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DIFFUSION INDUCED BY GRAIN BOUNDARIES: A SHE MODEL*

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Abstract. Classical motion of electrons in a two dimensional superlattice is considered. The lattice unit cell is a square with a small side. When electrons hit a cell side, they are reflected with a probability $\mathcal{R}$ and transmitted with probability $\mathcal{T}$. A diffusion approximation of the model is performed and leads to a diffusion equation in position-energy variables (SHE model). The diffusion constant can be expressed explicitly in terms of reflection-transmission coefficients. The mathematical problem is a two dimensional version of a previous work in the one dimensional case [N. Ben Abdallah, P. Degond, A. Mellet, F. Poupaud, *Electron transport in semiconductor superlattices*, Quarterly Appl. Math. **2003**, 61 (1) 161-192], and appears in the modeling of gas sensors.

1. Introduction

Polycrystalline semiconductors, in thin layers, are used in many technological applications such as gas detectors [20, 21, 24]. The polycrystal is a collection of microscopic crystal grains separated from each other by very thin regions called grain boundaries. At the grain boundary, charges can be trapped thus creating and/or modulating a localized potential barrier. This in turn modifies the probability that an electron hitting the grain boundary is transmitted to a neighboring grain or reflected back. The reflection-transmission phenomenon is responsible for the surface conductivity of the gas sensor, and is used to measure the concentration of the gas [20]. The principle of operation is as follows: as the gas molecules are deposited on the sensor surface, they are ionized and adsorbed. They are more likely to be trapped at the grain boundaries. The value of the trapped charge is directly related to the gas concentration; this relationship depends on the adsorption mechanism [5, 27]. Of course, the higher the gas concentration is the bigger the trapped charge. Its value, together with the doping concentration and the macroscopic electron density, determine the electrostatic structure at the grain boundary. This in turn determines the reflection-transmission coefficients across the grain boundary from which the conductivity of the gas sensor can be deduced. To summarize, the value of the gas concentration determines the conductivity of the sensor. By measuring the current flowing through the sensor, its conductivity is measured which allows us to deduce the gas concentration. The aim of this paper is to show how the conductivity can be deduced from the reflection-transmission coefficients of the grain boundaries. This is done by deriving a diffusion model whose diffusion coefficients are directly expressed in terms of the reflection-transmision coefficients. The grains are assumed to be arranged in a periodic bidimensional lattice, and the scattering coefficients at the grain boundaries are assumed to be known. We do not consider here the way to compute these coefficients from the electrical structure of the grain boundary. The scaled length of a simple grain is denoted by α and is assumed to be very small. Electrons are submitted to a macroscopic electrostatic potential and flow according to Newton's law in the grain. When they hit the grain boundary, they have a probability $\mathcal{R}$ to be reflected back following Descartes law and a probability $\mathcal{T}$ to be tranmitted to the neighboring grain

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