Nanostructured surfaces

Theoretical calculations of mechanical stresses in the system quantum dot - substrate

O.I. Moroz[1], M.V. Makarets[1]

[1] *Department of Physics, Taras Shevchenko National University of Kyiv, st. Volodymyrska, 64/13, Kyiv 01601, Ukraine*
E-mail: sasha_moroz_91@mail.ru

One of the methods of forming quantum dots is based on semiconductor nanostructures self organization during its epitaxial growth [1]. Mechanical stresses in epitaxial film of future quantum dot (QD) material and in its islands on the surface of the substrate are critical in the transition from the film's growth to growth of islets (Stranski-Krastanov mechanism[2,3]). These stresses are important in the further growth of QD in size, changing of its shape and its distribution on the substrate.

In this regard there is still the urgent task to find the mechanical stresses and deformations in InAs/GaAs systems and to estimate the size of QD, the achievement of which in the process of growth process there is running the conditions for the formation of structural defects.

Considering the elastic properties of the system, we will not take its full account of atomic structure, despite the fact that QD as well as substrate contains thousands of atoms. [4]. This assumption can consider the system as a complete environment. We also believe that as a zero approximation for the deformation description in the system can be applied the linear theory of elasticity.

Within these assumptions the stresses are satisfied with the Lame equation:

(1)

We make the step: the deformations in QD-substrate we will describe with the equations of elasticity theory for two isotropic environments. Then the equation (1, 2) takes the form of:

, (2)

Using the Lame's equation (2) and above assumptions formulated the components of vector displacement can be found in both environments.

, (3a)

, (3b)

, (3c)

. (3d)

where – the components of vector displacement in both environments.

Due to the Hooke's law the components of mechanical stresses will be written through the deformation:

, (4a)

, (4b)

, (4c)

, (4d)

where , – the deformation of components.

So we have got the deformations and stresses in the model of QD-substrate that allows us to assess of heir depending on the linear dimensions of quantum dots on the interface.

It has been established at the ideal stitching of atomic QD planes and substrates the only source of mechanical stresses and deformations is a mismatch of lattice period. Analytical estimates and numerical calculations show that the maximum stresses in the system occur at the edges of QD-substrate interface, so there will be created conditions for the emergence of defects.

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