Modeling of mechanical stress fields in multi-layered structures of diode lasers

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Comprehensive models of an operation of light-emitting diodes (LEDs) and diode lasers should contain mutually interrelated parts describing at least their optical, electrical and thermal properties [1]. Then all physical phenomena taking place inside a device volume and crucial for a device operation are characterized including influences of position-dependent temperature increases, carrier concentrations, current densities, and radiation intensities. Rarely any influence of mechanical properties is taken into account in such self-consistent approaches, mostly because of complexity of rigorous mechanical models which additionally are supposed to need truly time-consuming and arduous computer calculations to be implemented. However, mechanical stresses are known to influence considerably semiconductor band gaps and effective masses [2]. Besides, stress-related piezoelectric effects affect considerably carrier transport and recombination properties [3-7].

The above effects are especially strong materials having the structure of wurtzite, e.g. mostly all nitride semiconductors. Therefore it is an important task to develop a comprehensive model for determination of mechanical stress in the multi-layered structures based on such materials. The commonly used simple equation, which relates the mechanical strain only to the difference between lattice constants of substrate and epitaxial layer,

$$\varepsilon = \frac{a_s - a_f}{a_f} \tag{1}$$

where ε denotes mechanical strain of thin film layer deposited on the thick substrate and a_s and a_f are lattice constants of the substrate and the film respectively, is in many cases too simple to be applicable to the real devices. The major drawback of the above approach is the fact that it neglects several effects. In particular

1. In multi-layer structures the influence of all layers interaction should be considered
2. Due to the differences of thermal expansion coefficients, a new stress may be introduced even to the fully relaxed structure during the significant change of temperature, e.g. while cooling down newly created device from the epitaxy conditions to the room temperature.
3. When the layer thickness exceeds *critical thickness* [8,9], the misfit dislocations emerge which are the cause of stress relaxation and considerable strain reduction.

The model presented in this paper aims to include above effects and therefore give more accurate stress estimation while still it remains simple and efficient, thanks to the analytical form of all equations.

There are several assumptions necessary for analytical approach to be valid:

1. all layers are thin as compared to the substrate,
2. transversal structure sizes are much larger than layer thicknesses, and
3. layers have isotropic transversal properties, i.e. along the 0*z* axis perpendicular to layer heteroboundaries.

This allows to consider the strain only in the *xy* plane with a single elasticity modulus for each layer G^i

$$G^i = C_{11}^i + C_{12}^i - 2\,\frac{\left(C_{13}^i\right)^2}{C_{33}^i} \tag{2}$$

where $C_{ab}{}^i$ are elasticity coefficients for transversally isotropic materials.

It is important to notice that the introduction of concept of critical thickness and stress relaxation due to the misfit dislocations changes dramatically the required approach of stress estimation. It can be shown [10] that neglecting this effect the overall stress in the structure does not depend on its thermal history. Therefore only differences of the lattice constants in the operation temperature generate mechanical stress. From the equilibrium condition the following relation must be valid for the structure consisting on N layers

$$\sum_{i=1}^{N} d^i \sigma^i = 0 \tag{3}$$

where d^i is the i-th layer thickness. As there are no misfit dislocations in the structure the overall strain is constant and of the same value in every layer. From the Hooke's law the stress in each layer is proportional to this strain and layer's elasticity modulus

$$\sigma^i = G^i \left(\varepsilon + \varepsilon_m^i\right) \tag{4}$$

where ε_m^i is the *molecular strain*, resulting from lattice mismatch and calculated from the equation (1).

