A Physically-Based Analytic Model for Stress-Induced Hole Mobility Enhancement

B. Obradovic, P. Matagne, L. Shifren, X.Wang, M. Stettler, J. He[1], and M. D. Giles
Intel TCAD, Hillsboro, OR, 97124, USA[1] Intel PTD Q&R, Hillsboro, OR, 97124, USA
email: borna.obradovic@intel.com

Introduction

A novel computationally efficient model for stress-modulated hole mobility, suitable for a continuum transport simulators, has been developed and implemented. The physically-based model captures bandstructure modulation due to stress, and reproduces the experimental mobility behavior over a wide range of stress, electric fields, and current directions.

In the model, a simplified heavy-hole valence bandstructure is represented by a pair of intersecting ellipsoids in k-space, as shown in Figure 1. This models a slice of the full bandstructure through the (100) plane (the conduction plane). The essence of the behavior under compressive stress is illustrated in Figure 2. Uniaxial stress along the direction of current flow lowers the energy of the W regions relative to the H region. This results in a repopulation of holes into the W region, which is more favorable for conduction than the H region due to the larger gradient in K-space along the current flow direction [1]. Thus, mobility is enhanced. Conversely, a longitudinal tensile or transverse compressive stress results in an H to W repopulation, and a corresponding reduction of mobility. Additionally, stress leads to a change in the curvature of the bands, leading to modulation of mobility. *The effects of within-band repopulation and bandstructure curvature modulation are the physical basis of the model.*

The analytic model is constructed by parameterizing the relative energy shift of the two ellipsoids and their curvatures as functions of the in-plane stress tensor, expressed in the crystal coordinates of the Si unit cell. The relative fractional populations f_W and f_H of the W and H ellipsoids are calculated, based on the stress-dependent energy separation Δ, and Maxwell-Boltzmann statistics (using the carrier temperature). Next, the in-plane mobility tensor in the principal coordinates is computed, based on the curvature of the ellipsoids (stress dependent) and their relative populations. Finally, the mobility tensor is rotated into the direction of the local (in-plane) electric field. In this coordinate system, the tensor has only two relevant components, μ_{11} and μ_{21}, representing current flow in the direction of the field, and perpendicular to it. For MOS devices with typical channel orientations ([110]), the perpendicular component of the current vanishes, but the mobility tensor is not isotropic under general stress conditions and field orientations. The dependence on carrier energy (or lateral field, for drift-diffusion) is introduced through the carrier temperature term in the Boltzmann statistics. This results in reduced mobility enhancement for high-energy carriers (Figure 3.), since the W–H asymmetry is reduced at high carrier temperature (Figure 4.), as shown in full band Monte Carlo calculations [1].

The model is validated and calibrated using a set of wafer bending experiments (Figure 5). Devices of various lengths (with built-in stress) are subjected to additional longitudinal or transverse stress from the wafer bending, for a total stress range (bending plus structural) of 700 MPa tensile to 800 MPa compressive. The overall agreement to data is found to be very good, with only a slight increase (~10% for typical cases) in the required CPU time.

[1] M.D. Giles at al., "Understanding Stress Enhanced Performance in Intel 90 nm CMOS Technology", VLSI Symposium 2004 (to be published)
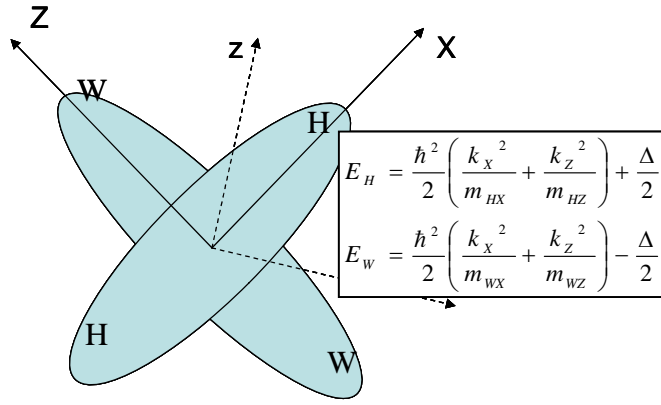
Figure 1. The simplified heavy-hole valence band is shown. Capital letters represent the principal directions in k-space [110]; lowercase letters represent the local (field-aligned) coordinate system. Typical current direction is 110.

$$E_H = \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_{HX}} + \frac{k_z^2}{m_{HZ}}\right) + \frac{\Delta}{2}$$

$$E_W = \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_{WX}} + \frac{k_z^2}{m_{WZ}}\right) - \frac{\Delta}{2}$$
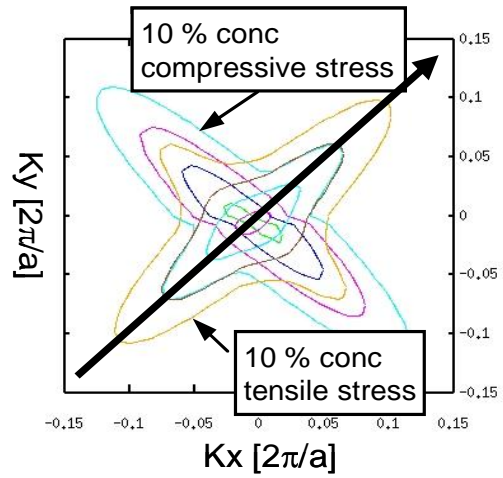

