

Chapter 3

Optical Absorption Coefficient

As mentioned above (Section 1.4.3), Kovalev et al. (1996) who studied the optical absorption of porous silicon suggests that porous silicon behaves like an indirect band-gap semiconductor, of which optical transition is phonon-assisted for photon energies up to 3 eV, as agreed with Datta and Narasimhan (1999). However, Kovalev et al. (1998) found that the spatial confinement of electrons and holes inside a nanocrystalline silicon increases the uncertainty of their crystal momentum, thus, resulting in optical transitions in which phonons are not involved. This indicates that the non-phonon assisted transitions probably consist in the optical absorption of porous silicon, contrasting with former suggestions.

Here, we have attempted to study such contradiction by calculating optical absorption coefficients in porous silicon which are contributed only from non-phonon assisted process. The non-phonon assisted processes can occur only when they involve with localized states because wave functions of localized states widely spread in momentum space so that the non-phonon assisted process can take place. On the other hand, such process cannot occur in transitions between delocalized states with well defined wave vectors. Then we neglect all transitions between delocalized states in our calculation. However, there are still some difficulties in optical absorption calculation due to unclear band structure of porous silicon, i.e., the position of bottom of the conduction band and top of the valence band in momentum space. Then we assume that all interested transitions are direct gap transitions, as a result, though the calculated absorption coefficients are

overestimated in magnitude but still be enough to determine the energy region of the non-phonon assisted process.

Before the calculation, let us now consider the quantum mechanical theory of absorption in this Section. Some basic approximations required will be mentioned first. Then the interaction between a radiation field and electrons in a medium will be studied by using standard quantum mechanics. For more understanding, a good review of basic concept of absorption in semiconductor can be found in Ph.D. thesis of Wichit Srirakool (1984).

3.1 Basic Approximations

We can express the kinetic energy of a system of N electrons in the presence of an electromagnetic field as follows

$$\sum_{i=1}^N \left[\frac{1}{2m} \left(\mathbf{p}_i + \frac{e}{c} \mathbf{A}(\mathbf{r}_i, t) \right)^2 \right] \quad (3.1)$$

$\mathbf{p}_i^2/2m$ stands for the kinetic energy of an individual free electron, e is the absolute value of the electronic charge and \mathbf{A} is the vector potential of the electromagnetic field. The choice of the Coulomb gauge implies that $\nabla \cdot \mathbf{A} = 0$. Moreover, all non-linear terms in the vector potential are also ignored because we deal with small amplitude of electromagnetic wave. Subsequently, the Hamiltonian describing the interaction of the electrons with the radiation field becomes

$$H' = \frac{e}{mc} \sum_{i=1}^N \mathbf{A}(\mathbf{r}_i, t) \cdot \mathbf{p}_i \quad (3.2)$$

which is treated as a time-dependent perturbation on the electronic states and will induce electrons to make transitions between occupied bands and empty

bands. According to the transition probability rate, the relationship between the electronic structure and optical constants can be derived.

The basic approximations used are the adiabatic scheme, the one-electron approximation and the effective mass approximation. These approximations can simplify the complicated many-body problem into a solvable eigenvalue equation. Many-body effects caused by electron-electron interactions are not studied significantly.

3.2 Quantum Theory of Absorption

If the perturbation term is $\hat{L} \exp(\pm i\omega t)$ and the time dependence is totally included in the exponent, the transition probability per unit time from the initial state $|i\rangle$ with energy E_i to the final state $|j\rangle$ with energy E_j becomes

$$P = \frac{2\pi}{\hbar} \left| \langle j | \hat{L} | i \rangle \right|^2 \delta(E_j - E_i - \hbar\omega) \quad (3.3)$$

The perturbation $\hat{L} \exp(-i\omega t)$ induces a transition with absorption of a photon of energy $\hbar\omega$ whilst $\hat{L} \exp(i\omega t)$ induces a transition with emission of a photon of energy $\hbar\omega$. The Dirac delta function indicates the conservation of energy. Since we examine the absorption only, the emission term is now disregarded.

Now, our observation is confined to the transitions from the valence band to the conduction band. The ground state of the electronic system can be expressed as a Slater determinant composed of all one-electron states in the valence band. It can be assumed that only one electron is excited to an excited state in the conduction band. Thus, the Slater determinant relating to the excited state will consist of $(N - 1)$ one-electron states in the valence band and only 1 one-electron state in the conduction band. So the matrix element of transition from

the ground state to the excited state as a result of the radiation field is only the transition from a one-electron state in the valence band to a one-electron state in the conduction band.

