Strain-dependent hole masses and piezoresistive properties of silicon Kazunori Matsuda

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Since piezoresistive properties of silicon were discovered by Smith fifty years ago, its effects have been widely used in the frame work of mechanical sensors. Recently, strained silicon has been extensively investigated to explore high speed MOSFETs. However, piezoresistivity in p-type silicon still has not been fully clarified due to the complexity of the valence band structure.

Previous model exploits decoupling of the degenerate valence band and attributes the piezoresistance effect to the hole transfer between the splitting bands while hole conductivity masses do not depend on strain. This model is based on the highly stressed approximation proposed by Bir and Pikus, and by cyclotron resonance at low temperature, where the band splitting is much more higher than 2kT, so it is not the case at room temperature¹.

Whereas, the density-of-states (DOS) effective masses play an important role in the depletion region of reverse biased bipolar device, such as piezo-capacitance effect, piezo-tunneling effect and piezo-junction effect and so on². However the highly stressed approximation can not explain the piezo-capacitance effect in the depletion layer of MOS capacitors because this approximation leads the DOS effective mass values for both heavy and light holes to be compatible.

In this paper, new model which includes strain-dependent hole massed in weakly stressed silicon is presented, which is the case at room temperature. The band mixing (BM) mass change effect due to the mixing between the light hole and the spin-orbit split-off bands, and the degeneracy lifting (DL) mass change effect caused by the decrease of the interaction between the heavy- and light-hole bands are taken into account.

The valence band of strained silicon is obtained by the empirical pseudo potential method. Its results are compared with results of the analytical solution of strain Hamiltonian deduced by Kim and Cardona³. The strain-dependent effective masses and the DOS masses for both heavy and light holes are obtained at the band minimum (i.e. gamma point in k-space) for independent crystallographic axes.

The piezoresistive coefficients are calculated on the base of this result by the relaxation-time approximation in Boltzman transport theory, taking into account both hole transfer and mass change effects for nondegenerated silicon at room temperature⁴. As a consequence, physical origin of longitudinal and transversal piezoresistive properties are discussed with BM and DL mass changes.

The results of strain-dependent DOS mass change are verified by the depletion layer capacitance and the threshold voltage of MOSFET because the letters shift with the mechanical stress due to change in the ratio of DOS masses of holes to electrons changes as discussed in our previous paper⁵.

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Figure 1. (a) Constant energy surfaces of heavy and light hole bands with <110> stress and without stress. (b)(c)(d) Rough estimation of effective masses change in <100> stress, <110> stress and <111> stress. (e) Density-of-states (DOS) masses change by applying uni-axial stresses for independent crystallographic directions.

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