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Mechanism of Mechanoluminescence in Elemental and III-V Semiconductors

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Abstract— *The present paper reports the theory of mechanoluminescence (ML) produced during the cleavage of elemental and III-V group semiconductors. For the ML excitation in elemental and III-V semiconductors, the following models may be proposed: (i) charging of newly created surfaces, (ii) thermal generation of charge carriers, (iii) recombination of fracture-generated defects, and (iv) formation of crack-induced localized states.*

Since Ge, Si, InP and GaAs are centrosymmetric, charging of newly created surfaces may not take place due to the piezoeletrification. As these semiconductors have covalent bonding, the charging of newly created surfacesmay not takeplace due to the baro-diffusion of charged ions near the trip of the moving cracks. There may be the possibility of charging of newly created surfacesdue to the movement of charged dislocations.

Keywords— *Mechanoluminescence , Semiconductors*

1. INTRODUCTION

Mechanoluminescence (ML) is a type of luminescence produced during any mechanical action on solids like grinding rubbing, cutting, cleaving, shaking, scratching, compressing or by crushing of solids. The phenomenon of ML is known for a long time. ML can also be excited by thermal shocks caused by drastic cooling or heating of materials or by the shockwaves produced during exposure of samples to powerful laser pulses. ML also appears during the deformation caused by the phase transition or growth of certain crystals. ML also appears during separation of two dissimilar materials in contact. ML has also been called by many other names like triboluminescence, trennugslicht, piezoluminescence, deformationluminescence and stress-activated luminescence. ML is a useful tool for investigating molecular and microscopic events accompanying formation of cracks and details of failure modes in a variety of materials. The knowledge of ML is useful in understanding various properties of solids such as acoustic emission, exo-electron emission, deformation bleaching of coloured crystals etc. ML is also useful in understanding certain parameters of other types of luminescence.

2. MECHANISM OF ML IN ELEMENTAL AND III-V SEMICONDUCTORS

The mechanisms of ML in elemental and III-V semiconductors have not been studied in detail. For the ML excitation in elemental and III-V semiconductors, the following models may be proposed:

i) charging of newly created surfaces,

ii) thermal generation of charge carriers,

iii) recombination of fracture-generated defects, and

iv) formation of crack-induced localized states.

All three above models may not provide a dominating process for the ML in elemental and III-V semiconductors, while the ML model involving formation of crack-induced localized states supports the process.

The radiative recombination of electron and holes may give rise to mechanoluminescence. Electronic excitations resulting in charge carrier production would likely be associated with localized states of energy greater than or equal to that of the conduction band. The total number of photons produced during the creation of unit surface area are $3X10^8$, $1.52X10^{10}$, $7X10^6$ and $3X10^4$ for Ge, Si, InP and GaAs semiconductors, respectively. The band gaps of Ge, Si, InP and GaAs are 0.67, 1.14, 1.35 and 1.43 eV, respectively. It follows that the number of photons emitted decreases with increasing energy of the band gap. This fact support the ML model involving formation of crack-induced localized states.

3. THEORY

Linke have measured the time-resolved crack velocity during the cleavage of alkali halide crystals. They have shown that initially the crack moves at low velocity, but very soon it attains a fixed velocity after attaining a certain crack length. If a crystal having length L, breadth W and thickness H is cleaved along the plane parallel to creation of new surfaces is given by 2Wv, where v is the average velocity of cleavage plane or the velocity of crack propagation. If B is the number of free charge

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carriers produced during the creation of unit surface area, then the rate of generation of the charge carriers

$$g = 2BWv \quad (1)$$

In intrinsic semiconductors the number of electrons is equal to number of holes. In this case, luminescence is produced during the radiative recombination of holes and electrons. If α_1 and α_2 are the recombination coefficient for radiative and non-radiative transitions, then the rate equation

$$\frac{dn}{dt} = g - \alpha n^2 \quad (2)$$

Where $\alpha = (\alpha_1+\alpha_2)$ and n is the number of carriers in the respective band at any time t.

$$\text{or } \frac{dn}{g-\alpha n^2} = dt \quad (3)$$

$$\frac{dn}{g\left[1-\frac{2\alpha n}{\sqrt{4\alpha g}}\right]^2} = dt \quad (4)$$

Integrating equation (4) and putting $f = \frac{2\alpha n}{\sqrt{4\alpha g}}$, we get (5)

$$\int \frac{df}{1-f2} = \sqrt{\alpha g} \int dt \quad (6)$$

Putting $f = \tanh\theta$, we obtain,

$$1 - f^2 = 1 - \tanh^2\theta = \operatorname{sech}^2\theta \quad (7)$$

Thus, from equation (5), we get

$$\int d\theta = \sqrt{\alpha g} \int dt$$

$$\text{or} \quad \theta = \sqrt{\alpha g t} + c \quad (8)$$

where c is an integration constant.

