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Dispersion Relation Due to the Interaction of the Atoms of Titanium and Oxygen Owing to Electron Trapping by the Anode (TiO_2) of a Dye-sensitized Solar Cell

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ABSTRACT

Titanium dioxide is an important raw material for the fabrication of the anode of a dye-sensitized solar cell. The fact it that electrons are trapped within this anode as they flow through it. These trapped electrons tend to set the atoms of titanium dioxide into vibration. Here this vibration (interaction) has been investigated. The aim of the research was to generate the dispersion relation owing to the interaction between the atoms of titanium and oxygen in a unit cell of the crystal of TiO_2. Certain assumptions were made before formulation the mathematical mode that generated the dispersion relation. The result showed a dispersion relation at various angular steps.

Key words: Titanium dioxide, dispersion relation, solar cell, dectrons

INTRODUCTION

The present inefficiency of the Dye-sensitized solar cells has been partly due to electron trapping by the anode (Tachibana *et al*., 2000). The anode of a standard dye-sensitized solar cell is made of an oxide of Titanium, known as titanium dioxide (TiO_2) (Yu and Chen, 2009; Snaith and Ducati, 2010; Efurumibe *et al*., 2012). Here the impact of electron trapping on TiO_2 crystal was investigated. Titanium dioxide is a naturally occurring oxide of titanium with the chemical formula TiO_2. It has a wide range of applications, ranging from paint to sunscreen to food colouring and to nanotubes. When used as nanotubes, for example as in dye-sensitized solar cells, they allow electrons to pass through them. Some of these electrons passing through these tubes (usually used as the anode) are trapped within the tubes, thereby causing the atoms of the tube to become unstable. This leads to interatomic vibration which leads to intermolecular vibration of the nanotubes. The aim of this work was to obtain the dispersion relation (Yeap *et al*., 2011) due to the interaction between atoms of TiO_2 used as nanotubes in dye-sensitized solar cells.

FORMULATION OF THE MODEL

Before the mathematical model, certain assumptions were made. These assumptions made here are based on the proper understanding challenges of electron transport through the anode (TiO_2) of a dye sensitized solar cell. From literature, through the anode (TiO_2) of a dye sensitized solar cell is a porous one. Figure 1 for a simple structure of the anode showing the pores and electrons movement through the pores. In this model, the pore structure is considered only in one dimension

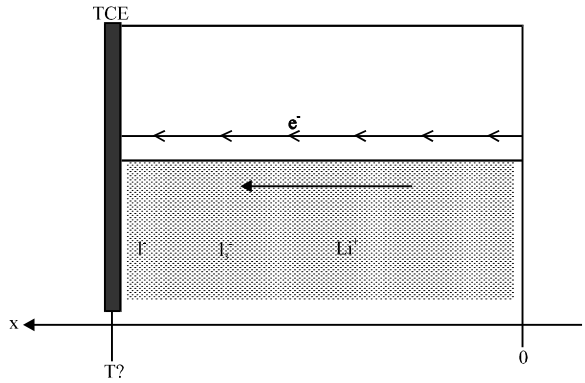

Fig. 1: Simplified structure of a single pore in one-dimension with effective pore length T?

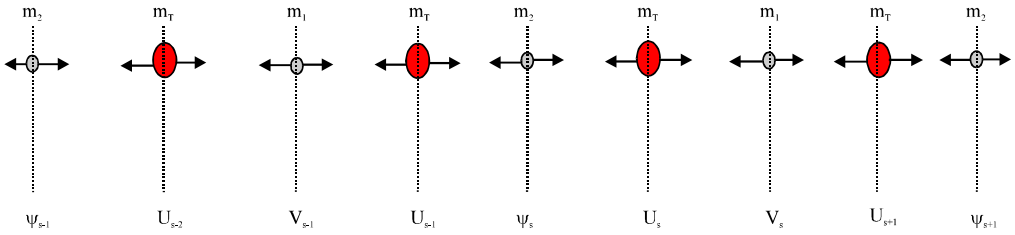

Fig. 2: Displacement modes of the atoms of TiO_2. The arrows indicate the interaction between the atoms in one dimension (the x-axis)

and that is along the x-axis, as shown in Fig. 1. And thus the vibration of the atoms is also considered in one dimension only.

