The role of trap depth and trap centers in thermoluminescence from semiconductor nanostructures

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Abstract

The absorption of radiation of energy greater than the band gap energy results in the ionization of valence electrons, producing free electrons in the conduction band and free holes in the valence band. The free electrons may become trapped at trap centers just below the conduction band and holes may be trapped at trap centers just above the valence band. The trapped electrons may be released back to the conduction band if they absorb enough energy E (called activation energy or trap depth), from where recombination with trapped holes is possible resulting in thermoluminescence (TL)). On the other hand, trap depth is the energy difference between the trap and the corresponding delocalized band. The temperature dependence of trap depth has been reported in recent experiments. We explain the role of trap depth and trap centers in thermoluminescence from semiconductor nanostructures.

Keywords: Thermoluminescence (TL), trapping, detrapping, recombination, Quantum confinement, trap center.

Resumen

La absorción de radiación de energía es mayor que los resultados de energía de ancho de banda en la ionización de electrones de valencia, produciendo electrones libres en la banda de conducción y los huecos libres en la banda de valencia. Los electrones libres pueden quedar atrapados en los centros de trampa justo debajo de la banda de conducción y los agujeros pueden ser atrapados en los centros de masa justo encima de la banda de valencia. Los electrones atrapados pueden ser liberados de nuevo a la banda de conducción si absorben suficiente energía E (llamada energía de activación o profundidad de la trampa), desde donde la recombinación con los agujeros atrapados es posible resultando en Termoluminiscencia (TL)). Por otro lado, la profundidad de la trampa es la diferencia de energía entre la trampa y banda correspondiente deslocalizada. La dependencia de temperatura de la profundidad de la trampa ha sido reportada en experimentos recientes. Explicamos el papel de la profundidad de la trampa y centros de trampa en Termoluminiscencia de nanoestructuras semiconductoras.

Palabras clave: Termoluminiscencia (TL), trampas, recombinación, Confinamiento cuántico, centro de trampa.

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I. INTRODUCTION

It is clearly reported that TL is the thermally stimulated emission of light due to absorption of energy from radiation [1-3].There are three essential ingredients necessary for the production of thermoluminescence [1]. Firstly, the material must be an insulator or semiconductor-metals do not exhibit luminescent properties. Secondly, the material must have at some time absorbed energy during exposure to radiation. Thirdly, the luminescence emission is triggered by heating the material [1]. The application of thermal energy causes the production of free electrons and holes which randomly move with in the conduction and valence bands respectively; which may later be trapped at trap centers. Luminescence can result because of two cases. One is due to the recombination of free electrons with trapped holes and the other is due to the recombination of free holes with trapped electrons.

II. THE ROLE OF TRAP DEPTH AND TRAP CENTERS

In order to understand the role of trap centers and trap depth in TL phenomena consider the following energy band scheme (Fig. 1). In this energy band scheme, there are just two localized levels, one situated between the demarcation level and the delocalized band (*i.e.*, D_e and E_c, or D_h and E_v and the other situated somewhere between D_e and D_h.

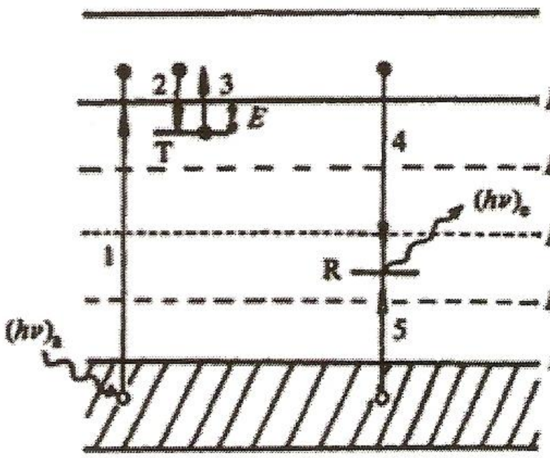

FIGURE 1. Simple two-level model for thermoluminescence. Allowed transition: (1) ionization; (2) and (5) trapping; (3) thermal release; (4) radiative recombination and emission of light [1].