From equations (6) and (7), we get

$$\tanh^{-1} f = \sqrt{\alpha g t} + c$$

$$\text{or } f = \tanh\left(\left(\sqrt{\alpha g}.t\right) + g\right. \quad (9)$$

Where K is another constant.

From equation (5) and (9), we get

$$\frac{2\alpha h}{\sqrt{4\alpha g}} = \tanh\left(\sqrt{\alpha g}.t\right) + K \quad (10)$$

At $= 0,\ n = 0,$ thus from equation (10), we get

$$k = 0$$

Thus , from equation (10) , we get

$$\frac{2\alpha h}{\sqrt{4\alpha g}} = \tanh\left(\sqrt{\alpha g}.t\right)$$

$$\text{or} n = \sqrt{\frac{g}{\alpha}} \tanh t\sqrt{\alpha g} \quad (11)$$

Case I : Rise of ML Intensity

The rise of intensity of bimolecular ML may be given by

$$I_r = \alpha_1 n^2 = \frac{\alpha_1 g}{\alpha} \tanh^2 t\sqrt{g\alpha} \quad (12)$$

$$\text{or} I_r = \frac{\alpha_1 g}{\alpha}\left[\frac{2t\sqrt{g\alpha}}{2}\right]^2$$

$$\text{or} I_r = \alpha_1 g^2 t^2 \quad (13)$$

Equation (13) indicates that I_r should increase quadratically with t.

Equation (13) shows that when a semiconductor material is cleaved, initially, the ML intensity should increase quadratically with time (t) and finally it should attain a saturation value I_{rs} given by the equation

$$I_{rs} = \frac{\alpha_1 g}{\alpha_1 + \alpha_2}$$

or

$$I_{rs} = \frac{2\alpha_1}{\alpha_1+\alpha_2} BWV \quad (14)$$

Case II: Decay of ML Intensity

When the light source will be switched off, the rate of generation, g, of carriers will become zero and equation (2) may be expressed as

$$\frac{dn}{dt} = -\alpha n^2 \quad (15)$$

If the cleavage is completed at

$t = t_m$, then taking $= \sqrt{\frac{g}{\alpha}}$, at $t = t_m$, we get

$$n = \sqrt{\frac{g}{\alpha}} . \frac{1}{(\sqrt{g\alpha})(t-t_m)+1} \quad (16)$$

Thus, the decay of ML intensity may be given by

$$I_d = \alpha_1 n^2$$

$$I_d = \frac{\alpha_1 g}{\alpha} . \frac{1}{\left[(\sqrt{g\alpha})(t-t_m)+1\right]^2} \quad (17)$$

For $\sqrt{g\alpha}(t - t_m) > 1$, we get

$$I_d = \frac{\alpha_1}{\alpha^{2(t-t_m)^2}} \quad (18)$$

The above equation shows that the decay of ML intensity should follow the power law.

For $t = t_m$, using equation (17) the maximum ML intensity may be expressed as

$$I_m = \frac{\alpha_1 g}{\alpha} = \frac{2\alpha_1 BWV}{\alpha} \quad (19)$$

From equation (17) and (19), we get

$$I_d = \frac{I_m}{\left[(\sqrt{g\alpha})(t - t_m) + 1\right]^2}$$

Or $\frac{I_m}{I_d} = \left[(\sqrt{g\alpha})(t - t_m) + 1\right]^2$

Total ML Intensity

The total ML intensity may be expressed as

$$I_T = \int_0^{t_m} \frac{\alpha_1 g}{\alpha} \tanh^2 t\sqrt{g\alpha}dt + \int_{t_m}^{\infty} \frac{\alpha_1 g}{\alpha} \frac{dt}{\left[\sqrt{g\alpha(t-t_m)} - 1\right]^2} \quad (20)$$

Integrating eqn. (20), we get

$$I_T = \frac{\alpha_1 g^{1/2}}{\alpha^{3/2}} \left[t_m\sqrt{g\alpha} - \tanh t_m\sqrt{g\alpha} + 1\right] \quad (21)$$

For $t_m\sqrt{g\alpha > 1}$, $\tanh t_m \sqrt{g\alpha} = 1$, thus eqn. (21) may be expressed as

$$I_T = \frac{\alpha_1 g t_m}{\alpha}$$

Or

$$I_T = \frac{\alpha_1 g t_m}{\alpha}$$

$$I_T = \frac{2\alpha_1 BWH}{\alpha}$$

Or

$$I_T = \frac{\alpha_1 BA}{\alpha} \quad (22)$$

Where A is the area of newly created surfaces.

4. CONCLUSION

(i) The mechanism related to the formation of crack-induced localized states is responsible for the ML excitation produced during the cleavage of elemental and III-V semiconductors.

(ii) When an elemental or III-V semiconductors is cleaved, initially, the ML intensity increases with time, attains a peak value at the timet_m corresponding to completion of the fracture of the materials, and then it decreases following power law decay.

(iii) From the measurement of the ML intensity, the velocity of crack propagation in a material can be determined by using the relation $v = H/t_m$.

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