Figure 2 depicts inter atomic interaction between the oxygen atoms and titanium atom for a unit cell of the crystal. The following specific assumptions were made:

- The subscript "1" in Fig. 2 represents the first oxygen atom at the right of titanium atom while the subscript "2" represents the second oxygen atom at the left of titanium atom
- The subscript "s" represents lattice site of interaction and that defines the original position of the atoms
- The subscript "s+1" represents the first displaced position of the atoms to the right while the subscript "s-1" represents the first displaced position of the atoms to the left
- U_s, V_s and ψ_s represent the displacement of the titanium atom, the first oxygen atom and the second oxygen atom, respectively at 's' position. U_{s+1}, V_{s+1} and ψ_{s+1} represent the first displacement of the respective atoms to the right. U_{s-1}, V_{s-1} and ψ_{s-1} represent the first displacement of the respective atoms to the left

MATHEMATICAL MODELLING OF THE INTERACTION

Here we aimed to obtain the dispersion relation (Benhaliliba and Belasri, 2006) due to the interaction. We employ Fig. 2 in this modeling. Following Hook's law we write:

$$M_T \frac{\partial^2 Us}{\partial t^2} \quad K(\psi_s - U_s) + K(V_s - U_s) \tag{1}$$

$$M_1 \frac{\partial^2 Vs}{\partial t^2} = K(U_s - V_s) + K(U_{s+1} - V_s) \quad (2)$$

$$M_2 \frac{\partial^2 \psi s}{\partial t^2} K(U_{s-1} - \psi_s) + K(U_s - \psi_s) \quad (3)$$

The three relations reduce to:

$$M_T \frac{\partial^2 Us}{\partial t^2} K(\psi_s + V_s - 2U_s) \quad (4)$$

$$M_1 \frac{\partial^2 Vs}{\partial t^2} K(U_s + U_{s+1} - 2V_s) \quad (5)$$

$$M_2 \frac{\partial^2 \psi s}{\partial t^2} K(U_{s-1} + U_s - 2\psi_s) \quad (6)$$

Applying the travelling wave solution:

$$U_s = U \exp I(sqa - wt) \quad (7)$$

$$V_s = V \exp I(sqa - wt) \quad (8)$$

$$\psi_s = \psi \exp I(sqa - wt) \quad (9)$$

$$U_{s+1} = U \exp I[(s+1)qa - wt] \quad (10)$$

$$U_{s-1} = U \exp I[(s-1)qa - wt] \quad (11)$$

Where:

W = Angular frequency of the travelling wave
t = Time taken
q = Wave vector
a = Lattice constant (It is equivalent to the distance covered by the wave in one cycle)
K = Stiffness coefficient

Next the derivative of the solutions are carried out to obtain the forms of Eq. 4, 5 and 6:

$$\frac{\partial Us}{\partial t} = iwU \exp i(sqa - wt) \quad (12)$$

$$\frac{\partial^2 Us}{\partial t^2} = i^2 \ w^2 \ U \exp i(sqa - wt) \quad (13)$$

$$\frac{\partial^2 Us}{\partial t^2} = -w2U_s \quad (14)$$

Similarly:

$$\frac{\partial^2 Vs}{\partial t^2} = -w^2 V_s \tag{15}$$

$$\frac{\partial^2 \psi s}{\partial t^2} = -w^2 \psi_s \tag{16}$$

$$\begin{aligned} Us+1 &= U \exp i[(s+1)qa-wt] \\ &= U \exp i[(sqa+qa)-wt] \\ &= U \exp I(sqa-wt).expiqa \end{aligned}$$

$$Us+1 = Us.expiqa \tag{17}$$

Similarly:

$$U_{s-1} = U_s exp\ (-iqa) \tag{18}$$

Substituting Eq. 14, 15, 16, 17 and 18 into equations 4, 5 and 6:

$$-M_T\, w^2 U_s = K(\psi_s + V_s - 2U_s) \tag{19}$$

$$-M_1\, w^2 V_s = K(U_s + U_s expiqa - 2V_s) \tag{20}$$

$$-M_2\, w^2 \psi_s = K(U_s exp(-iqa) + U_s - 2\psi_s) \tag{21}$$

Sorting Eq. 19, 20 and 21 into terms of U_s, V_s and ψ_s, we obtain:

$$(2K - M_T w^2)U_s - KV_s - K\psi_s = 0 \tag{22}$$

$$(2K - M_1 w^2)V_s - K(1 + expiqa)U_s = 0 \tag{23}$$

$$(2K - M_2 w^2)\psi_s - K(exp(-iqa) + 1)U_s = 0 \tag{24}$$

Following matrix algebra we have:

$$\begin{vmatrix} 2k-M_T w^2 & -K & -K \\ -K(1+exp(iqa)) & 2k-M_1 w^2 & 0 \\ -K(exp(-iqa)+1) & 0 & 2k-M_2 w^2 \end{vmatrix} = 0$$

$$\begin{aligned} &[2K-M_T w^2 (4K^2 - 2KM_2 w^2 - 2KM_1 w^2 + M_1 M_2 w_2 - 0) \\ &+K(-2K^2 + KM_2 w^2 - 2K^2 expiqa + KM_2 w^2 expiqa - 0) \\ &-K(0-(-2K^2 exp(-iqa) + KM_1 w^2 exp(-iqa) - 2K^2 + KM_1 w^2] = 0 \end{aligned} \tag{25}$$

$$[8K^3-4K^2M_2w^2-4K^2M_1w^2+2KM_1M_2w^4-4K^2M_Tw^2 +2KM_TM_2w^4+2KM_TM_1w^4-M_TM_1M_2w^6-2K^3 +K^2M_2w^2-2K^3expiqa+K^2M_2w^2expiqa-2K^3exp(-iqa) +2K^3exp(-iqa)+K^2M_1w^2exp(-iqa)-2K^3+K^2M_1w^2]=0 \quad (26)$$

$$[-M_TM_1M_2w^6+4K^2w^2(-M_2-M_1-M_T)+2Kw^4(M_1M_2+M_TM_2+M_TM_1) +K^2w^2(M_2+M_2expiqa+M_1exp(-iqa)+M_1)+constant]=0 \quad (27)$$

$$Constant = 8K^3-2K^3-2K^3expiqa-2K^3exp(-iqa)-K^3$$

Equation 27 reduces to:

$$[-M_TM_1M_2w^6+2Kw^4(M_1M_2+M_TM_2+M_TM_1)+F(w^2)+constant]=0$$

$$F(w^2)=K^2w^2(-4M_2+M_2+M_2expiqa-4M_1+M_1exp(-iqa)+M_1-4M_T)$$
$$=K^2w^2(-3M_2+M_2expiqa-3M_1+M_1exp(-iqa)-4M_T)$$

Since oxygen atoms have the same mass we can write:

$$M_1 = M_2 = M$$

Thus:

$$F(w^2) = K^2w^2[-6M-4M_T+M(expiqa+exp(-iqa))]$$

From trigonometric identities we have that:

$$expiqa = cosqa+isinqa$$

$$exp(-iqa) = cosqa-isinqa$$

$$expiqa+exp(-iqa) = 2cosqa$$

Thus:

$$F(w^2) = K^2w^2(2Mcosqa-6M-4M_T) \quad (28)$$

Also the constant term reduces to:

$$Constant = 4K^3-4K^3cosqa = 4K^3(1-cosqa) \quad (29)$$

qa = Phase angle of the elastic wave generated due to the vibration of the atoms
w = Frequency of the elastic wave

Equation 27 therefore reduces to:

$$-M_TM^2w^6+2Kw^4(M^2+2MM_T)+K^2w^2(2Mcosqa-6m-4M_T)+4K^3(1-cosqa)=0 \quad (30)$$

At relatively long wavelength, qa will tend to zero leading to:

$$4K^3(1-cosqa)=0$$

Therefore, Eq. 30 reduce to:

$$(w^2)^2-2Kw^2(M^2+2MM_T)/M_TM^2-K^2(2Mcosqa-6m-4M_T)/M_TM^2=0 \quad (31)$$

The above equation gives a form of quadratic equation:

$$ax^2+bx+c$$

with the roots determined from:

$$x=\left(-b\pm\sqrt{(b\text{^}2-4ac)}\right)/2a$$

Comparatively:

$$a=1,\ x=w^2,$$
$$b=-2K(M^2+2MM_T)/M_TM^2$$
$$c=-K^2(2Mcosqa-6m-4M_T)/M_TM^2$$

The masses: M and M_T have been obtained as approximately:

$$M=2.6788\times10^{-26}kg$$
$$M_T=3.4158\times10^{-25}kg$$

'b' was obtained as: 0.0166

Again, Sokolov *et al.* (1999) has obtained the value of K as: -4×10^{-8} N m^{-1}.