Thus, one level acts as trap (T) and the other acts as recombination center(R). The trap is situated above the equilibrium Fermi level E_f and thus is empty in the equilibrium state (*i.e.*, before the absorption of radiation). It is therefore a potential electron trap. The recombination center, on the other hand, is situated below the Fermi level and is thus full of electron and is a potential hole trap [1].

The absorption of radiation of energy $(h\nu)_a > E_c - E_v$ (*i.e.*, greater than the band gap energy results in the ionization of valence electrons, producing free electrons in the conduction band and free holes in the valence band (transition 1). The free carriers may either recombine with each other or become trapped at the trap centers. In order for recombination to occur holes first become trapped at centers (R) (transition 5). Recombination takes place via the annihilation of the trapped holes by free electrons (transition 4). If the recombination transition is assumed to be radiative, then luminescence will result [1]. The free electrons may also become trapped at level T (transition 2) in which case recombination can only take place if the trapped electrons absorb enough energy E(called trap depth) to be released back to conduction band, from where recombination is possible. Thus, the luminescence emission is delayed by an amount governed by the mean time t spent by the electrons in the trap, given by the Arrhenius Eq. [1].

$$p = t^{-1} = sexp\left(-\frac{E}{K_B T}\right),$$

where s is trapping parameter, T is the temperature and $K_B$is the Boltzmann constant. Here p is defined as the probability per unit time of the release of an electron from the trap. It is found that s varies with temperature like T^{-b}, where $-2 < b < 2$. If the trap depth E is such that at the temperature of irradiation T_o, $E \gg K_B T_o$, then, any electron which becomes trapped will remain so for a long period of time, even after the removal of the irradiation there will exist a substantial population of trapped electrons [1]. Furthermore, because the free electrons and holes are created in pairs and are annihilated in pairs, there must exist an equal population of trapped holes at level R. If the temperature of the sample is raised to a higher temperature T such that $E \leq K_B T$, the probability of detrapping p will increase and the electrons will now be released from the trap in to the conduction band. Thermoluminescence now results when the free electrons recombine with the trapped holes. For a spherical quantum dot of well defined size distribution, the calculated temperature dependent thermoluminescence intensity (I_{th}) is given by [2]:

$$I_{th} = CR_{rad} d^3 \exp\left(\frac{-2E}{K_B T}\right),$$

where C is arbitrary constant, R_{rad} is the radiative recombination rate and d is the diameter of the dot.

As the temperature rises the electrons are released from the trap and recombination takes place reducing the concentration of trapped holes and increasing the thermoluminescence intensity. As the electron traps are progressively emptied the rate of recombination decreases and thus the thermoluminescence intensity decreases accordingly. This produces the characteristic thermoluminescence peak [1].

III. RESULTS AND DISCUSSION

For a fixed value of b (which is approximately equal to 1.99) the calculated thermoluminescence intensity has a peak value at a temperature of 50K and starts decreasing slowly after this temperature. It is also found that the thermoluminescence intensity increases following the reduction in size [2]. This is due to the quantum confinement effect which allows direct band to band radiative recombination following the widening of band gap [4]. From this result one can easily understand that the TL intensity increases with increasing the band gap of the dot; because the reduction in size allows the increment of band gap. Concerning trap depth, experimental reports show that it increases with increasing temperature [5].

