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MODEL OF PHOTOCATHODE FOR CW ELECTRON GUN

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Abstract

The rapid development of X-ray Free Electron Lasers (XFEL) requires continuous wave (CW) electron guns to provide high brightness electron bunch. Most of the proposed CW gun for free electron laser use semiconductors as photocathodes due to their high quantum efficiency and potentially low thermal emittance. We manage to establish a model to explain the photoemission of semiconductors with incident photon energy above or below the theoretical threshold and derive the expression for quantum efficiency and thermal emittance. For the incident photon energy near or below the threshold of the cathode, things will be subtle and we should be careful to consider the details we used to neglect. The results of quantum efficiency and thermal emittance agree well with the published work.

INTRODUCTION

The next generation of the XFEL is the most powerful scientific instrument for cutting edge research areas, such as material science and biology. To achieve the desired x-ray performance, many researches have been dedicated to making XFELs with high brightness and high repetition rate. This will give a great challenge to the fabrication and conditioning of the photocathode. High quantum efficiency (QE) is required to achieve high repetition rate. Thermal emittance is now of greater importance to high brightness, for it has gradually become the dominant term for beam emittance due to the development of electron gun technologies. Both characters are closely related to the photoemission of the cathode. Therefore, understanding the mechanism of photoemission will be helpful to the design of the cathode. Recently, some researchers [1, 2] have discovered that it is possible to obtain extremely low thermal emittance from semiconductors with photon energy lower than the emission threshold. These results cannot be explained by the previous model. In this paper, we would like to establish our photoemission model to explain the experimental results and explore the subtle nature near the threshold region.

MODEL OF SEMICONDUCTOR PHOTOCATHODE

Our model is shown in Fig. 1. We consider the photoelectrons provided by defect level and valance band. First, we define n_d as the ratio between the density of defect level and valance band. To estimate the value of n_d, we can do the following derivation. The electrons at defect level should follow the Fermi-Dirac statistics as

$$f(E_A) = \frac{1}{1+2\exp((E_A - E_F)/k_B T)}, \quad (1)$$

where E_A is the energy of a defect level beyond the bottom of the valance band, and E_F is the Fermi energy. The factor 2 is required in the expression for defect levels or impurities, representing two spins. The electrons occupied at the defect level can be calculated as

$$N_{\text{defect}} = N_A \times f(E_A), \quad (2)$$

where N_A is the density of acceptors. To estimate the electron density of the valance band, we use the effective mass approximation. The energy of electrons can be transferred to the free particle form near the bottom or top of the band. The density of states $g(E)$ can be defined as

$$\frac{2}{8\pi^3}\int d^3k = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{\frac{3}{2}}\int \sqrt{E}dE = \int g(E)dE \cdot \quad (3)$$

Based on the expression of the density of states, we can normalize the contribution of the defect level as

$$n_d = \frac{N_{\text{defect}}}{(2m_e^*/\hbar^2)^{\frac{3}{2}}/2\pi^2} \cdot \quad (4)$$

Thus, the distribution of excited electrons with regard to the energy can be expressed as

$$N(E) = n_d\sqrt{E}\delta(E-\hbar\omega+E_g-E_A) + \sqrt{E(E-\hbar\omega+E_g)}\,. \quad (5)$$

When the photon energy is below the threshold, the contribution from defect level will become remarkable. The formation of defect level starts from the vacancies of atoms, which is very universal during the fabrication process. If the atom happens to be a positive ion, then the vacancy behaves as a negative charge. It will attract a hole

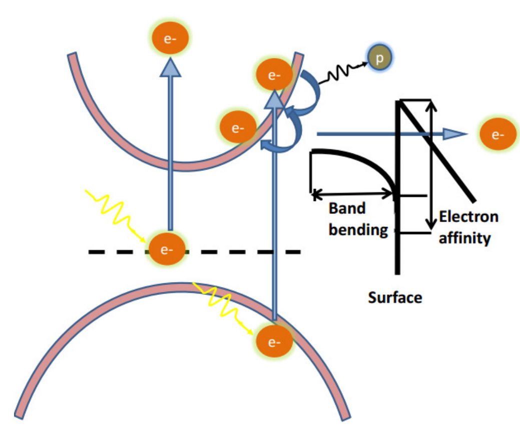

Figure 1: Model of photoemission for semiconductors.

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and form the defect level. In this case, the defect level is the acceptor level. If the initial atoms are negative ions, the defect level will be the same as the donor level. As shown in Fig. 1, the electrons from the defect level will always have higher energy than those from the valance band. This will considerably influence the value of the thermal emittance.

