# A Simple, Unified 3D Stress Model for Device Design in Stress-Enhanced Mobility Technologies

A. Kumar, K. Xiu, W. Haensch IBM Semiconductor Research and Development Center T.J. Watson Research Center Yorktown Heights, NY, USA arvkumar@us.ibm.com

*Abstract*—A simple, physical model relating 3D stress field to carrier mobility enhancement is presented. The model is valid for both holes and electrons on orientations of interest for both conventional planar and FinFET technologies, and is well-suited for efficient implementation in a TCAD environment.

Keywords-Charge carrier mobility, stress, numerical simulation

### I. INTRODUCTION

Improving channel mobility through stress engineering is a powerful method of boosting device performance [1-8]. The mobility enhancement-stress relation is usually characterized using piezoresistance coefficients [1-3], which linearize this relation and are valid for low stress levels. However, today's stress elements induce high stress levels with complex R. Robison<sup>1</sup>, M. Bajaj<sup>2</sup>, J.B. Johnson<sup>1</sup>, S. Furkay<sup>1</sup>, R.Q. Williams<sup>1</sup>

IBM Semiconductor Research and Development Center <sup>1</sup>Essex Junction, VT, USA <sup>2</sup>Bangalore, India

geometry [4] such that the nonlinear and 3D character of this relation becomes critical, presenting a challenge for efficient implementation in a TCAD environment. In this work we introduce a simple methodology such that the mobility dependence on stress field is expressed as a universal curve of an effective stress parameter  $S_{\text{eff}}$  that is a simple function of the diagonal components of the stress tensor. This universal behavior can be modeled with a very efficient analytic mobility calculation which supplants the need for look-up tables or a real-time self-consistent multi-band computation.

We show that these simple relations can be used for both holes and electrons. We consider the cases of current flow along <110> on (001), as in conventional planar devices, and along  $<\overline{1}$  10> on (110), as is important for FinFETs [7].



**Fig. 1:** (001) <110> hole phonon mobility enhancement for (a) uniaxial and biaxial stress and (b) other stress combinations as a function of the stress component varied, at vertical field F=0.5 MV/cm. In (c) all points from (a) and (b) are replotted as function of effective stress field  $S_{\text{eff}}$ . Inset shows the direction convention used in this work.



**Fig. 2:** (110)<  $\overline{1}$  10> hole phonon mobility enhancement for (a) uniaxial and biaxial stress and (b) other stress combinations as a function of the stress component varied, at vertical field *F*=0.5 MV/cm. In (c) all points from (a) and (b) are replotted as function of effective stress field *S*<sub>eff</sub>.

	(001) <110> holes	(110) < 1 10> holes	(001) <110> electrons	(110) < 1 10> electrons
αx	1	1	1	1
αy	-0.4	-0.3	-1.7	0.8
αz	-0.6	-0.7	0.7	-1.8
βxx	0	0	0	0
βуу	0.00006	0.0001	0	0
βzz	0.00011	0	0	0
βxy	0	0	0	0
βyz	-0.00018	0	0	0
βxz	-0.00004	0	0	0

TABLE I: Values of coefficients used in expression for Seff

#### II. UNIFIED MODEL

The basis of the Unified Model (UM) is full-band calculations [5-8] of the mobility response to a 3D stress field. To exemplify the method, Fig. 1(a) shows phonon mobility enhancement  $\gamma_{ph}$  for (001)<110> holes at vertical field *F*=0.5 MV/cm and temperature 25C for six cases of uniaxial and biaxial stress, while Fig. 1(b) shows  $\gamma_{ph}$  for a multitude of other cases in which one component is varied while the other two are fixed. Fig. 1(c) replots the same data in (a) and (b), but as a function of an effective stress field *S*<sub>eff</sub>:

$$S_{\rm eff} = \Sigma \alpha_{\iota} S_{\rm ii} + \Sigma_{(j \ge i)} \beta_{\rm ij} S_{\rm ii} S_{\rm jj} \quad . \tag{1}$$

As apparent from Table I which summarizes the coefficient values for each case,  $S_{\text{eff}}$  is approximately a linear combination of  $S_{xx}$ ,  $S_{yy}$ , and  $S_{zz}$ , with small second-order terms necessary for high stress in the hole cases. Remarkably, when the mobility enhancement is plotted against this effective stress field with appropriately chosen coefficients, the data points fall on a universal curve, allowing the mobility dependence on a 3D stress field to be captured in a very simple way. Fig. 2(a-c) shows a similar analysis for  $(110) < \overline{1}$  10> holes, while Figs. 3(a-b) and 4(a-b) demonstrate that the  $S_{\text{eff}}$  concept works well for (001) < 110> and  $(110) < \overline{1}$  10> electrons, respectively. Interestingly, note that  $(\alpha_x + \alpha_y + \alpha_z) = 0$  for all cases.

