Extended Abstracts of the 2004 International Conference on Solid State Devices and Materials, Tokyo, 2004, pp. 450-451

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Electron Transport Model for Strained Silicon-Carbon Alloy

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1. Introduction

There is growing interest in using the new group IV alloys such as SiGeC and $Si_{1-x}C_x$ for fabricating Si heterostructure devices. Recently, strained $Si_{1-x}C_x$ on Si has been the subjected of intense interest because the tensile strain due to the lattice constant of $Si_{1-x}C_x$ being smaller than that of Si leads to a lifting of the degeneracy in both the conduction and valence bands. Thus the $Si_{1-x}C_x$ channel embedded in Si has been proposed as an alternative to a strained Si channel. Since graded buffer is not necessary for the fabrication of a strained $Si_{1-x}C_x$ layer, high crystalline perfection of a $Si_{1-x}C_x$ channel is obtained. But despite this apparent importance all electron transport models for strained $Si_{1-x}C_x$ published so far are limited generality (e.g. neglect the influence of Carbon on phonon scattering [1,2]) and are not verified experimentally by measurement of mobility in strained $Si_{1-x}C_x$ layers. This paper aims at closing this gap.

2. Mobility Model

Within our model the conduction band structure of strained $Si_{1-x}C_x$ grown on (001) Si substrate is described by six ellipsoidal and nonparabolic valleys, two of which shifted downwards in energy under the biaxial tensional strain. The valley shifts and the effective masses are modeled as a function of relative C content x as described in Ref. [3]. The non parabolicity is set to $\alpha=0.5eV^{-1}$ independently of x. The phonon system considers all relevant scatterings in the Si-like band structure with its six valleys along the Δlines for Si. Phonon energies determining the thresholds for optical phonon emission are distinctly different in Si and C. This effect is taken into account by considering the phonon scattering rates of Si and C linearly weighted by their relative fraction in the alloy. The C phonon energies for interband scattering between the valleys on the axes are extracted from Ref. [4]. Essentially the same values as in Si are taken for corresponding coupling constants.

3. Results and Discussion

Fig.1 and Fig. 2 show the good agreement between the results of the transport model and the Monte Carlo simulations [5] proving the validity of our model. From the theoretical standpoint the proper modeling of impurity scattering is still a controversial issue. On the other hand reliable experimental data for electron mobility as function of doping is readily available in Si. Therefore as an engineering compromise the ionized impurity scattering model of Ridley is adopted with a doping dependent adjustment to mobility measurements to account for all additional effects like degeneracy [6] (see Fig. 3). In $Si_{1-x}C_x$ the only additional modification of Ridley model consists of a linear interpolation of dielectric constant between its values in Si and C. Hence all scattering model parameters of transport model presented here have been delivered exclusively from available literature data on unstrained Si and C. Alloy scattering is modeled according the model of Harrison and Hauser. The unknown scattering potential was chosen such that the experiment data of Ref [9, 10] for strained $Si_{1-x}C_x$ are reproduced. In Fig. 4 electron mobility is displayed as function of C content for doping $N_D=10^{17}cm^{-3}$. The mobility components perpendicular and parallel to $Si_{1-x}C_x$ /Si interface in strained $Si_{1-x}C_x$,μ_{zz} and μ_{xx}, as well the mobility in relaxed $Si_{1-x}C_x$, μ, are shown for majority electron in Fig. 5. The influence of impurity scattering on the electron mobilities for various carbon mole fraction is shown in Fig. 6. The electron mobility decreases with increasing carbon content up to x=1% due to the alloy scattering. For high impurity concentrations impurity scattering is by far the dominant scattering process, while for moderate dopant concentration effect of alloy scattering is still relatively strong. This consideration explains the carbon content dependence of the mobility at different doping levels. Since the contribution of the alloy scattering rate to the total scattering rate at low doping is still large, increasing carbon content always results in a mobility reduction. At a high doping level, alloy scattering is relatively unimportant compared with impurity scattering. Consequently, the mobility reduction due to alloy scattering becomes smaller at a higher doping level. In addition, electron mobility tends to saturate for doping level exceed $10^{19}cm^{-3}$ because of electron screening in impurity scattering. This behave is confirmed by recent experimental result (i.e. The mobility in strained $Si_{1-x}C_x$ is almost the same as that in bulk Si for doping level above $10^{19}cm^{-3}$) [10]Both results of our model and experiment on electron transport in strained $Si_{1-x}C_x$ alloys indicate that the effect of alloy and impurity scattering dominates over the expected gain due to strain.