When the photon energy is lower than the threshold energy, the electrons from the valance band can still emit into the vacuum because the band bending at the surface reduces the effective electron affinity. The band bending is formed by the interaction between the surface state and the bulk. If the surface state is n-typed while the bulk is p-typed, which is usually the case for photocathodes, then the abundant electrons at the surface will move toward the bulk. Therefore, a p-n junction will form and the surface electric field is built. The electron traversing the band bending region will obtain extra energy in the longitudinal direction. We can estimate the band bending energy by assuming all the holes in the band bending region are occupied with electrons such that

$$E_b = \frac{N_A e d^2}{2\varepsilon\varepsilon_0}. \quad (6)$$

Absorbing a photon, some of excited electrons will move towards the surface for emission. They will experience scattering during the process. For semiconductors, electron-phonon scattering is dominant rather than the electron-electron scattering in metals. One collision will induce the electron to emit a phonon and lose energy E_{ph}. The direction of electron movement tends to maintain because it prefers to small angle scattering [3]. Therefore, it is a good assumption that the photoelectrons follow ballistic transport. We can calculate the transporting time as

$$t = \frac{s}{x \times \sqrt{2E/m}}, \quad (7)$$

where x is $\cos\theta$ and θ is the angle between the direction of electron movement and the normal direction of the surface, and s is the distance from surface.

The phonon scattering is mainly of two kinds, one is optical phonon scattering, the other is inter-valley scattering. The former can happen to all electrons with any energy while the latter can only happen when the electron have higher energy than the bottom of the other valley. The scattering rate $\lambda(E)$ is much higher for inter-valley scattering than for optical phonon scattering. This means the high energy electrons will lose energy more quickly than the low energy ones. The scattering rate $\lambda(E)$ can be calculated by the methods described by Fawcett [4]. Therefore, the energy loss ΔE can be expressed as

$$\Delta E = t \times \lambda(E) \times E_{ph}. \quad (8)$$

When the electrons arrive at the surface, they have some probability to tunnel through the vacuum barrier. We consider the triangle barrier model. This consideration is necessary, for when the photon energy is below the threshold, a large part of the excited electrons do not have enough energy to overcome the barrier. If we still use the step function, many photoelectrons will be deleted artificially and the analysis will result in a serious deviation from the reality. Therefore, we should carefully deal with the tunnel probability and take the expression for triangle barrier derived in the previous work [5]:

$$D(E) = \frac{4\sqrt{EH(E)}}{2\sqrt{EH(E)} + (H(E)+E)(e^{\theta(E)} - \frac{1}{4}(1-e^{-\theta(E)}))}, \quad (9)$$

$$H(E) = \sqrt{(E-E_a)^2 + (\frac{p_0^2\hbar^2(e\beta\xi)^2}{2m})^{\frac{3}{2}}}, \quad (10)$$

and

$$\theta(E) = \begin{cases} 0 & E > E_a \\ \frac{2}{e\hbar\beta\xi}\sqrt{2m(E-E_a)^3} & E < E_a \end{cases}, \quad (11)$$

where ξ is the electric field, m is the electron mass, and p_0 is equal to 0.51697. The field enhancement factor β is considered for the electric field in the expression D(E).

Under the above assumptions and derivations, we can derive the expression of the QE for semiconductors:

$$\mathrm{QE} = (1-R(\omega))\frac{\iiint N(E)F(s)T(E,s,x,\lambda(E))dEdsdx}{\int N(E)dE\int_{-1}^{1}dx}, \quad (12)$$

$$T(E,s,x,\lambda(E)) = D((E - \frac{s}{x\sqrt{2E/m}} \times \lambda(E) \times E_{ph})x^2 + E_{bend}), \quad (13)$$

and

$$F(s) = \alpha(\omega)e^{-\alpha(\omega)s}, \quad (14)$$

where $T(E,s,\cos\theta,\lambda(E))$ is the emission possibility of electrons excited from the depth s with energy E and direction θ. $\alpha(\omega)$ represents the light-absorption factor and $R(\omega)$ is the reflectivity.

To derive the thermal emittance, we can calculate MTE first and obtain the thermal emittance through

$$\varepsilon_n = \frac{1}{m_0 c}\sqrt{\langle x^2\rangle\langle p_x^2\rangle} = \sigma_x\sqrt{\frac{\mathrm{MTE}}{m_0c^2}}. \quad (15)$$

It has been supposed that the transverse position is irrelevant to the transverse momentum. Surface roughness is believed to have some unfavourable effect on the thermal emittance, but we will neglect its contribution in the following discussion and there exists fabrication methods to minimize the roughness. We assume the conservation of transverse momentum at the interface. Thus, the MTE can be expressed as

$$\mathrm{MTE} = \frac{\iiint N(E)F(s)T(E,s,x,\lambda(E))(1-x^2)EdEdsdx}{\iiint N(E)F(s)T(E,s,x,\lambda(E))dEdsdx}. \quad (16)$$