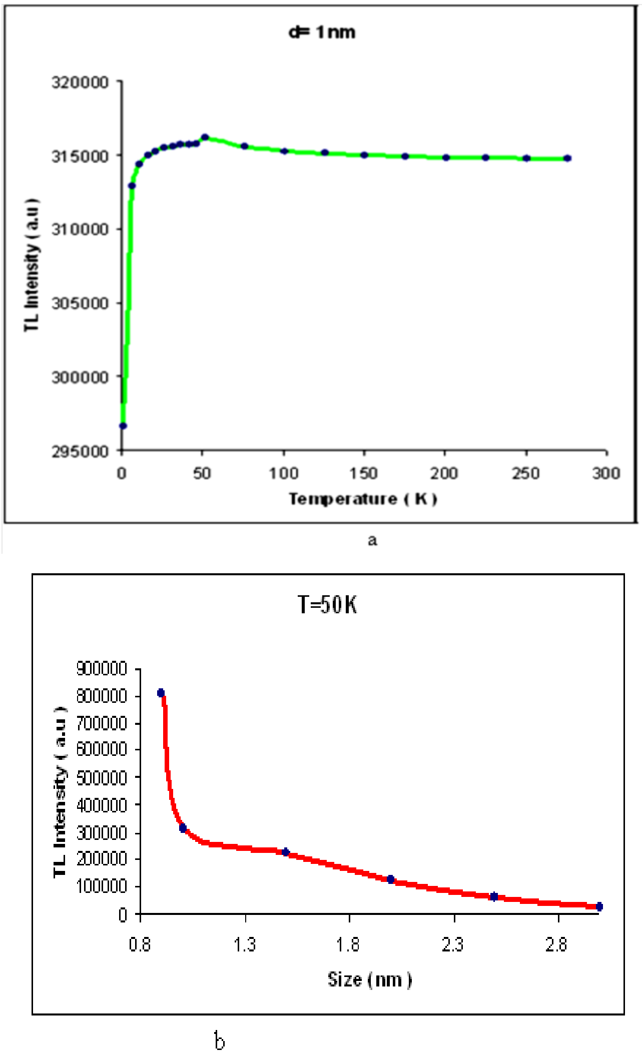

FIGURE 2. (a) TL intensity versus temperature for d=1nm: (b) TL intensity versus size for T=50K [2].

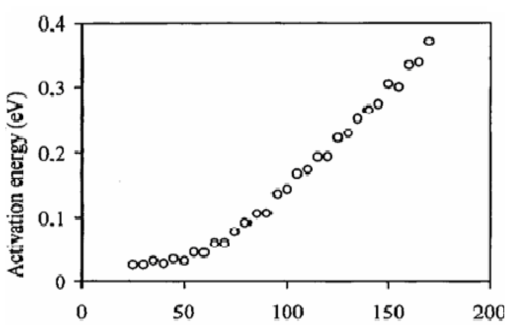

FIGURE 3. The experimentally reported activation energy versus temperature for silicon nanostructures [5].

III. CONCLUSION

In this work we have explained the role of trap depth and trap centers in thermoluminescence from semiconductor nanostructures. From calculated values and experimental reports we have seen that the TL intensity increases with increasing temperature and attains its maximum value near 50K and then starts decreasing slowly. It is also observed that the TL intensity increases following reduction in size. This can be explained in terms quantum confinement effect which allows band gap widening and direct band to band radiative recombination following the reduction in size. We have seen that the trap depth increases with increasing temperature. This implies that the deeper the trap centers, the larger the trap depth and hence relatively high temperature is required to detrap the electrons.

In general we have observed that the temperature dependence of the TL intensity is much similar to that of the photoluminescence and electroluminescence intensities. This shows that the mechanism of luminescence in the three types of luminescence is in general similar to one another.

REFERENCES

[1] Mckeever, S. W. S., *Thermoluminescence of Solids*, Cambridge solid state science series, Oklahoma state university **396**, 1-100 (1988).

[2] Gemechu, D. N. and Ghoshal, S. K., *Thermoluminescence from Silicon quantum dots: A model study*, Lat. Am. J. Phys. Educ. **5**, 428-431 (2011).

[3] Pal, U., Melendrez, R., Chernov, V. and Barboza-Flores, M., *Thermoluminescence properties of ZnO and ZnO: Yb nanophosphors*, Appl. Phys. Lett. **89**, 1-3 (2006).

[4] Kittle, Ch., *An Introduction to Solid State Physics*, 7th Ed. (University of California, Berkeley, 2005), p. 673.

[5] Skryshevskii, Y. A. and Skryshevskii, V. A., *Thermally Simulated Luminescence*, J. Appl. Phys. **89**, 2711-2714 (2001).