Figure 2. The heavy hole population in k-space is shown under longitudinal compressive and tensile stress. Depending on the stress, the population is shifted from a symmetric distribution (unstressed) to one that is predominantly in W or H (compressive or tensile)
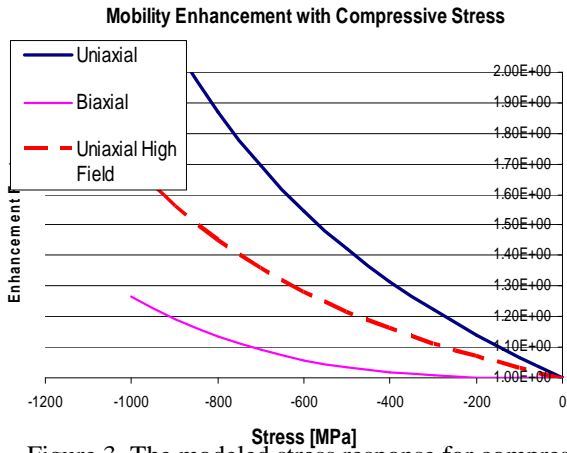

Figure 3. The modeled stress response for compressive stresses is shown. The behavior is strongly non-linear at high stress values, in sharp contrast to the Piezo model.
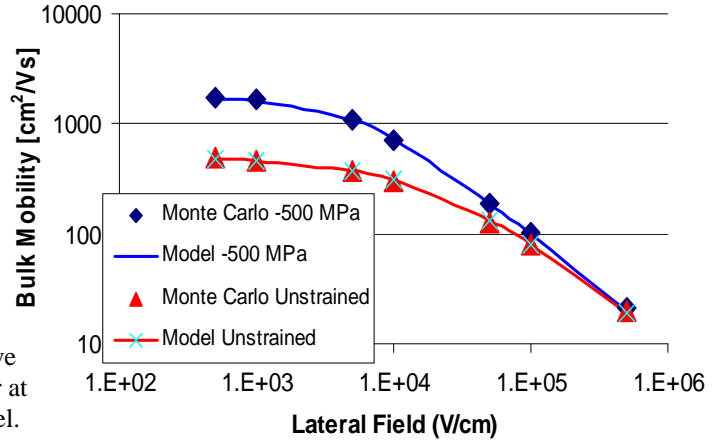

Figure 4. The high-field (lateral) behavior of the model (solid lines) is compared to Monte Carlo simulation (points). Saturation velocity is unchanged by stress. Thermal symmetrization of W and H populations is used to match intermediate-field behavior.

$$\mu_{enh} = 2\frac{m_t m_l}{m_t + m_l}\left[\cos^2\theta\left(\frac{f_1}{m_{t1}} + \frac{f_2}{m_{t2}}\right) + \sin^2\theta\left(\frac{f_1}{m_{l1}} + \frac{f_2}{m_{l2}}\right)\right] \quad \text{Eq.1}$$

$$f_W = \frac{\exp\left(\frac{\Delta}{2kT}\right)}{\exp\left(\frac{\Delta}{2kT}\right) + \exp\left(-\frac{\Delta}{2kT}\right)}, \quad f_W = \frac{1}{1 + \exp\left(-\frac{\Delta}{kT}\right)}, f_H = \frac{1}{1 + \exp\left(\frac{\Delta}{kT}\right)} \quad \text{Eq.2}$$

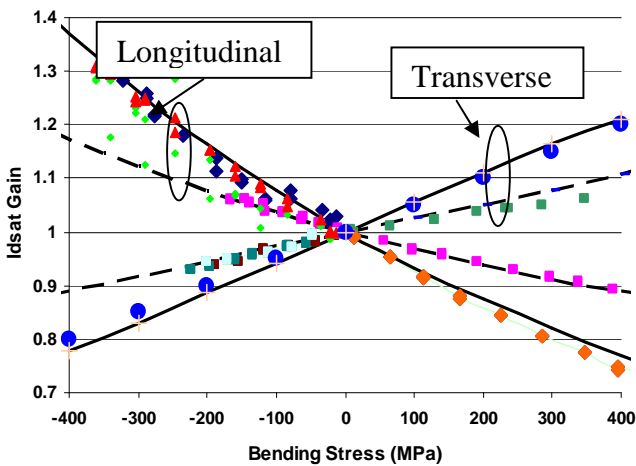$$S = \begin{pmatrix} b+a & s \\ s & b-a \end{pmatrix} \quad \text{Eq. 3.}$$

Figure 5. Comparison of predicted Idsat gain (lines) to wafer bending data (points) for long channel (1 μm – solid line) and short-channel devices (55 nm – dashed line). All devices have built-in stress in addition to the bending stress.

Figure 6. Equation 1. specifies the mobility enhancement (relative populations (f), current direction (θ), carrier temperature T, and the curvature masses) Equation 2. defines the components of the in-plane stress tensor :shear (s), biaxial (b), asymmetric (a).

A full journal publication of this work will be published in the Journal of Computational Electronics.