COUPLED-FIELD THEORY FOR GRADE 2 PIEZOELECTRIC MEDIA: APPLICATION TO QUANTUM DOTS

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1. General

Quantum dots (QDs) are often grown with a periodic distribution within a piezoelectric matrix (barrier). An example of such quantum structures (QSs) is shown in Figure 1. The initial misfit strains within the embedded quantum dots stemming from the lattice mismatch between the QDs and the surrounding matrix result in the electro-elastic fields within both the QDs and the barrier. The lattice mismatch provides the needed driving force for the generation of the self-organized QDs during Stranski-Krastanov growth mode via molecular beam epitaxy (MBE). This intrinsic strain field, which affects the interatomic distances and consequently alters the energy level and the bonding electrons, influences the electronic and optical properties of semiconductor crystalline QDs [2]. Therefore, an accurate determination of the strain field associated with QSs is beneficial for predicting the creation and evolution of semiconductor QSs as well as the design of optoelectronic and microelectronic devices. It is well-known that, if the principal feature of interest is to model the nanoscopic variation of field variables within solids, the size independent classical theory cease to hold. For enhancing the solution, the employed theory must be capable of capturing not only the size effect, but also resolve the strain gradient across the interfaces with sufficient accuracy. To this end, a mathematical framework for the calculation of the electromechanical fields associated to electro-elastic inclusions with an arbitrary distribution of eigenfields - eigenstrain field, $\boldsymbol{\epsilon}^*(\boldsymbol{x})$, eigenstrain gradient field, $\boldsymbol{\eta}^*(\boldsymbol{x})$, eigenelectric field, $\mathbf{E}^*(\boldsymbol{x})$, and eigenelectric gradient field, $\boldsymbol{\zeta}^*(\boldsymbol{x})$- in grade 2 piezoelectric media is developed.

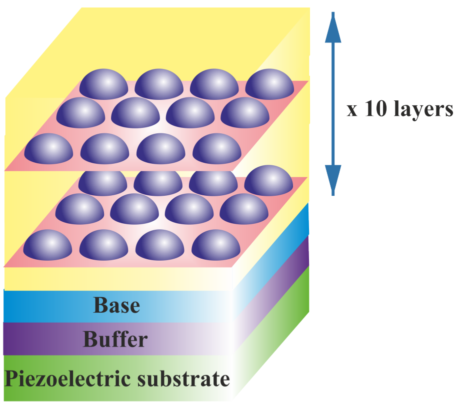

Figure 1: A sample of periodic distribution of semi spherical inclusions within a piezoelectric barrier in solar cells.

2. Formulation

In the absence of body forces and electric charge density, the equilibrium equations and charge equation of electrostatics are given as [1], [3]

(1a) $$(t_{ij} - \mu_{ijk,k})_{,j} = 0,$$

(1b) $$D_{i,i} = 0.$$

Respectively, where **t** is Cauchy stress tensor, **μ** is the double stress tensor, and **D** is the grade 2 electric displacement tensor. The presence of a given distribution of eigenfields is conveyed to the above equations through the field quantities **t**, **μ**, and **D**.

3. Numerical results

For illustration, consider a periodic distribution of spherical inclusions within a piezoelectric barrier. Assume that the direction of polarization coincides with the x_3 axis. Let the spheres have radius, R= 3 nm and period of distribution 12 nm in x_1-, x_2-, and x_3- directions. For convenience, suppose that the elastic behavior of the medium is isotropic, while it is transversely isotropic with respect to its piezoelectric properties. Moreover, let $\epsilon^*_{ij}(\boldsymbol{x}) = \delta_{ij}$ inside each sphere and $\epsilon^*_{ij}(\boldsymbol{x}) = 0$ outside the sphere. Under the above mentioned assumptions, the strain component $\epsilon_{33}(0, 0, x_3)$ has been calculated and plotted as a function of x_3 in Fig. 2. In this figure, l_1 is a characteristic length of the piezoelectric medium. The case of $l_1 = 0$ corresponds to classical piezo-electric material. Figure 2 shows that the gradient effects in grade 2 piezoelectricity are more notable near the boundaries and the jump of $\epsilon_{33}(0, 0, x_3)$ is decreases by increasing the gradient effects (l_1).

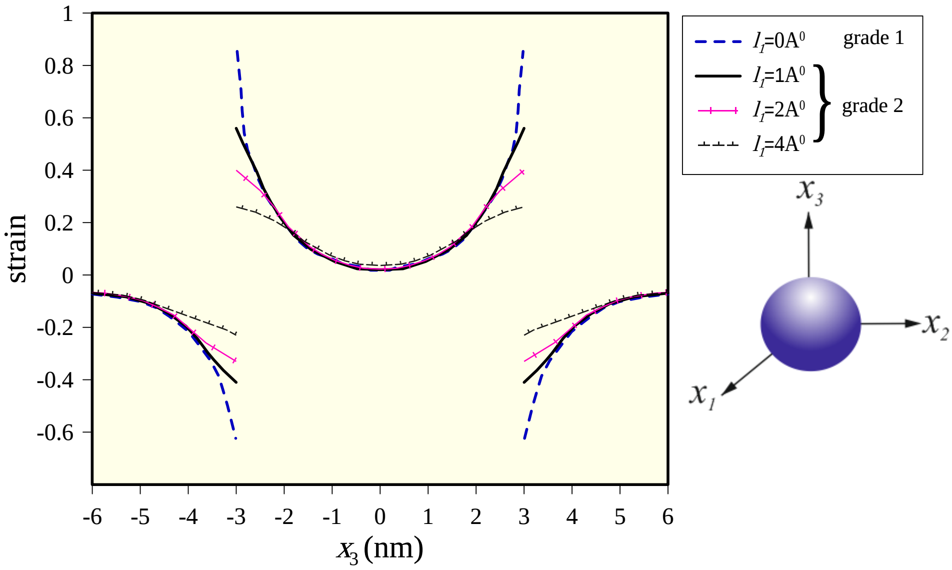

Figure 2: Variation of $\epsilon_{33}(0, 0, x_3)$ versus x_3 associated with the spherical QDs.

References

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