4. Summary

In summary, we have presented an accurate and experimentally verified model for electron transport in strained $Si_{1-x}C_x$ alloys.

References

[1] M. Eeshov and V. Ryzhii, J. Appl. Phys, **76** (1994)1924.
[2] P. Dollfus et al., IEEE Trans. Electron Dev., **47** (2000)1247.

[3] S. T. Chang, C. Y. Lin and C. W. Liu, J. Appl. Phys, **92** (2002). 3717
[4] F. Nava et al., Solid State Commu., **33** (1980) 475.
[5] SILVACO TCAD package, MOCASIM: Monte Carlo simulator (2002).
[6] F. M. Bufler, "Full band Monte Carlo Simulation of Electrons and Holes in Strained Si and SiGe," Munich: Herbert Utz Verlag, 1998. (http://utzverlag.com)
[7] W. R. Thurber, R. L. Mattis, and Y. M. Liu, J. Electrochem. Soc., **127** (1980) 1807.
[8] A. B. Sproul, M. A. Green, and A. W. Stephens, J. Appl. Phys., **72**, (1992) 4161.
[9] H. J. Osten et al., J. Appl. Phys, **82** (1997) 4977.
[10] S. Yagi et al., Jan. J. Appl. Phys, **41** (2002), 2472.

Acknowledgements

This work is supported by the National Science Council, Taiwan, ROC, under the contract Nos. of NSC92-2112-M-005-010 (C. Y. Lin), NSC 92-2215-E-033-004 (S. T. Chang)

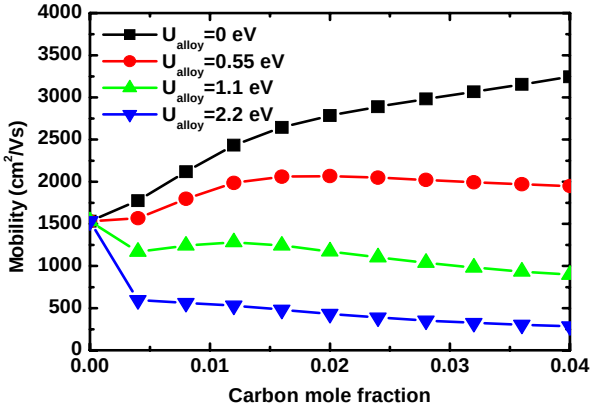

Fig. 1 In-plane low-filed mobility in strained $Si_{1-x}C_x$ alloy as a function of carbon content x with different alloy scattering potential. Solid lines are results of an analytical transport model. Symbols are results of Monte Carlo Simulation [5] with the same scattering processes.

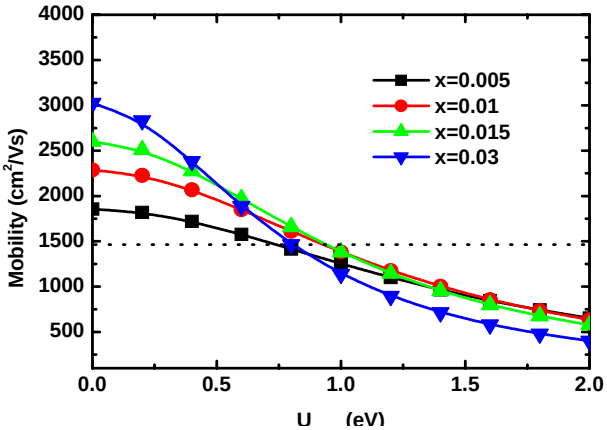

Fig. 2 In-plane low-filed mobility in strained $Si_{1-x}C_x$ alloy as a function of scattering alloy potential with different carbon content x. Solid lines are results of an analytical transport model. Symbols are results of Monte Carlo Simulation [5] with the same scattering processes.

