ANALYSIS OF QUANTUM DOTS INDUCED STRAIN AND ELECTRIC-FIELD IN PIEZOELECTRIC SEMICONDUCTOR SUBSTRATE BY THE GREEN'S FUNCTIONS

Canyun Wang¹, Mitsunori Denda² and Ernian Pan 3

 Mathematics and Modelling Department Schlumberger-Doll Research Old Quarry RD, Ridgefield, CT 06877-4108, USA ² Mech. Aero. Engineering Department Rutgers University Piscataway, NJ 08854-8058, USA denda@rutgers.edu

³ Advanced Material and Structure Center College of Engineering, University of Akron Akron, OH 44325-3905, USA

The electron and hole energy levels, wave functions and other characteristics in the self-organized quantum dots (QDs) are dependent on the state of strain and electric field produced during the growing process of QDs in a semiconductor substrate [1] [2]. The calculation of the strain and electric field in the QDs simulation process involves material anisotropy induced coupling between the elastic and electric fields and it must include the full three-dimensional and usually intricate shapes of the QDs. A new Green's function approach which takes into account QDs of arbitrary shape and semiconductor substrates with the most general class of anisotropy and piezoelectricity is presented in this paper.

The problem is formulated as an Eshelby inclusion problem [3] of which the solution can be expressed by a volume-integral equation that involves the Green's functions and the equivalent body-force of eiegenstrain. The volume integral is subsequently reduced to a line integral based on exploring a unique structure of the Green's functions obtained by Radon transform. The final equations are cast in a form that most of the computation results can be repeatedly used for QDs at different locations - a very attractive feature for simulating large systems of QD arrays. The proposed algorithm has been implemented and validated by comparison with analytical solutions. Numerical simulations are presented for pyramidal QDs in the substrates of Gallium Arsenite (GaAs) [001] and GaAs [111].

References

[1]M. Notomi, J. Hammersberg, H. Weman, S. Nojima, H. Sugiura, M. Okamoto, T. Tamamura and M. Potemski, "Dimensionality effects on strain and quantum confinement in lattice-mismatched InAsxP1-x/InP quantum wires," *Physical Review B* **52**, 11147-11158, 1995.

[2] G. Medeiros-Ribeiro, "Epitaxial growth of strained nanocrystals," Physica Status Solidi 230, 443-450, 2002.

[3] J.D. Eshelby, "Elastic inclusions and inhomogeneities," *Progress in Solid Mechanics (edited by I. N Sneddon and R. Hill)* **2**, 89–140, 1961.

Keywords: quantum dot, Green's functions, Radon transform