If ψ_{kv} and ψ_{kc} are defined as one-electron wave functions in the valence and conduction bands respectively and k 's are their corresponding wave vectors. Then the matrix element of the transition will be

$$\langle j | H' | i \rangle = \frac{e}{mc} \langle \psi_{kc} | \mathbf{A} \cdot \mathbf{p} | \psi_{kv} \rangle \delta_{sc,sv} \quad (3.4)$$

where sv and sc represent the spins of the two wave functions respectively. Through this work, we will neglect the spins and handle the energy states as a single state. When we approach the final expression for the absorption coefficient, spin will be re-introduced to cover the spin degeneracy.

The vector potential can be exhibited in the form of frequency and the polarization vector $\hat{\mathbf{e}}$ which is in the same direction as the field, i.e.

$$\mathbf{A}(\mathbf{r}, t) = A_0 \hat{\mathbf{e}} \exp[i(\mathbf{q} \cdot \mathbf{r} - \omega t)] + c.c. \quad (3.5)$$

where \mathbf{q} is the wave vector of the radiation and $c.c.$ is the complex conjugate of the previous term. Again, we will not consider the $c.c.$ which is the emission term. So the transition probability per unit time is

$$P = \frac{2\pi}{\hbar} \left(\frac{eA_0}{mc} \right)^2 \left| \langle \psi_{kc} | e^{i\mathbf{q} \cdot \mathbf{r}} \hat{\mathbf{e}} \cdot \mathbf{p} | \psi_{kv} \rangle \right|^2 \delta(E_c - E_v - \hbar\omega) \quad (3.6)$$

where E_v and E_c are the corresponding energies of the states in the valence and conduction bands, respectively. The magnitude of a typical photon wave vector is always small compared to the magnitude of the wave vectors for the electronic wave functions whose magnitude is of the order of a few angstroms. Thus the

exponential term in eq.(3.6) becomes unity and

$$P = \frac{2\pi}{\hbar} \left(\frac{eA_0}{mc} \right)^2 | \hat{\mathbf{e}} \cdot \mathbf{M}_{cv}(\mathbf{k}_c, \mathbf{k}_v) |^2 \delta(E_c - E_v - \hbar\omega) \quad (3.7)$$

where $\hat{\mathbf{e}} \cdot \mathbf{M}_{cv}(\mathbf{k}_c, \mathbf{k}_v) = \langle \psi_{k_c} | \hat{\mathbf{e}} \cdot \mathbf{p} | \psi_{k_v} \rangle$. The magnitude of \mathbf{M}_{cv} in the $\hat{\mathbf{e}}$ direction is

$$|\mathbf{M}_{cv}| = \hat{\mathbf{e}} \cdot \int_{\Omega} \psi_{k_c}(\mathbf{k}_c, \mathbf{r}) (-i\hbar\nabla) \psi_{k_v}(\mathbf{k}_v, \mathbf{r}) d\mathbf{r} \quad (3.8)$$

In order to get the rate of the transition per unit volume, $W(\omega)$, we have to sum eq.(3.7) over all possible states in the unit volume, i.e. we must sum over all wave vectors \mathbf{k}_c and \mathbf{k}_v (and over spin degeneracy). If there are more than one valence band or more than one conduction band, they must also be included. Since \mathbf{k}_c and \mathbf{k}_v are confined to the first Brillouin zone with a density $\Omega/(2\pi)^3$ (Ω stand for the volume of the crystal), the transition rate per unit volume is

$$W(\omega) = \frac{2\pi}{\hbar} \left(\frac{eA_0}{mc} \right)^2 \Omega \int \int_{\text{Brillouin zone}} \frac{d\mathbf{k}_c}{(2\pi)^3} \frac{d\mathbf{k}_v}{(2\pi)^3} \mathbf{M}_{cv}^2 \delta(E_c - E_v - \hbar\omega) \quad (3.9)$$

The absorption coefficient is also described as the energy absorbed in unit time and in unit volume divided by the energy flux.

