

A Finite Element Method for Modelling Electromechanical Wave Propagation in Anisotropic Piezoelectric Media

S. Rahman^{1,*}, H. P. Langtangen² and C. H. W. Barnes¹

¹ *Cavendish Laboratory, Cambridge University, JJ Thomson Avenue,
Cambridge, CB3 0HE, United Kingdom.*

² *Simula Research Laboratory, Martin Linges v 17, Fornebu P. O. Box 134,
1325 Lysaker, Norway.*

Received 23 June 2006; Accepted (in revised version) 26 July 2006

Available online 30 September 2006

Abstract. We describe and evaluate a numerical solution strategy for simulating surface acoustic waves (SAWs) through semiconductor devices with complex geometries. This multi-physics problem is of particular relevance to the design of SAW-based quantum electronic devices. The mathematical model consists of two coupled partial differential equations for the elastic wave propagation and the electric field, respectively, in anisotropic piezoelectric media. These equations are discretized by the finite element method in space and by a finite difference method in time. The latter method yields a convenient numerical decoupling of the governing equations. We describe how a computer implementation can utilize the decoupling and, via object-oriented programming techniques reuse independent codes for the Poisson equation and the linear time-dependent elasticity equation. First we apply the simulator to a simplified model problem for verifying the implementation, and thereafter we show that the methodology is capable of simulating a real-world case from nanotechnology, involving SAWs in a geometrically non-trivial device made of Gallium Arsenide.

PACS: 02.70.Dh, 41.20.Jb, 46.25.Hf

Key words: Finite element method, piezoelectric surface acoustic waves, Gallium Arsenide.

1 Introduction

In the process of designing quantum electronic devices based on surface acoustic waves (SAWs) traversing piezoelectric media, it is necessary to determine the effect, on these

*Corresponding author. *Email addresses:* S.Rahman.00@cantab.net (S. Rahman), hp1@simula.no (H. P. Langtangen), chwb101@cus.cam.ac.uk (C. H. W. Barnes)

waves of obstacles such as electrical gates on the surface, and also the effect of the SAW on the low-dimensional quantum mechanical systems such as quantum wires and quantum dots. In general, the gates have a non-trivial geometry, which necessitate numerical simulation tools. The finite element method is well suited to handle complex geometries and is widely used to model piezoelectric devices [1–6] and has recently been applied to modelling of SAWs [7–9]. The effect on the low-dimensional quantum mechanical systems would be analyzed through coupling the SAW simulator to both stationary and time-dependent Schrödinger equations [10]. This would require the development of a fast SAW simulator but also flexible and portable code.

SAWs are modes of propagation of energy along the free surface of a material such that there is no decay along the direction of propagation but there is exponential decay into the bulk. SAWs have been used in electrical technologies such as SAW filters [11,12] and ultrasonic imaging [13] for many years and have also been a useful tool in probing quantum electronic structures, for example, quantum Hall liquids [14]. Recently, much experimental work has been performed in the field of acoustic charge transport whereby a SAW across a GaAs/AlGaAs heterostructure is used to capture a single electron and then transport it along a one-dimensional quantum wire [15]. This would be useful in developing an accurate current standard, but more challenging proposals to use this in the burgeoning field of quantum information processing have been proposed [16–20]. SAWs have also been utilized for both static quantum dot [21] and photo-luminescence experiments [22,23]. The time and resources required to build such devices are immense, and therefore the mathematical modelling of these devices before the physical construction is advantageous. This approach requires the solution of the continuum electromechanical equations of motion in a piezoelectric medium. The method of partial waves [12] can be used to obtain simple analytical expressions for the waves in the bulk material, but the solutions say nothing about the effect of gates on the surface. Attempts to solve the governing equations analytically for devices which do have surface gates [24–26] involve simplifications, and the accuracy of these approximations remains uncertain.

There is a vast amount of literature on the three-dimensional finite element analysis of piezoelectric devices [1–6], and these methods are exploited in the field of ultrasonics to design control systems involving piezoelectric actuators and sensors [27]. Commercial software such as ANSYS and ABAQUS can be used to simulate electromechanical phenomena but lack the flexibility to couple to quantum mechanical calculations such as iterative Poisson-Schrödinger. Therefore it is often necessary to develop ones own computer code for modelling such devices.

In this paper, we formulate and evaluate a finite element based solution method for the equations governing SAWs in piezoelectric media, and we formulate it in a flexible and portable manner to allow the ability to interface with other code. The implementation is performed in an object-oriented style in order to incorporate existing solvers and to enhance portability of the code. Such a tool can be valuable in the design of micro- and nano-scale devices. We describe a set of boundary conditions that are capable of efficiently exciting SAWs and demonstrate the propagation of SAWs through a GaAs-