Calculation of alloy scattering mobility in SiGe FETs based on atomistic tight-binding approach

Hong-Hyun Park, Changwook Jeong*, Seonghoon Jin, Woosung Choi,
Young-Tae Kim*, Ui-Hui Kwon*, Keun-Ho Lee*, and Youngkwan Park*
Samsung Semiconductor Inc., San Jose, California, USA
*Semiconductor R&D Center, Samsung Electronics, Hwasung-si, Gyeonggi-do, Korea
e-mail: honghyun.p@samsung.com

ABSTRACT

The use of SiGe alloy as a channel material is a promising way to overcome the low mobility problem of conventional Si-based field effect transistors. This paper presents an atomistic approach to alloy scattering mobility calculation and shows its application to SiGe channel field effect transistors.

INTRODUCTION

The calculation of alloy scattering mobility has become an important device modeling issue to determine the expected device performance of SiGe-based FETs. Usually, the calculation of alloy scattering mobility assumes an alloy scatterer in a simple analytical form with some fitting parameters [1], which is a good practical approach but has a limited predictability. Recently, Mehrotra et al. presented an atomistic approach to calculate the alloy scattering mobility in bulk SiGe materials, which describes an alloy system in atomistic level and requires no fitting parameters for the mobility calculation [2].

In this paper we extend the atomistic approach to be applicable to general devices as well as bulk materials. Also, we investigate the alloy scattering mobility in SiGe bulk, thin film, and thin film FETs.

CALCULATION METHOD

The following briefly shows a few steps to calculate the alloy scattering hole mobility in the channel region of a device.

Step 1: Perform a device simulation at a certain bias condition to obtain the solution and information needed for the following mobility calculation.

Step 2: Solve Schrodinger equations in a desired channel region of the device assuming no atomistic randomness due to alloy atoms. Alloy-averaged Hamiltonian matrices($H_{VCA}(\vec{k})$) are solved and corresponding eigenfunctions($|\vec{k}\rangle$) and velocities($v(\vec{k})$) are obtained.

Step 3: Calculate the ensemble average of the momentum relaxation time due to alloy scattering.

$$\frac{1}{\tau_x(\vec{k})} = \int d\vec{k}' \left\langle \frac{2\pi}{\hbar} \left| \left\langle \vec{k} \left| H_{alloy}(\vec{k}) - H_{VCA}(\vec{k}) \right| \vec{k}' \right\rangle \right|^2 \delta\left(E(\vec{k}) - E(\vec{k}')\right) \right\rangle \left(1 - \frac{v_x(\vec{k}')}{v_x(\vec{k})}\right)$$

, where $H_{alloy}(\vec{k})$ is a Hamiltonian matrix of a randomly generated SiGe alloy structure.

Step 4: Calculate the hole mobility according to Kubo-Greenwood formula.

$$\mu_x = \frac{\frac{q}{k_B T} \int d\vec{k}\, \tau_x(\vec{k}) \left| v_x(\vec{k}) \right|^2 f(E(\vec{k}))\left(1 - f(E(\vec{k}))\right)}{\int d\vec{k} \left(1 - f(E(\vec{k}))\right)}$$

RESULTS AND DISCUSSIONS

Hole alloy scattering mobility for SiGe bulk, thin film, and the channel of thin film transistors are calculated. $sp^3d^5s^*$ tight-binding basis with spin-orbit coupling and a valence band offset of 0.54eV between Si and Ge have been used throughout our calculations. Results and discussions are shown in the following page with figures and captions.

REFERENCES

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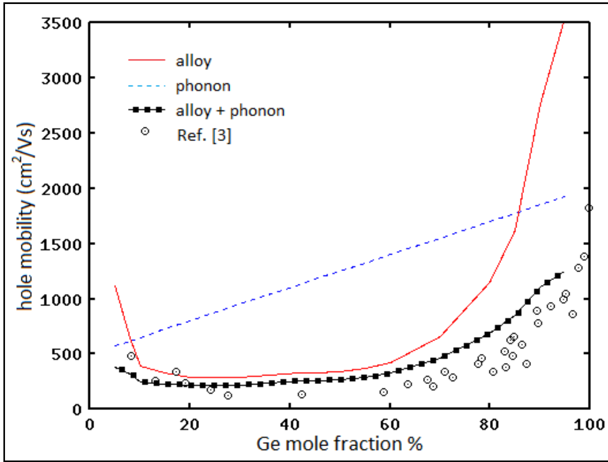


Fig. 1. Calculated hole mobility(red), estimated hole phonon mobility(dashed blue), and the total of the two(marked black) versus alloy mole fraction in bulk SiGe. Our calculation shows good agreement with Ref. [3].