The average energy density u in a medium of radiation field indicated by the vector potential in eq.(3.5) is related to the optical constants through the equation

$$u = \frac{1}{2\pi c} n^2 A_0^2 \omega^2 \quad (3.10)$$

where n is refractive index of crystalline silicon. Additionally, the energy density associated with a single photon of energy $\hbar\omega$ appears to be the same. The product of the average energy density u and the velocity of the propagation in the medium c/n is the energy flux. Thus, we can simply expressed the absorption coefficient

in terms of $W(\omega)$ as

$$\alpha(\omega) = \frac{\hbar\omega W(\omega) n}{uc} \quad (3.11)$$

or

$$\alpha(\omega) = \frac{4\pi^2 e^2 \Omega}{m^2 c n \omega} \int \int_{\text{Brillouin zone}} \frac{d\mathbf{k}_c}{(2\pi)^3} \frac{d\mathbf{k}_v}{(2\pi)^3} \mathbf{M}_{cv}^2 \delta(E_c - E_v - \hbar\omega) \quad (3.12)$$

In porous silicon, the wave vector can no longer be a good quantum number because translational symmetry is destructed by the random vacancy potentials. This leads to the conversion of the integration over all wave vectors to the integration over all energies. Using one of the definitions of the density of states

$$\rho(E) = \frac{1}{(2\pi)^3} \frac{d\mathbf{k}}{dE}$$

and a property of the delta function, eq.(3.12) can be rewritten as follows

$$\alpha(\omega) = \frac{4\pi^2 e^2 \Omega}{m^2 c n \omega} \int_{-\infty}^{\infty} dE \rho_v(E) \rho_c(E + \hbar\omega) \mathbf{M}_{cv}^2. \quad (3.13)$$

This suggests that the absorption coefficient depends on the density of states at the initial energy, the density of states at the mapping energy, and also the matrix element linking the initial and the final states through the interaction Hamiltonian which is so called momentum operator.

Hence, the density of states and the matrix element of transition becomes the two basic physical quantities required for the determination of the absorption coefficient of porous silicon.

It should be noted that eq.(3.13) is valid only at absolute zero temperature. In such a condition, all the valence band states are occupied and all the conduction band states are empty and there is no thermal excitation. Then, introduction of the thermal factor, which describes the occupancy at such a temperature, to the expression for the absorption coefficient is necessary if one would

like to compare our results with experiments. This thermal factor can also be called the occupancy factor and defined in terms of the Fermi function $f(E)$ as follows

$$f(E)[1 - f(E + \hbar\omega)] - f(E + \hbar\omega)[1 - f(E)] = f(E) - f(E + \hbar\omega), \quad (3.14)$$

where $f(E)$ represents a probability that the state of energy E is occupied and $1 - f(E)$ represents the probability that the state of energy E is unoccupied. Then the first term of the left-hand side is interpreted as the optical absorption occurrence whereas the second term is interpreted as the probability of occurring of emission. So eq.(3.14) can be interpreted as the total probability of occurring of optical absorption.

Multiplying the integrand in eq.(3.13) by this factor, we can get

$$\alpha(\omega) = \frac{4\pi^2 e^2 \Omega}{m^2 c n \omega} \int_{-\infty}^{\infty} dE \rho_v(E) \rho_c(E + \hbar\omega) M_{cv}^2 [f(E) - f(E + \hbar\omega)] \quad (3.15)$$

Eventually, the final expression for the absorption coefficient must include the spin degeneracy of each single state either by multiplying the right hand side of eq.(3.15) by a factor two and considering all single state wave function for the matrix element or by applying double-state density of states for both bands together with considering double-state wave functions for the matrix element. Both procedures will generate the same results which indicate that there is no interaction between two different spin states.

3.3 Matrix Element of Transition

The matrix element of transition defined in eq.(3.8) is clearly a function of the interaction Hamiltonian and the wave functions of initial and final states. The

wave function of an electron in a solid is always evaluated through a model because it cannot be exactly known. This also includes a crystalline semiconductor which its band structure is significantly complicated as well as the density of states of both valence and conduction bands do not go along with the theory, which shown perfect parabolic shapes. The interband absorption performed by assuming the two parabolic bands is just an approximate issue.

In this Section, our attention is to determine an appropriate matrix element of transition which physically agrees with our model.

It has been stated by Kohn and Luttinger (1957) that a state closed to a band extremum can be demonstrated as a Bloch periodic function at the extremum modulated by gradually varying envelope function. This well-known idea has been widely applied to porous silicon by a number of authors (Hybertsen, 1994 and Xie et al., 1994). Consequently, the state near band edge $\psi(\mathbf{r})$ can be written as the superposition between the Bloch function at $\mathbf{k} = 0$, $u_0(\mathbf{r})$ and the envelope function, $\phi(\mathbf{r})$

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \phi(\mathbf{r}) u_0(\mathbf{r}) \quad (3.16)$$

with normalizations

$$\frac{1}{\Omega} \int |u_0(\mathbf{r})|^2 d\mathbf{r} = 1 \quad (3.17)$$

and

$$\int |\phi(\mathbf{r})|^2 d\mathbf{r} = 1 \quad (3.18)$$

Let us now consider a transition from a state in the valence band to a state in the conduction band. If both states can be represented by wave function as shown in eq.(3.16), the matrix element of transition, which is essentially the overlap of the two wave functions by the momentum operator, is defined in

eq.(3.8) as

$$\mathbf{M}_{cv} = \frac{1}{\Omega} \int \phi_c^*(\mathbf{r}) u_c^*(\mathbf{r}) (-i\hbar\nabla) \phi_v(\mathbf{r}) u_v(\mathbf{r}) d\mathbf{r} \quad (3.19)$$

where c and v indicate the conduction and valence bands respectively. To facilitate the writing, the subscript "0" of $u_0(\mathbf{r})$ has been neglected.

