^2/(8Pi^2ma^2)`,labels=[`q
(1/a)`,`Energy`],color=green,discont=true,thickness=2);

>
```



Appendix IV

$$-\hbar^2\frac{\partial^2\Psi}{\partial x^2} = \hbar^2 k^2\Psi = p^2\Psi \text{ , for } \Psi = e^{i(kx-\omega t)}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V(x)\Psi(x) = E\Psi(x)$$

$$P(x) = \Psi(x)\Psi^*(x)$$

$$\int_{-\infty}^{\infty} P(x)\,dx = 1$$

$$< f(x,p) >= \int_{-\infty}^{\infty} \Psi(x)F(x)\Psi^*(x)\,dx$$

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} = E\Psi(x) \text{ , for } 0 < x < L_x$$

$$\Psi(x) = A\sin(\frac{\sqrt{2mE}}{\hbar}x) + B\cos(\frac{\sqrt{2mE}}{\hbar}x)\text{, for } 0 < x < L_x$$

$$\Psi(0) = 0 \text{ and } \Psi(L_x) = 0$$

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