NEW MODELS OF SEMICONDUCTOR MATERIALS AND HETEROSTRUCTURES FOR IR LASERS AND PHOTODETECTORS

O. Davarashvili, L. Akhvlediani, M. Enukashvili, N. Kekelidze

Accepted for publication February, 2006

ABSTRACT. It was stated by us that in the connection with the diffusional mismatch in semiconductor heterostructures IV-VI the pressure exceeding the limit of elasticity can originate. For lasers it leads to the increase of threshold currents almost by a range and to the decrease of operating temperature. When the critical deformation resource is used up, the widening of elastic deformation diapason is used on account of elasticity modulus modification by doping with impurities, decreasing the crystal constant of solid solution. Accordingly it causes a significant weakening of mismatch effect.

Widening of elastic deformation diapason also allows to create the conditions in epitaxial layers for displacing impurity level into the depth of the forbidden gap. If at the same time the impurity is capable of stabilizing the Fermi level then for the given impurity and certain composition of solid solutions the transformation metal-dielectric is carried out.

The work presents formulation of conditions for creation the dielectric state in given IV-VI semiconductors, which are necessary for rising sensitivity of IR photodetectors.

Lately considerable breakthrough has been traced in working out IR tunable lasers and photodetectors on the basis of IV-VI semiconductors. This is connected firstly with creation of new heterostructures and homogenous heavily doping crystals.

If the width of forbidden gap and effective mass of current carriers in different semiconductors are basically determined through their chemical composition (chemical formula), then most characteristics: type of conductivity, mobility of carriers, lifetime, coefficients of absorption and heat conduction, etc., significantly depend on doping impurities. According to totality of these parameters for different tasks the most effective materials are selected. Particularly, for semiconductor lasers and photodetectors optimization of their characteristics: threshold current (operating temperature), capacity of radiation, sensitivity, etc., are carried out in consideration with influence of doping on electrical, optical and thermal characteristics of materials. Although our latest research [1] showed that new important resource in perfecting their characteristics represented mechanical elastic properties (elasticity modulus, limit elastic deformation), modified at doping by certain impurities.

In the present statement we consider the situations, when at widening diapason of elastic deformation in semiconductor lasers threshold current decreases, and resistivity and consequently sensitivity considerably rises in photodetectors.

It is well-known that due to decrease of active volume and limitation effects a considerable decrease of threshold current is achieved in lasers on the basis of heterostructures. In most cases for widening spectral diapason multicomponent solid solutions are used as active layers. Due to experiments and calculations in the process of heterostructure creation an obvious interdiffusion of solid solution components takes place [1]. Consequently even in structures, assumed as isoperiodic, in emitters and active ranges of lasers an mismatched area forms. In most cases they are inevitable, even when changing the profile of composition in the heterostructure. The strain corresponding to mismatch exceeds limit of elasticity- their relaxation causes mismatch dislocation from the sticking centre [1,2]. Because of the increase of nonradiative recombination the threshold current rises considering:

$$I_{\text{th}} \sim \left(\frac{\tau_{\text{эф}}}{\tau} \right)^{-1} = \frac{d + 2S\tau}{d}, \tag{1}$$

where τ is the carrier's lifetime considering the centres of recombination under mismatch; τ is lifetime in active area; d is the thickness of active range; S is the velocity of surface recombination (in the given case distributed in certain thickness in the active range of lasers). In its turn:

$$S = \sigma \cdot \upsilon \cdot N, \tag{2}$$

here $\sigma = a^2$ is the square of recombination; υ is thermal velocity of current carriers; *a* is a crystal parameter constant; *N*- density of centres of recombination, equaling to:

$$N = \frac{1}{a^2} \cdot \frac{\Delta a}{a}. \tag{3}$$

Assuming that at weak mismatch $\frac{\Delta a}{a}$ equals to its maximum. Let consider as a sample heterostructures in IV-VI semiconductors PbSeTe-PbSnSeTe. The mismatch $\frac{\Delta a}{a}$ in the active range at epitaxial temperature corresponds to $(1 \div 3)\cdot 10^{-3}$. On the other hand out of measuring the lifetime in the active range of heterostructures and amplitudes of dependence of internal friction more than half of the whole amount of defects are revealed at deformation $(1 \div 2)\cdot 10^{-3}$. Therefore, considering $\upsilon = 3.10^7$ cm/s, $\tau = 5\cdot 10^{-9} \div 10^{-8}$ s, $d = 0.4$ µm because of diffusional mismatch the measured threshold current I_{th} increases by an order and more.