The integration in eq.(3.19) can be splitted out into two integrals according to an assumption that the envelope function is gradually varying

$$\begin{aligned} \mathbf{M}_{cv} = & \left[\int \phi_c^*(\mathbf{r}) \phi_v(\mathbf{k}_v, \mathbf{r}) d\mathbf{r} \right] \left[\frac{1}{\Omega} \int u_c^*(\mathbf{r}) (-i\hbar\nabla) u_v(\mathbf{r}) d\mathbf{r} \right] \\ & + \left[\int \phi_c^*(\mathbf{r}) (-i\hbar\nabla) \phi_v(\mathbf{k}_v, \mathbf{r}) d\mathbf{r} \right] \left[\frac{1}{\Omega} \int u_c^*(\mathbf{r}) u_v(\mathbf{r}) d\mathbf{r} \right]. \end{aligned} \quad (3.20)$$

On the basis of the fact that $u_c(\mathbf{r})$ and $u_v(\mathbf{r})$ are orthogonal, the last term of eq.(3.20) is vanished and can then be rewritten as

$$\mathbf{M}_{cv} = \mathbf{M}_b \mathbf{M}_{env} \quad (3.21)$$

by defining

$$\mathbf{M}_b = \frac{1}{\Omega} \int u_c^*(\mathbf{r}) (-i\hbar\nabla) u_v(\mathbf{r}) d\mathbf{r} \quad (3.22)$$

and

$$\mathbf{M}_{env} = \int \phi_c^*(\mathbf{r}) \phi_v(\mathbf{r}) d\mathbf{r}. \quad (3.23)$$

Afterward, the matrix element of transition is squared and averaged over all directions and eq.(3.24) is achieved

$$|\mathbf{M}_{cv}^2| = |\mathbf{M}_b^2| |\mathbf{M}_{env}^2|. \quad (3.24)$$

$|\mathbf{M}_b^2|$ can be obtained by band-structure calculation as follows (Hybertsen, 1994)

$$\frac{|\mathbf{M}_b^2|}{2m_e} = 4 \text{ eV}. \quad (3.25)$$

Now on, only envelope matrix element will be substantially determined.

3.3.1 Envelope Matrix Element

Our density of states is derived through modelling potential fluctuation wells by harmonic wells and the obtained model provides Gaussian wave functions [see Appendix C]. However, the delocalized wave function obviously is plane wave. So the envelope function in our model is assumed to be a superposition of the obtained Gaussian wave function (C.7) and plane wave in order to cover both localized and delocalized states (Sritrakool, Sa-yakanit and Glyde, 1985). Then the envelope functions of the valence and conduction bands are

$$\phi_v(\mathbf{k}_v, \mathbf{r}) = \left(\frac{2\mu_v}{\pi}\right)^{3/4} \exp[i\mathbf{k}_v \cdot \mathbf{r}] \exp[-\mu_v |\mathbf{r} - \mathbf{r}_i|^2] \quad (3.26)$$

and

$$\phi_c(\mathbf{k}_c, \mathbf{r}) = \left(\frac{2\mu_c}{\pi}\right)^{3/4} \exp[i\mathbf{k}_c \cdot \mathbf{r}] \exp[-\mu_c |\mathbf{r} - \mathbf{r}_j|^2] \quad (3.27)$$

where \mathbf{r}_i and \mathbf{r}_j are the centers of the envelope functions and, $\mathbf{k}_{v,c}$, which stand for the wave vector of carriers, will be discussed later. The localization parameter $\mu_{v,c}$ is related to the variational parameter through

$$\mu_{v,c} = \frac{m\omega_{v,c}}{2\hbar} = \frac{z_{v,c}}{4L^2}. \quad (3.28)$$

Then, the envelope matrix element which is defined relying on eq.(3.23) is

$$\mathbf{M}_{env} \sim \int \exp[-i(\mathbf{k}_c - \mathbf{k}_v) \cdot \mathbf{r}] \exp[-\mu_v |\mathbf{r} - \mathbf{r}_i|^2] \exp[-\mu_c |\mathbf{r} - \mathbf{r}_j|^2] \quad (3.29)$$

where the normalized factors of the envelope functions are temporarily ignored.

