A 2-D modeling of Metal-Oxide-Polycrystalline Silicon-Silicon (MOPS) structures for the determination of interface state and grain boundary state distributions.

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Abstract

The aim of this work is the study of the Metal-Oxide-Polycrystalline Silicon-Silicon (MOPS) structure. This study is carried out by means of the two-dimension numerical resolution of Poisson's equation with a model of state continuum in the bandgap and at the Si/SiO_2 interface. By fitting experimental C(V) data with computed results, both grain boundary state and interface state distributions are determined.

1. Introduction

The Metal-Oxide-Polycrystalline Silicon-Silicon (MOPS) structure can be an active zone of a thin film transistor fabricated onto an integrated circuit (3-D architecture). A numerical modeling is used for the study of the interface and polysilicon grain boundary trap distributions. This study is based on the resolution of the Poisson's equation to calculate the electrostatic potential variation induced by a gate voltage in a polysilicon MOS capacitor. We perform a numerical integration of this equation with a proper choice for the geometrical modeling of the polycrystalline silicon layer. Inside the grain boundary and at the Si/SiO_2 interface, we consider a U-shape distribution of states, with three kinds of traps: band tail states, dangling bond states and discrete states with proper parameters for each distribution. By fitting experimental data with numerical data, bulk state and interface state parameters are determined. We firstly explain the numerical method we use to solve the Poisson's equation, then we specify the simulation domain and finally we present and discuss the results of the simulation.

2. Resolution of Poisson's equation

The modeling is based on the two dimensional numerical solution of Poisson's equation:

$$\text{div } \varepsilon \text{ grad } \Phi = q (n - p + N_A^- - N_D^+ + N_{TA}^- - N_{TD}^+)$$

where ε is the local permittivity (silicon or oxide), Φ the electrostatic potential, n and p the electron and hole concentrations expressed in Maxwell-Boltzmann's statistics. The ionised trap density $N_{TA}^- - N_{TD}^+$ is computed with the Shockley, Read and Hall [1] model for the tail states and discrete states and with the Sah-Shockley [2] model for the dangling bonds states. N_A^- et N_D^+ are acceptor and donor ionised doping impurity densities. The method used to solve the Poisson's equation is the finite-difference method.

The resulting capacitance value can be expressed as a function of Φ from $C = \frac{dQm}{dVg}$, where Vg is the applied voltage and Qm the electric charge given by a two numerical integration:

$$Qm = \varepsilon_{ox} \cdot \iint_{\Sigma} [\overrightarrow{\text{grad}}\Phi]_{x=0} \cdot \vec{n} \, dS$$

3. Simulation domain

The polycrystalline silicon layer is modeled as a juxtaposition of monocrystalline grains separated by a 1 nm thick amorphous region perpendicular to the oxide-polycrystalline silicon interface (Figure 1).

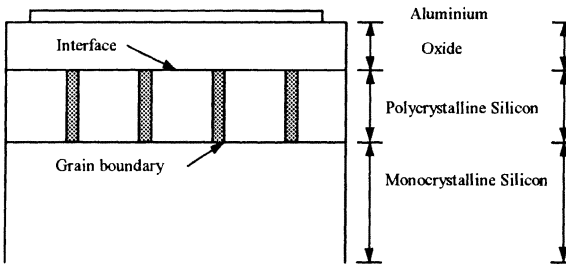

Figure 1: Schematic representation of the structure

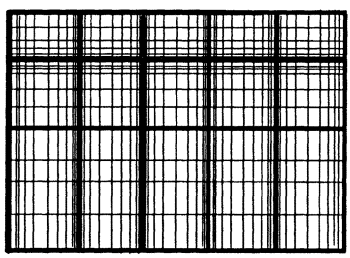

Figure 2: Mesh of the structure

The n-type polycrystalline silicon (300 nm thick, 2×10^{16} cm^{-3}) is deposited and *in-situ* doped by Very Low Pressure Chemical Vapor Deposition (VLPCVD) on a highly doped monocrystalline silicon substrate (0.02 Ω.cm). The oxide layer (150 nm thick) is obtained by thermal oxidation at 1050 °C. Subsequent aluminium deposit and photolithography give the final structure. Mean grain size (parallel to interface) is 300 nm. Figure 2 shows the mesh used for the discretization of the geometrical structure.

4. Trap distribution

Inside the grain boundary and at the Si/SiO_2 interface, we consider a U-shape distribution of states, with three kinds of traps: band tail states, dangling bond states and discrete states (Figure 3) with proper parameters for each distribution.