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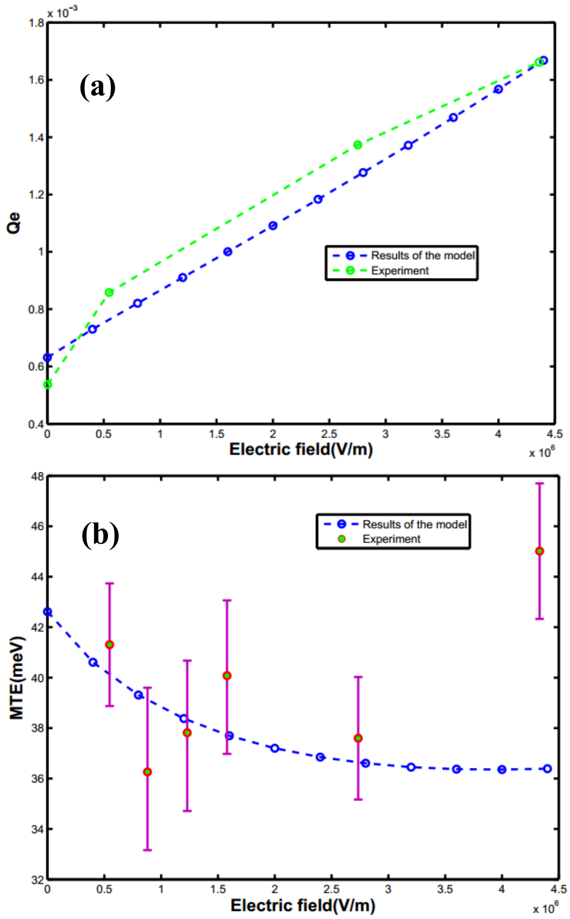

Figure 2: Comparison between calculation results of our model and the published data [1] in (a) QE and (b) MTE.

RESULTS

Our model succeeds in explaining the performance of the cathode when the incident photon energy is lower than the threshold. We take cesium antimonide with an incident photon energy of 1.8 eV as an example. The applied electric field is taken as a variable. We can see the calculation results fit well with the published work [1] for both QE and MTE. There exists an initial decrease for MTE with the enhancement of electric field. This is because the rise of the electric field enables the low energy valance band electrons to tunnel through the barrier with higher probability and reduce the ratio of defect level, resulting in the decrease of the average energy. Therefore, the participation of valance band is important to obtain low thermal emittance.

If we fabricate a perfect crystal, *i.e.* without any defect level, it will exert great influence on the thermal emittance. We take the applied electric field as a variable and calculate the situation with and without the consideration of defect level respectively. The results are shown in Fig. 3. We can see that the MTE will generally be larger with the consideration of defect level. This phenomenon is more visible at the low electric field. This is because the electrons from defect level have higher energy than those from valance

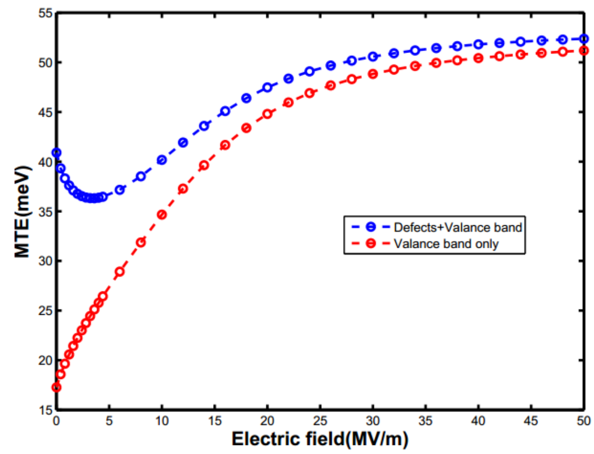

Figure 3: The difference in MTE with and without consideration of defect level.

band. When the electric field is low, the valance band electrons have little chance to tunnel through the barrier. But the defect level electrons are hardly affected. Therefore, the defect level electrons account for a large part of photoelectrons at the low gradient.

With the enhancement of the electric field, the effective electron affinity decreases and valance band electrons gradually become the dominant part of the photoelectrons. Thus, both lines have similar trends and values at large gradient. The case without defect level is similar to the situation at low temperature, for at that time the electron density is quite low at defect level and can be neglected.

CONCLUSION

In conclusion, we propose a model of photoemission of semiconductors and derive the expressions for QE and MTE. We take Cs_3Sb as an example and the results given by this model agree well with the published work. We also discover that perfect crystal may have lower thermal emittance at low electric field, but this advantage will be small at high gradient.

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