Applying the Gaussian integration formula,

$$\int_{-\infty}^{\infty} \exp[-ax^2 + bx] dx = \left(\frac{\pi}{a}\right)^{1/2} \exp\left[-\frac{b^2}{4a}\right], \quad (3.30)$$

eq.(3.29) then becomes

$$\begin{aligned} \mathbf{M}_{env} \sim & \left(\frac{\pi}{\mu_v + \mu_c} \right)^{3/2} \exp [- (\mu_v \mathbf{r}_i^2 + \mu_c \mathbf{r}_j^2)] \\ & \exp \left[\frac{\{i (\mathbf{k}_c - \mathbf{k}_v) + 2 (\mu_v \mathbf{r}_i + \mu_c \mathbf{r}_j)\}^2}{4 (\mu_v + \mu_c)} \right]. \end{aligned} \quad (3.31)$$

The magnitude of squared of envelope matrix element is

$$|\mathbf{M}_{env}^2| \sim \left(\frac{\pi}{\mu_v + \mu_c} \right)^3 \exp \left[- \frac{(\mathbf{k}_c - \mathbf{k}_v)^2}{2 (\mu_v + \mu_c)} \right] \exp \left[- \frac{2\mu_v\mu_c}{\mu_v + \mu_c} (\mathbf{r}_i - \mathbf{r}_j)^2 \right]. \quad (3.32)$$

Since we obviously concern with a random system, it is important to average the result over all random positions $\mathbf{r}_i, \mathbf{r}_j$ and the angle between wave vector \mathbf{k}_c and \mathbf{k}_v , θ , then

$$\begin{aligned} \langle |\mathbf{M}_{env}^2| \rangle_{\mathbf{r}_i, \mathbf{r}_j, \cos \theta} &= \frac{1}{2} \int_{-1}^1 d \cos \theta \int \frac{d\mathbf{r}_i}{\Omega} \int \frac{d\mathbf{r}_j}{\Omega} |\mathbf{M}_{env}^2| \\ &\sim \frac{1}{\Omega} \left(\frac{\pi}{\mu_v + \mu_c} \right)^3 \left(\frac{\pi (\mu_v + \mu_c)}{2\mu_v\mu_c} \right)^{3/2} \exp \left[- \frac{(k_c + k_v)^2}{2 (\mu_v + \mu_c)} \right] \\ &\quad \cdot \left(\frac{\mu_v + \mu_c}{k_c k_v} \right) \sinh \left(\frac{k_c k_v}{\mu_v + \mu_c} \right). \end{aligned} \quad (3.33)$$

Reintroducing the normalization factors into eq.(3.33) results in

$$\langle |\mathbf{M}_{env}^2| \rangle_{\mathbf{r}_i, \mathbf{r}_j, \cos \theta} = \frac{1}{\Omega} \left(\frac{2\pi}{\mu_v + \mu_c} \right)^{3/2} \left(\frac{\mu_v + \mu_c}{k_c k_v} \right) \sinh \left(\frac{k_c k_v}{\mu_v + \mu_c} \right) \exp \left[- \frac{(k_c + k_v)^2}{2 (\mu_v + \mu_c)} \right] \quad (3.34)$$

which represents the envelope matrix element used in our work. However, it still be in entangled form, $\langle |\mathbf{M}_{env}^2| \rangle_{\mathbf{r}_i, \mathbf{r}_j, \cos \theta}$. So, from now on, it will be simply rewritten as $|\mathbf{M}_{env}^2|$.

Further problem is how to determine k_c and k_v . According to the existence of the mobility edge as we discussed previously in Section 2.4, the change of state from localized to delocalized, in disordered systems, is undoubtedly sudden

instead of continuous. The states below the mobility edge are all localized and allow all k 's equal to zero. On the other hand, the states above the mobility edge are all delocalized and are assumed to have parabolic $E - k$ dispersion relationship similar to that of free carrier

$$k_c = \left(\frac{2m_e}{\hbar^2} (E - E'_c) \right)^{1/2} \quad (3.35)$$

and

$$k_v = \left(\frac{2m_h}{\hbar^2} (E'_v - E) \right)^{1/2} \quad (3.36)$$

Prior to numerical calculation, we also note that, in this calculation, the band gap of crystalline silicon is generally temperature dependent (Singh, 1995) :

$$E_g(T) = E_g(0) - \beta T \quad (3.37)$$

where $E_g(0)$ is the energy gap of crystalline silicon at 0K (1.17 eV) and $\beta = 0.5$ meV/K.