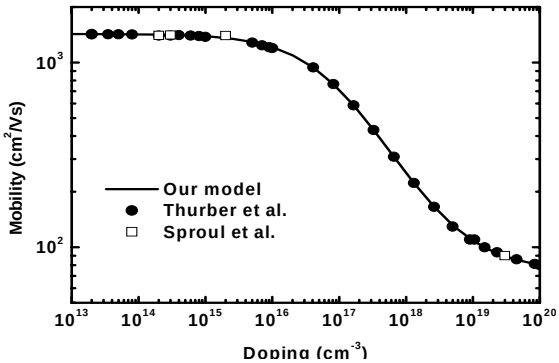

Fig. 3 Approximation of doping dependent experimental electron mobility data by Ref [6]. Data for solid symbol from Ref [7] and for open symbol from Ref. [8].

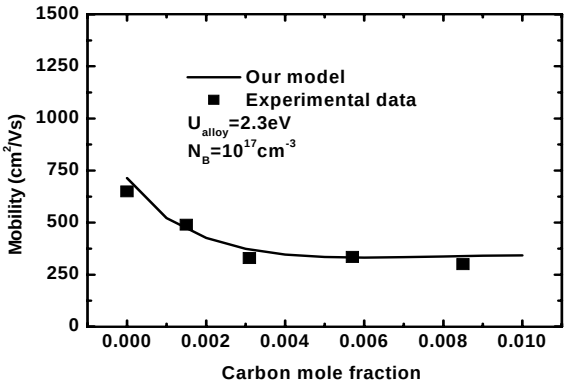

Fig. 4 Electron mobility of strained $Si_{1-x}C_x$ alloy for doping $N_D=10^{17}cm^{-3}$: solid line μ_{xx} of strained $Si_{1-x}C_x$ (in-plane mobility) and square dot is experimental data [9]. The value of 2.3 eV for U_{alloy} is used in our calculation.

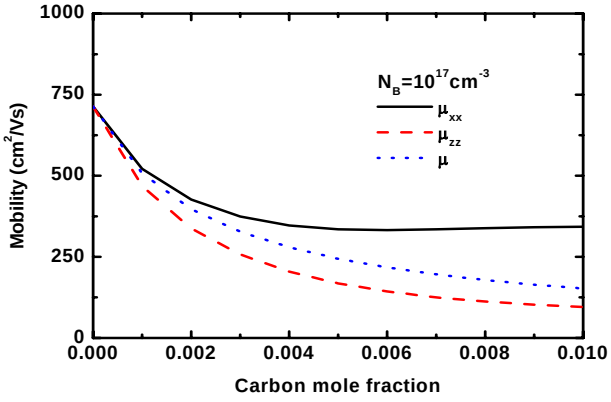

Fig. 5 Electron mobility of strained $Si_{1-x}C_x$ alloy for doping $N_D=10^{17}cm^{-3}$: solid lineμ_{xx} of strained $Si_{1-x}C_x$(in-plane mobility), dashed lineμ_{zz} of strained $Si_{1-x}C_x$(out-of-plane mobility), and dotted line μ of realxed $Si_{1-x}C_x$.

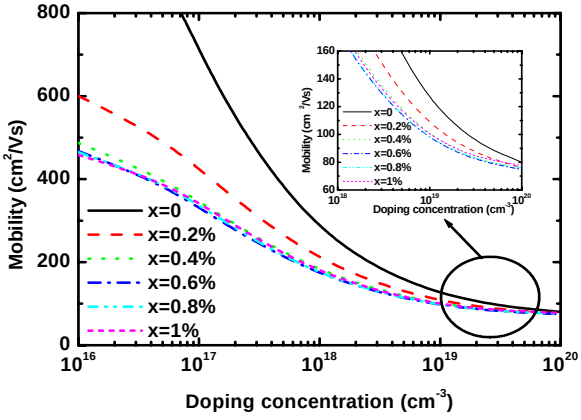

Fig. 6 The dependence of electron mobility on doping concentration for various carbon mole fraction. The local region is zoomed in as shown in the inset.