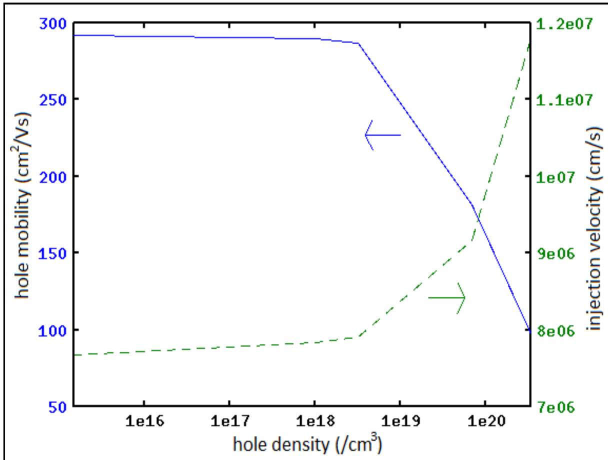


Fig. 2. Calculated hole alloy scattering mobility(blue) versus hole density in $Si_{0.7}Ge_{0.3}$ bulk. In degenerate semiconductors the alloy scattering mobility decreases due to rapid increase of alloy scattering rate even though the average carrier velocity increases as carrier density.

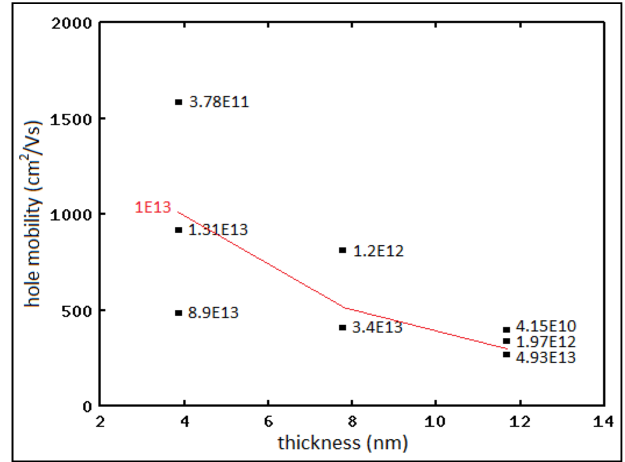
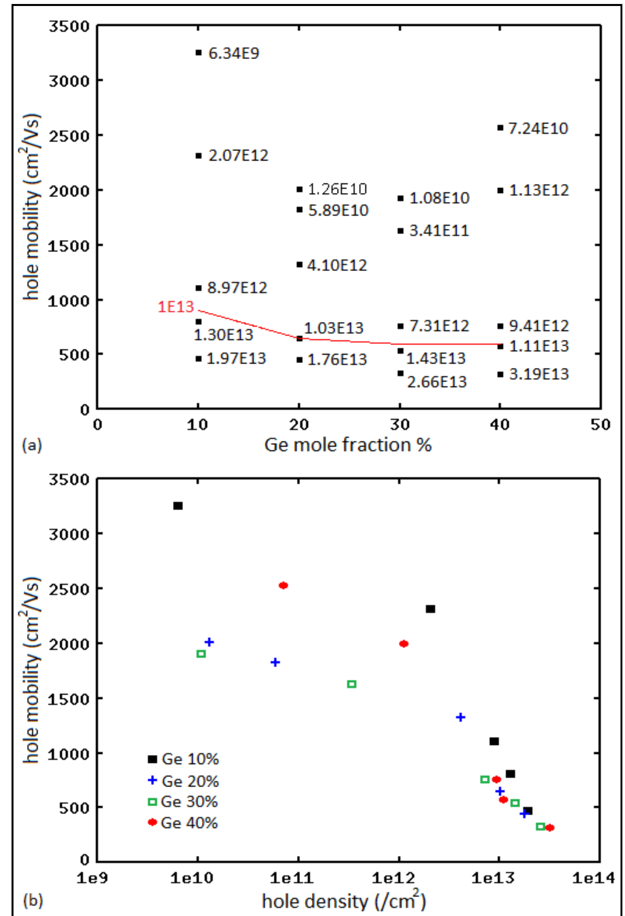


Fig. 3. Calculated hole alloy scattering mobility in thin film $Si_{0.7}Ge_{0.3}$ layers with different thicknesses and carrier densities. The transport and confinement directions are [110] and [1-10], respectively. The numbers at markers are the surface hole densities(/cm^2) and a red line indicates a hole alloy mobility with a fixed surface hole density of 1E13/cm^2.



Figs. 4(a) and 4(b). Calculated hole alloy scattering mobility in the channel of thin film SiGe transistors with various alloy mole fraction and gate bias conditions. The thickness of the thin films is 11.7nm, and the transport and confinement directions are [110] and [1-10], respectively. (a) The numbers at markers are the surface hole densities(/cm^2) and a red line indicates a hole mobility with a fixed surface hole density of 1E13/cm^2. (b) There is a tendency for the alloy scattering mobility to decrease with increasing the carrier density.