3.4 Numerical Results of Absorption Coefficient

In this Section the calculated results of optical absorption are presented. The calculation employs the model discussed previously with the density of states constructed in Chapter 2. The optical absorption coefficients are calculated using eq.(3.15) multiplied by two to include spin degeneracy, i.e.

$$\alpha(\omega) = \frac{8\pi^2 e^2 \Omega}{m^2 c n \omega} \int_{-\infty}^{\infty} dE \rho_v(E) \rho_c(E') |\mathbf{M}_{cv}^2(E, E')| [f(E) - f(E')] \quad (3.38)$$

where $E' = E + \hbar\omega$. The density of states, employed here, is PS DOS eq.(2.98) consists of the low-energy density of states $\rho_L(E)$ up to the energy E^* at which

it crosses the high-energy density of states $\rho_H(E)$. Thereafter, the high-energy density of states is displayed. Furthermore, we sensibly assume an effective unit band mass of $0.58m_0$ (Singh, 1995) in density of states of valence band. For conduction band, an effective unit band mass of $0.32m_0$ is presumed (Singh, 1995). However, in order to include the six valleys of conduction band, it is essential to multiply the density of states by six (Singh, 1995).

The matrix element of transition manipulated in this calculation is given by eqs.(3.24), (3.25) and (3.34). The values of k_v , k_c , μ_v and μ_c are determined through the method described in Section 3.3.1. In our model, we suggest that autocorrelation length L is approximately $a_0/\sqrt{\ln 2}$ (see Appendix A) which, therefore, is applied in the calculations.

In the calculations, we consider only 60%, 65%, 71% and 80% porosity which are valid in our model. The calculated results of optical absorption coefficients at 71% porosity as a function of photon energy at 300K, 100K and 7K are illustrated in Figures 3.2, 3.3 and 3.4, respectively and at 80% porosity at 300K, 100K and 7K are also shown in Figures 3.5, 3.6 and 3.7, respectively. Every curve exhibits a significant peak at slightly above their mobility gap with the magnitude of about 80 cm^{-1} when of about 0 cm^{-1} is found elsewhere. For 60% and 65% porosity, the calculated absorption coefficients are close to 0 cm^{-1} through all energy range of study as shown in Figure 3.1.

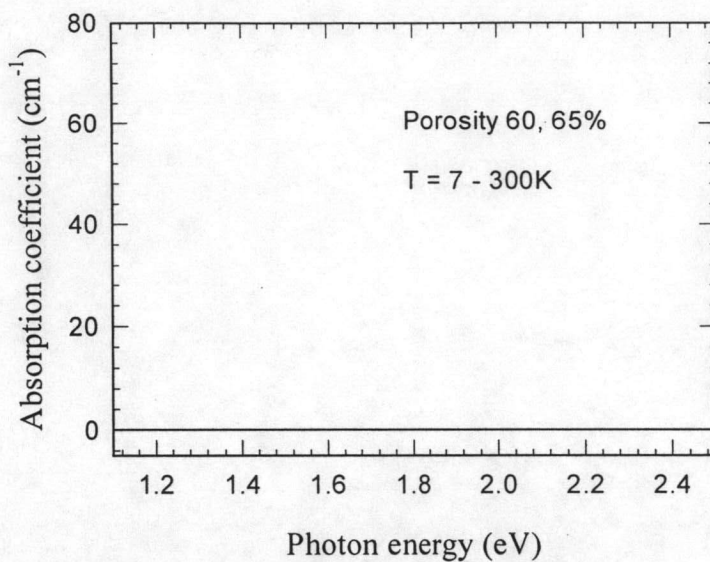


Figure 3.1: Calculated absorption coefficient as a function of photon energy at 60% and 65% porosity and $T = 7-300\text{K}$