These values were used to solve the problem. The constant 'c' was obtained as:

$$c=7.8693\times10^{46}-3.49717\times10^{45}cosqa$$

With these the following roots were obtained:

$$w1=sqrt(-0.0083+sqrt(-7.8693\times10^{46}+3.49717\times10^{45}cosqa))$$
$$w2=sqrt(-0.0083-sqrt(-7.8693\times10^{46}+3.49717\times10^{45}cosqa))$$

A MATLAB programme was afterwards written to plot the dispersion relation.

RESULTS

The result shown in the Fig. 3-8 were obtained here.

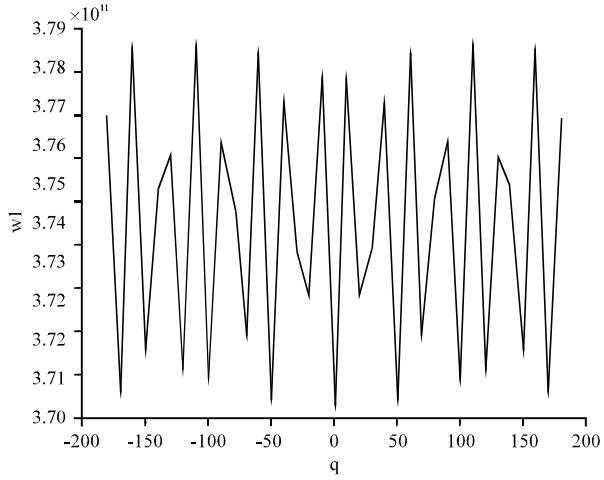

Fig. 3: Dispersion relation of the interaction for the first root in angular step of 10°

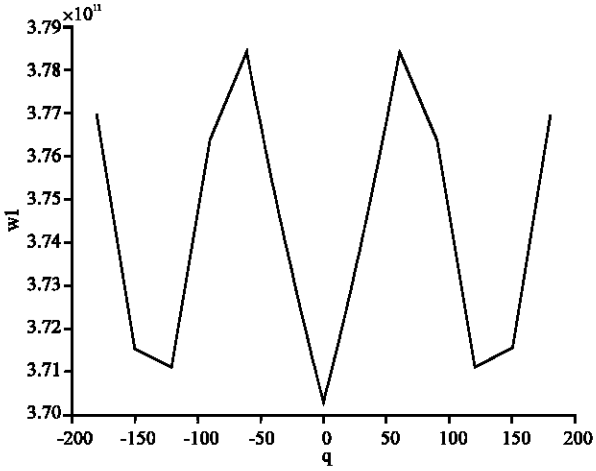

Fig. 4: Dispersion relation of the interaction for the first root in angular step of 30°

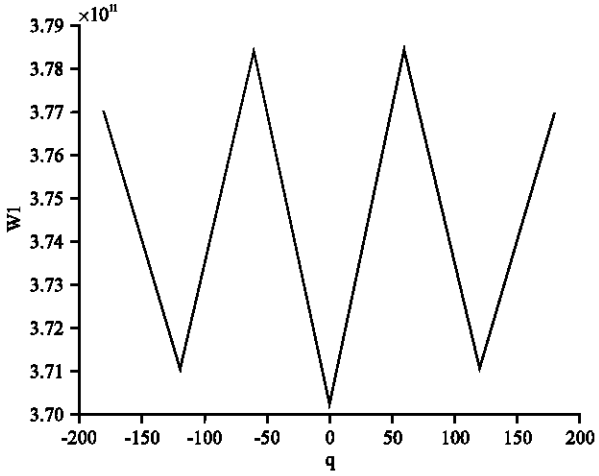

Fig. 5: Dispersion relation of the interaction for the first root in angular step of 60°