It is worth mentioning that the limit stress at research internal friction are determined by critical amplitudes of oscillation (when the derivative of the energy loss from the amplitude of oscillation considerably changes) with weak temperature dependence, i.e. with strong centers of sticking the dislocation. Although, for the initial crystals and layers with different density of dislocation plastic deformation generates in comparatively small or big amount of local volumes of different values. In epitaxial layers at large density of dislocation the limit of elasticity occurs at small mismatch. But even in this case the influence on this threshold current is significant. The calculations show that if mismatch represents the half of limit, then the threshold current increases $5 \div 6$ times.

When the resource for limit strain deformation in laser structures are excluded, then ultimate stress $\sigma_M = \frac{E}{1-\nu} \cdot \frac{\Delta a}{a}$ (where ν is Pausson coefficient) can be increased on behalf of the rise of elasticity modulus E (for photodetectors also due to increase of critical elastic deformation ε_{Cr}). The research [3] shows that elasticity modulus in IV-VI semiconductors rises 2.5-3 times, and the critical elastic deformation 3.5-4 times at doping by Cr, Ca Mn impurities on the level ≤ 0.01. All these impurities reduce the crystal constant even in the condition of its pressing the barrier for generation and motion of dislocation. Though, the most neutral in relation to radiative transition in IV-VI semiconductors is impurity of Mn.

The doping effect, for example, with chromium impurity, can be expressed by letting the coefficient $\frac{r_{Cr}}{r_{Pb}} C_{Cr}$ (where $r_{Cr} = 1.1$ Å, $r_{Pb} = 1.5$ Å radii of Cr and Pb atoms in the lattice of solid solution PbSnTe, $C_{Cr} \leq 0.01 -$ concentration of chromium impurity) in the expression of dislocation tightness (3). Clearly enough, this effective mismatch reduces by 2-3 orders and the threshold current will significantly be decreased, and the operating temperatures of lasers will rise.

The evaluations given above relate to double heterostructure lasers. In case when the width of mismatch area coincides with the thickness of active layer of the laser, then formable lead to displacement of the band edges. Considering isotopic and mobile deformational potentials displacement of the band edges at $\varepsilon \approx 2 \cdot 10^{-3}$ represents ~ 40 meV. At the same time the degeneracy of four ellipsoids of band structure for their different orientation is relative to the direction of deformation that causes decrease of density of state, and consequently to the threshold current. In this way diffusional mismatch can be used as a positive factor in creation of strained layers in this case.

One of the abovementioned impurities – chromium, along with widening the diapason of elastic deformation, has the feature of stabilization of Ferm level. In the condition of stabilization of Fermi level at the rise of concentration of the given impurity or others the

Fermi level does not change its position. When some impurity is high in concentration ($10^{19}\div10^{20}cm^{-3}$) nonstoichiometric and other electrically active defects can take multivalentive states, including donor and acceptor, certain relation of occupied states among them takes place and the state of Fermi level changes only in accordance to composition of solid solutions.

In solid solutions PbSnSe(Te) with the rising composition of tin the stabilized Fermi level displaces from the edge of the conductivity band to valence band, so that amount of vacancies rises in the sublattice of metal-equilibrium displaces on the side of acceptor states. Although the chromium level in PbTe is placed above the edge of conductivity band (~100 meV) the speed of its displacement with the composition (8 meV per 1%SnTe) exceeds almost two times the speed of reducing the width of the forbidden gap (4.8 meV per 1%SnTe) and therefore for some compositions of solid solutions it falls below the middle of the forbidden gap, transferring to acceptor state. If stabilized Fermi level of for some compositions coincides with the middle and is remote from the edges of bands at considerable energy – (7 ÷ 9) kT, then resistivity of the semiconductor significantly rises and it becomes possible to realize effective photodetector at maximum temperature.

Behaviour of the chromium level in PbSnTe is a matter of interest even at hydrostatic pressure the level is weakly displaced relatively in the middle of the forbidden gap. Obviously in some compositions of PbSnTe when the stabilized level of chromium lies in the forbidden gap, at pressing with negative coefficient of change of the forbidden gap width the transfer of dielectric-metal takes place with pressure. If in any way we achieve the stretching of semiconductor the reverse effect will be observed. According to the model of the dielectric state in the indicated semiconductor, using the mentioned methods at doping by impurities, the widening of the forbidden gap and penetrating in the depth of forbidden gap (or the cut) of donor or acceptor level can be assumed. The calculations show that for leaving of the forbidden gap edge with the energy 7 ÷9 kT by the Fermi level, the widening of the bands in the indicated semiconductors should be ~ 100meV (for compositions corresponding to $\lambda \leq 8$ μm). In the range of elastic deformation $8\cdot10^{-3}$, achieved at doping by chromium, the difference among the electron potentials and the holes should be 10 eV. It occurred that abovementioned options should be realized at stretching the semiconductor through the growth of thin strained layer, for example, PbSnTe on the substrate BaSeTe with crystal constant. For the concrete composition PbSeTe:Cr with the content of SnTe = 0.3 and Cr = 0.5 % at increase on the substrate BaSeTe with content of BaTe-0.15, the mismatch constitutes $5 \cdot 10^{-3}$ and the suitable pressure - 8 кbar. The width of the forbidden gap increases at 60 meV and reaches 140 meV (λ = 9 μm) at 100K, and the chromium level leaves the peak of the valence band at 60 meV. Relation of the specific resistance of semiconductor in strained and normal states according to calculation makes 4÷5 ranges. For covering the area of spectrum up to 20 μm by photodetectors the composition of solid impurities will be separately doped by gallium and vanadium.