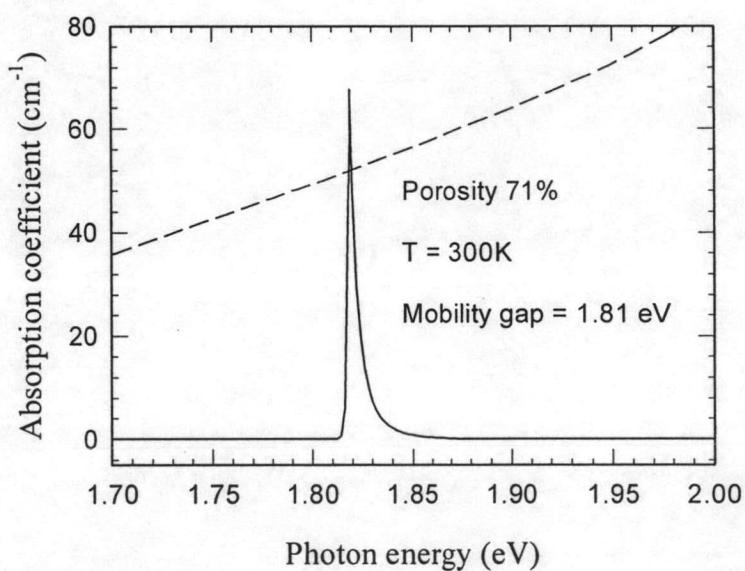


Figure 3.2: Calculated absorption coefficient as a function of photon energy at 71% porosity and $T = 300\text{K}$ (solid line) and experimental result of Kovalev et al. (1996) (dashed line)

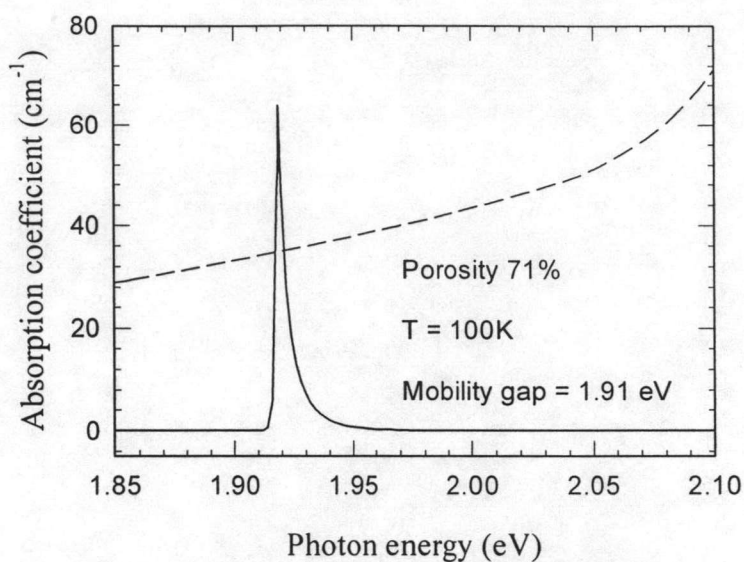


Figure 3.3: Calculated absorption coefficient as a function of photon energy at 71% porosity and $T = 100\text{K}$ (solid line) and experimental result of Kovalev et al. (1996) (dashed line)

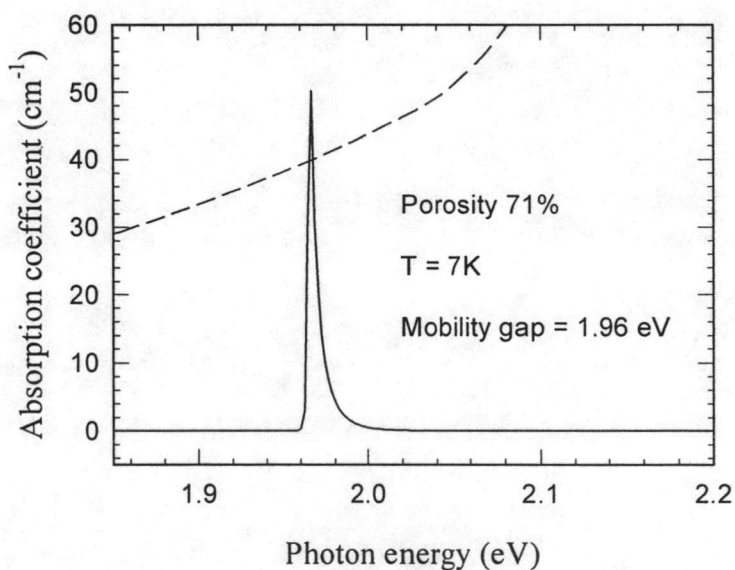


Figure 3.4: Calculated absorption coefficient as a function of photon energy at 71% porosity and $T = 7\text{K}$ (solid line) and experimental result of Kovalev et al. (1996) (dashed line)