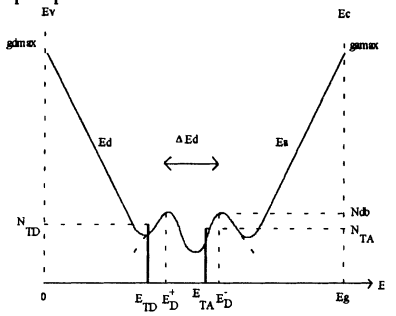

Fig 3: Schematic representation of state distributions

Band tails are caused by localisation of carriers within the wells and hills of potential fluctuations [3]. This exponential distribution may be derived from a Boltzman distribution of isolated defect centres. The trap density due to band tails is given by N_{TD} for the valence band tail and N_{TA} for the conduction band tail:

$$N_{TD} = \int_{Ev}^{Ec} f_D(E)\, g_D(E)\, dE \quad \text{and} \quad N_{TD} = \int_{Ev}^{Ec} f_A(E)\, g_A(E)\, dE$$

where $f_A(E)$ and $f_D(E)$ are the acceptor and the donor occupation functions and $g_A(E)$ and $g_D(E)$ the acceptor and donor distribution functions respectively. E_C and E_V are the conduction and valence band edge energies.

Dangling bonds are located in the middle of the bandgap and are characterised by their amphoteric character. These defects come from the polycrystalline silicon structure and correspond to no satisfied Si-Si bonds. The energy distribution is gaussian. The total density of ionised states is given by $N_{DB} = N_{D+} - N_{D-}$ where N_{D+} and N_{D-} are the donor and acceptor dangling bonds density respectively. These dangling bond state densities are given by:

$$N_D{+} = \int_{Ev}^{Ec} n_D(E)\, f^{+}(E)\, dE \quad \text{and} \quad N_D{-} = \int_{Ev}^{Ec} n_D(E)\, f^{-}(E)\, dE$$

where $f^{+}(E)$ et $f^{-}(E)$ are the distribution functions and $n_D(E)$ is the gaussian trap states distribution function.

Discrete states are traps due to uncontrolled impurities, which can give localised states in the band gap with either an energy E_{TA} for acceptor-like traps or either an energy E_{TD} for donor-like traps.

5. Numerical results

Numerical values for the physical parameters as the permittivity, the electron affinity, the densities of states in the conduction and valence band edge, the gap energies in the crystallite (1.12 eV) and in the grain boundary (1.7 eV) are taken from the literature. Fitting parameters are the doping of the polysilicon layer and the distribution of tail states and dangling bonds both at grain boundary and at Si/SiO_2 interface. Figure 4(a) shows the comparison of experimental and computed data for the high frequency and quasi-static C(V) plots. This fit is possible by adjusting both the interface states distribution Dit (b) and the grain boundary states distribution Dgb (c).

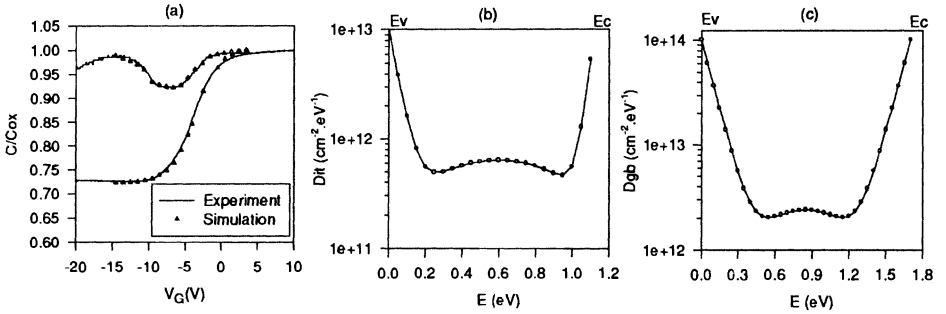

Figure 4: Example of the high frequency and quasi-static C(V) plots simulation (a), Distribution of interface state density (b), of grain boundary state density (c).

6. Conclusion

The polysilicon device performances depend on the polysilicon layer quality. Traps resulting from defects at grain boundary as well as at polysilicon/oxide interface affects the electronic behaviour of the device. By fitting experimental C(V) data with computed results, both grain boundary state and interface state distributions are determined. The differentiation of these distributions is needed if we want to qualify the efficiency of process like hydrogenation used to lowered these two trap distributions.

References

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[3] J. H. Werner, M. Peisl, "Exponential band tails in polycrystalline semiconductors films", Physical Review B, Vol.31, No.10, pp. 6881-6883, May 1985.