Thus, the negative effect of diffusional mismatch in laser structures can be surmounted by doping with active impurity layers, decreasing the crystal lattice parameters. The creation of dielectric states in narrow-band IV-VI semiconductors seems possible only in case of fulfillment of these three options:

a. Formation of pressure for interchanging the level of impurity in the forbidden gap with leaving the edges of bands at energy 7-9 kT.
b. Fulfillment of appropriation of this pressure for the diapason of elastic deformation of the observed composition of solid solutions.
c. Selection of substrate with the same crystallographic structure and the composition for the necessary mismatch.

In conclusion, it is worth mentioning that simultaneous stabilization of Fermi level and widening the diapason of elastic deformation at doping the IV-VI semiconductors by certain impurities transform the initially defective, nonstoichiometric material into perfect, homogeneous with wide possibilities for managing energetic spectrum the current carriers. This condition can play a decisive role in the further usage of IV-VI semiconductors in IR optoelectronics.

REFFERENCES

1. O. Davarashvili, M. Enukashvili, N. Kekelidze, M. Metskhvarishvili. Georgian Engineering News, **2,** 2002, 7.
2. O. Davarashvili, G. Darsavelidze, M. Enukashvili, N. Kekelidze, T. Mamedov, N. Akhmedadze. Research of Internal Friction in IV-VI Semiconductors, International Conference Proceedings "Fizika-2005", Baku, 2005.
3. O. Davarashvili, M. Enukashvili, N. Kekelidze, R. Mamedov, V. Zlomanov. Influence of Impurities on the Mechanical Properties of IV-VI Semiconductors. Thesis of the XI International Conference on Condensed Matter Physics. Ankara, 2004, 19.

Tbilisi State University

ო. დავარაშვილი, ლ. ახვლედიანი, მ. ენუქაშვილი,
ნ. კეკელიძე

ნახევარგამტარული მასალებისა და ჰეტეროსტრუქტურების ახალი მოდელები ინფრაწითელი ლაზერებისა და ფოტომიმღებებისათვის

დასკვნა

დადგინდა, რომ დიფუზური შეუთანხმებლობის გამო ნახევარგამტარულ IV-VI ჰეტეროსტრუქტურებში შეიძლება აღიძრას დაძაბულობა, რომელიც აჭარბებს დრეკადობის ზღვარს. ლაზერებისათვის ეს გამოიწვევს ზღურბლური დენების გაზრდას თითქმის ერთი რიგით და სამუშაო ტემპერატურების შემცირებას. წარმოდგენილ შრომაში შემოთავაზებულია დრეკადი დეფორმაციის დიაპაზონის მნიშვნელობის გაზრდა დრეკადობის მოდულის მოდიფი-კაციის მეშვეობით, როცა ზღვრული დეფორმაციის რე-

სურსები მთლიანად ამოწურულია. დრეკადობის მოდულის მოდიფიკაცია შესაძლებელია კრისტალური მესერის პარა-მეტრის შემცირებით მინარევებით ლეგირებისას. შესაბამი-სად არსებითად სუსტდება შეუთანხმებლობა.

დრეკადი დეფორმაციის გაფართოებისას შესაძლებელი ხდება, აგრეთვე, ეპიტაქსიალურ ფენებში მინარეული დონეების გადანაცვლება აკრძალული ზონის სიღრმეში. ამავე დროს, თუ მინარევს ფერმის დონის სტაბილიზაციის უნარი აქვს, მაშინ მოცემული მინარევისათვის განხორცი-ელდება მეტალი-დიელექტრიკი გადასვლა განსაზღვრული შემადგენლობის მყარ ხსნარში.

შრომაში ფორმულირებულია პირობები ვიწროზონიან IV-VI ნახევარგამტარში დიელექტრიკული მდგომარეობის შესაქმნელად, რომელიც აუცილებელია იწ ფოტომიმღებე-ბის მგრძნობიარობის ასამაღლებლად.