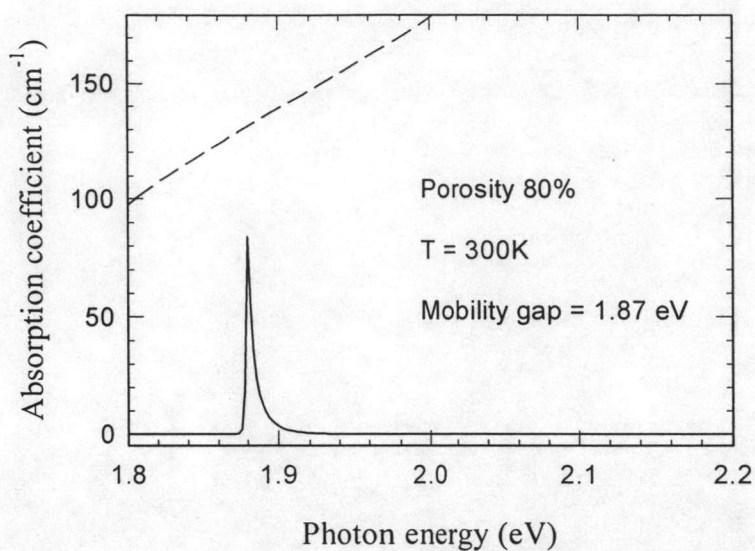


Figure 3.5: Calculated absorption coefficient as a function of photon energy at 80% porosity and $T = 300\text{K}$ (solid line) and experimental result of Kovalev et al. (1996) at 86% porosity (dashed line)

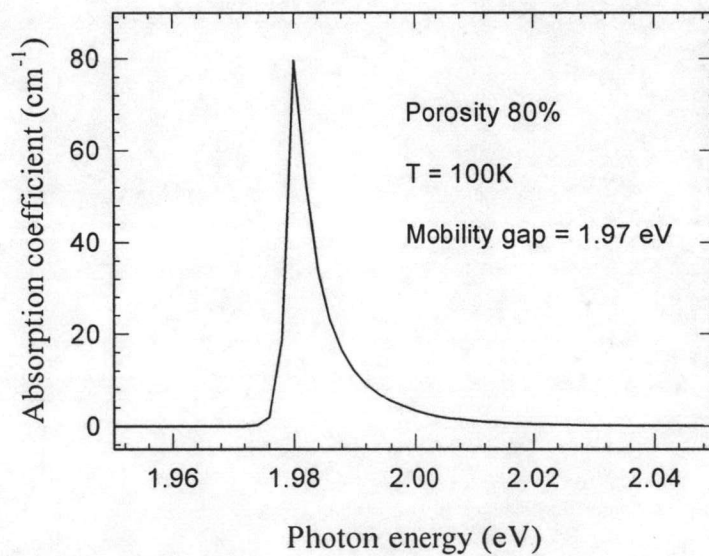


Figure 3.6: Calculated absorption coefficient as a function of photon energy at 80% porosity and $T = 100\text{K}$

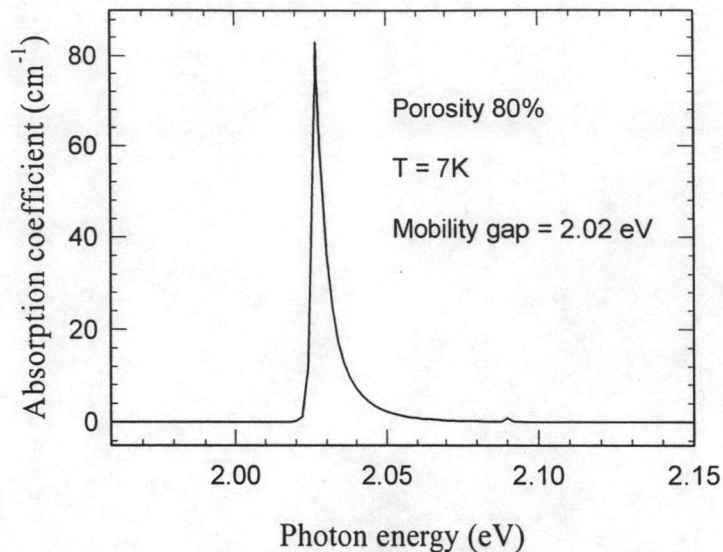


Figure 3.7: Calculated absorption coefficient as a function of photon energy at 80% porosity and $T = 7\text{K}$

These can be concluded that non-phonon assisted transition significantly involves with optical absorption only in a small range of energy ($\lesssim 0.05\text{ eV}$) with porosity above 70%. In addition, the magnitude of peak arised from calculated results are comparable with that of the experimental results (Kovalev et al, 1996). However, our results are overestimated due to the assumption of direct gap transition. This indicates that the calculated magnitude is substantially smaller and may be ignored when it is calculated rigorously. This also implies that non-phonon assisted process can be neglected in the optical absorption, at least in the energy range of study.