We now generalize our results as a function of vertical field *F*. Fig. 5(a-b) shows  $\gamma_{ph}$  as a function of  $S_{eff}$  for (001)<110> holes and electrons, for *F* from 0.25 to 1 MV/cm. Again, the data points all fall on universal curves simply characterized by field-dependent coefficients. For both holes and electrons, curves of the phonon mobility enhancement  $\gamma_{ph}$  (relative to the unstressed phonon mobility  $\mu_0$ ) can be fit to a sigmoid function



Fig. 3: (001) <110> electron phonon mobility enhancement (a) various stress combinations as a function of the stress component varied, at vertical field F=0.5 MV/cm. In (b) all points from (a) are replotted as function of  $S_{\text{eff}}$ .



**Fig. 4:** (110)< 1 10> electron phonon mobility enhancement (a) various stress combinations as a function of the stress component varied, at vertical field F=0.5 MV/cm. In (b) all points from (a) are replotted as function of  $S_{\text{eff}}$ .

TABLE II: Values of parameters in sigmoid fits.

	(001) <110> holes	(110) < 1 10>	(001) <110> electrons	<110) <110>
		holes		electrons
$\mu_0$	212	1235	810	326
$A_1$	2460	505-365 $F$ +164 $F^2$ , $F \le 0.5$ , 364, $F \ge 0.5$	565-81 <i>F</i> -44 <i>F</i> <sup>2</sup>	270
$A_2$	42	9136-25027 $F$ + 24494 $F^2$ , $F \le 0.5$ , 2746, $F \ge 0.5$	2028-1992 <i>F</i> + 920 <i>F</i> <sup>2</sup>	761
S <sub>0</sub>	-1338	$\begin{array}{l} -2084{+}6879F{-}\\ 6896F^2,  F{\leq}0.5,\\ -368, F{\geq}0.5\end{array}$	1334- 2646F+875F <sup>2</sup>	799
t	524	-650	882- 987F+604F <sup>2</sup>	417

$$\gamma_{\rm ph} = (1/\mu_0) \left( (A_1 - A_2) / (1 + \exp((S_{\rm eff} - S_0)/t)) + A_2 \right)$$
(2)

with parameters for each case shown in Table II. For (001)<110> holes the field dependence is sufficiently weak [6] that field-independent coefficients are used for simplicity. For (110)< $\overline{1}$  10> holes, field-dependent coefficients are used only below 0.5 MV/cm since the field dependence becomes significant only for low *F*. For (110)< $\overline{1}$  10> electrons, the field dependence is also very weak, so we have used field-independent coefficients. Sigmoid fits for (110)< $\overline{1}$  10> holes and electrons at *F*=0.5 MV/cm are shown in Figs. 2(c) and 4(b).

## III. IMPLEMENTATION

We have implemented the UM into the IBM continuum device simulator FIELDAY [9] by modifying the Mujtaba mobility model [10], with stress fields obtained from self-



**Fig. 6:** Comparison of phonon vs. total mobility enhancement for (001)<110> holes.



**Fig. 5:** Vertical field dependence for (001)<110> (a) holes and (b) electrons along with sigmoid fits.

consistent process simulation. Conventionally a piezoresistance coefficient relates the total mobility enhancement response from a stress field [3] while the enhancement calculated here is for the phonon mobility  $\mu_{ph}$  only. The phonon mobility  $\mu_{ph}$  is combined with other mobility components using Matthiessen's rule to obtain the total mobility  $\mu_{T}$ .

For the case of electrons, there is an ample body of literature [11-14] which suggests reduction of surface roughness (SR) with strain. To partially account for this, we choose for electrons to apply  $\gamma_{ph}$  to both phonon and SR components. On the other hand, for holes unchanged [15] or increased [6] SR scattering is suggested, so that we apply  $\gamma_{ph}$  to  $\mu_{ph}$  only and leave the other mobility components unchanged. For holes, inclusion of the unenhanced SR scattering dampens the total mobility, leading to saturation of  $\mu_{T}$  as shown in Fig. 6. This gives results consistent with calculations for purely uniaxial compression stress ( $S_{yy}=S_{zz}=0$ ) [1]. Implemented TCAD shows better agreement with 45nm hardware for both nFET and pFET using these assumptions.

# IV. DISCUSSION AND CONCLUSION

These expressions not only provide a simple methodology for handling arbitrary stress fields in TCAD but also provide intuitive formulas useful for stress engineering by indicating favorable directions for each type of stress. For example, the large negative  $\alpha_z$  for (110)< 1 10> electrons suggests transverse compressive strain to improve electron mobility in a FinFET configuration favorable for hole mobility [7].

In conclusion, we have developed a simple but powerful physically-based TCAD tool for stress engineering device design in future technologies. The model allows for arbitrary stress fields, thereby providing a unifying expression for uniaxial and biaxial stress. It extends the low-stress limit of piezoresistance coefficents to the high-stress regime required for current technologies. Dependence on vertical field is included, while generalization to account for temperature dependence is among the problems we have left for future work. Finally, the model allows for both holes and electrons under different orientations, making it a very versatile tool for predictive simulation in future technology nodes.

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