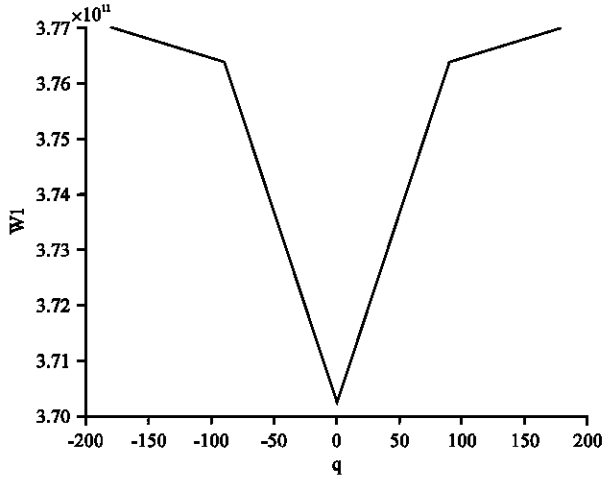

Fig. 6: Dispersion relation of the interaction for the first root in angular step of 90°

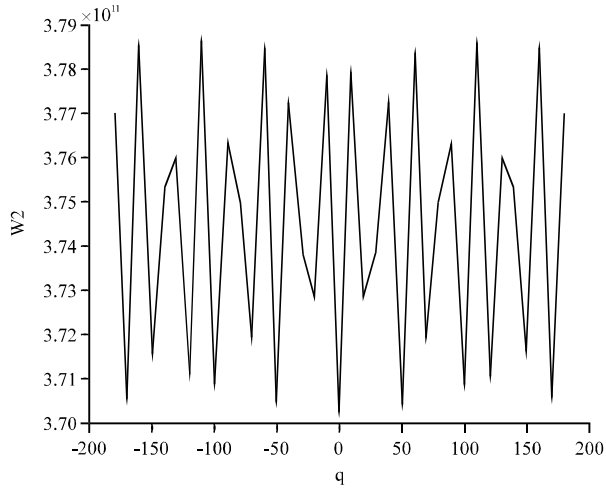

Fig. 7: Dispersion relation of the interaction for the second root in angular step of 10°

ANALYSIS OF RESULT

The dispersion relation plotted from the two roots w1 and w2 gave the same form of wave (Fig. 3-6). Figure 3 shows a number of interactions between the atoms within the first and second Brillouin zones (that is between: -90 and 90 and between -180 and 180) and the elastic wave (Yeap *et al*., 2011) generated due to the interaction propagates to the right and to the left with increased frequency. As the angular step increases, the interactions decrease, thereby reducing losses. These figures show detailed propagation of the elastic wave within the Brillouin zone boundaries (Fig. 4-8). Since angular distances are proportional to linear distances, it can invariably be said that increase in the thickness of the anode will lead to reduction in the atomic interactions within the anode, thereby improving the efficiency of the cell (Efurumibe *et al*., 2012). This is an indirect confirmation of the result obtained by Beermann *et al*. (2002). The optical branch of the phonon wave is the portion of the wave that goes while the acoustical branch is the portion that points downwards. Researches are on to improve the efficiencies of other solar cells (Konan *et al*., 2007).

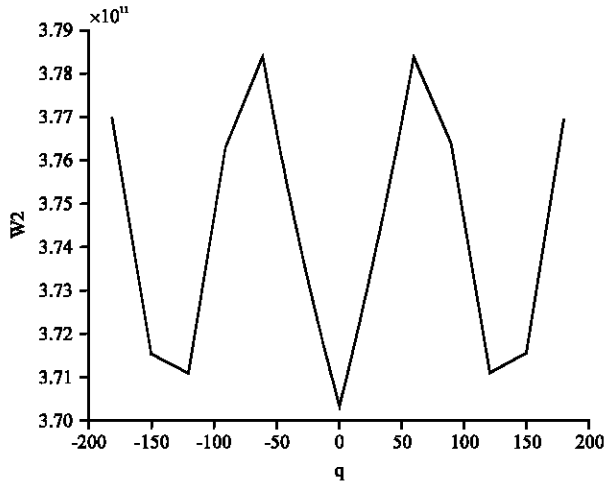

Fig. 8: Dispersion relation of the interaction for the second root in angular step of 30°

CONCLUSION

Looking at the results obtained, the conclusion is that the thickness of the TiO_2 should be improved in order to improve the efficiency of the dye-sensitized solar cell.

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