11-Surfaces, Interfaces and Thin Films

PS–11.01.18 AN ALGORITHM OF OPTIMAL CHOICE OF SUBSTRATES FOR HIGH-Tc SUPERCONDUCTORS: SEARCH OF COMPOUNDS AND CRYSTALLOGRAPHIC ORIENTATIONS. By A.N.Efimov* and A.O.Lebedev, Ioffe Physical-Technical Institute, Petersburg, Russia.

Concept of "small lattice mismatch" is most frequently used to choose the substrates. So, if both layer and substrates structure are cubic the strict coincidence of lattice parameters need to create the transient region without defects. In this case approach described above is conventional and proved to be correct.

Unfortunately, a lot of active materials being used by the modern functional electronics (opto-, acousto-, HTS-electronics) belongs to various systems (not only cubic), and in most general case the lattice metric match requirement is modified to the following:

$a_1 = a_2$, $b_1 = b_2$, $c_1 = c_2$, $\alpha_1 = \alpha_2$, $\beta_1 = \beta_2$, $\Gamma_1 = \Gamma_2$, where $a, b, c, \alpha, \beta, \Gamma$ – parameters of unit cell (lengths and angles, accordingly); subscript 1 denotes epilayer, 2 – substrate.

Obviously, it is impossible to find the substrate strictly satisfying to all these conditions simultaneously and in this case optimization problem consist in the correct choice of the well-founded goal-oriented function.

We have employed the following statement:

$$f = (E_1/E_0)^{0.5},$$

where f – goal-oriented function, E_1 – elastic energy of the epitaxial layer, E_0 – reduction coefficient, the later being equal to the energy of model "cubic-on-cubic" epitaxial pair if its lattice mismatch is equal 1% and thicknesses and elastic constants of model and real crystals are the same. For cubic crystals such goal-oriented function corresponds to the traditional definition of lattice mismatch. Below this function is called "misfit".

In the present study energy E has been calculated in terms of linear elasticity theory for the case of anisotropic body, pseudomorphic state of heterocomposition, non-strained substrate and small difference between unit cell parameters of layer and substrate.

For reduced rhombic cell of the layer there are 6 non-equivalent co-ordinate systems built on the reduced perovskite cell vectors. These settings can be corresponded to various types of orientation relationships "layer – substrate". We have calculated misfits for all possible types of relationships and have selected minimum from ones as a result.

An approach developed is realized within the computer program "COHERENT". For the number of the traditional epitaxial pairs the goal-oriented function as well as the maps of dominant epitaxial relationships are presented as functions of substrate orientation.

Correctness of algorithm is demonstrated by the interpretation of experimental data concerned with the HTS-layer perfection dependence on both the substrate composition and its crystallographic orientation.

It is shown that for creating of perfect singlecrystalline layers following additional conditions are essential:
- the goal-oriented function depends weakly on substrate orientation near the selected cut;
- energetical degeneration is absent, i.e. there is a considerable difference between the elastic energies of the main and "parasitic" epitaxial relationships. This restriction is necessary for suppression of polysynthetic twinning in epitaxial layers. The computer programs for solving of tasks described above are available from the authors.

PS–11.01.19 LATTICE-ADAPTABLE HETEROEPITAXY BY CONTROLLING OF SOLID SOLUTION COMPOSITION: CASE OF NON-CUBIC CRYSTALS. By A.N.Efimov*, A.O.Lebedev, Ioffe Physical-Technical Institute, S.-Petersburg, Russia

Such important characteristics of epilayer as an energy band gap, refractive index et al. may be controlled independently in the case of using multi-component solid solutions. Simultaneously, both lattice metric match and coincidence of thermal expansions can be obtained. For cubic crystals two-component solid solution allows to achieve the lattice metric match meanwhile three-component solid solution – both the lattice match and coincidence of thermal expansions. For non-cubic crystals seven-component solid solution is needed to agree six unit-cell parameters in the most general case. However, using of such multi-component systems is prevented by obstacles connected with the reproducibility of the control over the composition.

It is shown that the lattice metric match condition for cubic crystals, $a_1 - a_2 = 0$, can be transformed to:

$$d = ABC + 2DEF - BE^2 - CD^2 - AF^2 = 0 \quad (1) \quad \text{and}$$
$$j = AB + BC + CA - D^2 - E^2 - F^2 \leq 0 \quad (2), \quad \text{where}$$

$A = a_1^2 - a_2^2$; $B = b_1^2 - b_2^2$; $C = c_1^2 - c_2^2$;
$D = a_1 b_1 \cos\Gamma_1 - a_2 b_2 \cos\Gamma_2$; $E = c_1 a_1 \cos\beta_1 - c_2 a_2 \cos\beta_2$;
$F = b_1 c_1 \cos\alpha_1 - b_2 c_2 \cos\alpha_2$; $a, b, c, \alpha, \beta, \Gamma$– parameters of unit cell (lengths and angles, accordingly); subscript 1 denotes epilayer, 2 – substrate,
provided using the additional freedom degree such as crystallographic substrate orientation. The later conditions can be satisfied in the same way as for cubic crystals.

An example of such transient region for two-dimension case is presented in figure. There are variations of angles and lengths of bonding for interfacial atoms (see figure) but they are small if difference between metrics of layer and substrate is small too.

It should be pointed out that only condition (1) must be carried out strictly meanwhile an inequality (2) is condition that enables to reduce the number of possible crystal combinations.

It is proved by means of numerical statistical simulation that for non-cubic heterocompositions if two-component solid solution were used the lattice metric match condition could be carried out more frequently than for the case of cubic crystals.

Problem connected with the agreement on thermal expansions of layer and substrate (taking into account their anisotropy) is also considered.

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