Solving equations (3) and (4) we may obtain the final results

$$\varepsilon = -\frac{\sum G^i d^i \varepsilon_m^i}{\sum G^i d^i} \tag{5}$$

and

$$\sigma^i = G^i \left(\varepsilon_m^i - \frac{\sum G^i d^i \varepsilon_m^i}{\sum G^i d^i} \right) \tag{6}$$

When the effect of critical thickness is taken into consideration the above equation ceases to be valid. Due to the misfit dislocations the lattice constants of the structure layers are not necessary equal and depend on the layer thickness. Denoting the effective lattice constant of i-th layer in the strained structure as b^i, we may write that

$$b^i = \begin{cases} b^{i-1} & \text{where } h < h_c \\ a^i + \frac{h_c}{h^i}\left(b^{i-1} - a^i\right) & \text{where } h \geq h_c \end{cases} \tag{7}$$

In our model it is assumed that stress relaxation can only take place during epitaxy process. After this the change in temperature may noticeably change the stresses but no new relaxation take place.

The above method was applied to determine the mechanical stress in the modern nitride LED [11]. The results are presented at the fig. 1. As one can see, nearly uniform moderate compression stresses are determined for all layers with an exception of quantum wells, where these stresses are much stronger. Similar behaviour has been also found experimentally [12].

Conclusions

A simple, but still quite exact, analytical approach has been developed to determine stress fields in multi-layered structures of nitride devices. So, from now on, comprehensive optical-electrical-thermal models of the above devices may be supplemented by the mechanical part without an expensive increase in their computing time. Now an impact of mechanical stresses within nitride active regions on effective masses and band gaps as well as piezoelectric-related separation of electrons and holes in wide active-region QWs may be included in the most comprehensive models of nitride devices. However, analogous stress fields around quantum dots need more sophisticated approach to be determined which is now under our consideration.

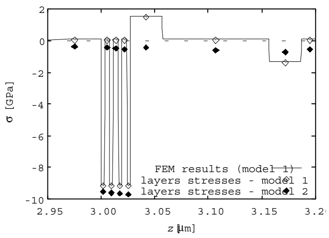

Fig. 1 Determined stress profile along 0z axis of sample LED

References

1. M. Osiński and W. Nakwaski, Chapter 5 in H. Li and K. Iga, *Vertical-Cavity Surface-Emitting Laser Devices* (Berlin: Springer), 2003
2. S. L. Chuang, *Physics of Optoelectronic Devices*, Chapter 4.5, New York: J. Wiley, 1995
3. S. H. Park and S. L. Chuang, *Appl. Phys. Lett.* **72**, p. 3103, 1998
4. L. Hsu and W. Walukiewicz, *Appl. Phys. Lett.* **73**, p. 339, 1998
5. R. D. Underwood, P. Kozodoy, S. Keller, S. P. Den Baars, and U. K. Mishra, *Appl. Phys. Lett.* **73**, p. 405, 1998
6. E. T. Yu, X. Z. Dang, L. S. Yu, D. Qiao, P. M. Asbeck, S. S. Lau, G. J. Sullivan, K. S. Boutros, and J. M. Redwing, *Appl. Phys. Lett.* **73**, p. 1880, 1998
7. H. S. Kim, J. Y. Lin, H. X. Jiang, W. W. Chow, A. Botchkarev, and H. Morkoç, *Appl. Phys. Lett.* **73**, p. 3426, 1998
8. Ch. Kim, I. K. Robinson, J. Myoung, K. Shim, M.-Ch. Yoo, K. and Kim, *Appl. Phys. Lett.* **69**, p. 2358, 1996
9. G. C. Osbour, *IEEE J. Quantum Electron.* **QE-22**, p. 1677, 1986
10. M. Dems and W. Nakwaski, *Semicond. Sci. Technol.* **18**, p. 733, 2003
11. T. Takeuchi, G. Hasnain, S. Corzine., M. Hueschen, Jr, R. Schneider, Ch. Kocot, M. Blomqvist, Y.-I. Chang, D. Lefforge, M. R. Krames, L. W. Cook, S. A. Stockman, *Jpn. J. Appl. Phys., Pt. 2* **40**, p. L861, 2001
12. J. Keckes, J. W. Gerlach, R. Averbeck, H. Riechert, S. Bader, B. Hahn, H. J. Lygauer, A. Lell, V. Härle, A. Wenzel, and B. Rauschenback, *Appl. Hys. Lett.* **79** p. 4307, 2001