Microelectronics Journal 40 (2009) 452–455

Contents lists available at ScienceDirect

Microelectronics Journal

journal homepage: www.elsevier.com/locate/mejo

Enhanced electrical properties of nominally undoped Si/SiGe heterostructure nanowires grown by molecular beam epitaxy

P. Das Kanungo *, A. Wolfsteller, N.D. Zakharov, P. Werner, U. Gösele

Max-Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany

ARTICLE INFO

Available online 29 July 2008

Keywords:
Nanowire
Silicon-Germanium
MBE

ABSTRACT

Electrical properties of epitaxial single-crystalline Si/SiGe axial heterostructure nanowires (NWs) on Si⟨111⟩ substrate were measured by contacting individual NWs with a micro-manipulator inside an scanning electron microscope. The NWs were grown by incorporating compositionally graded $Si_{1-x}Ge_x$ segments of a few nm thicknesses in the Si NWs by molecular beam epitaxy. The *I–V* characteristics of the Si/SiGe heterostructure NWs showed Ohmic behavior. However, the resistivity of a typical heterostructure NW was found to be significantly low for the carrier concentration extracted from the simulated band diagram. Similarly grown pure Si and Ge NWs showed the same behavior as well, although the *I–V* curve of a typical Si NW was rectifying in nature instead of Ohmic. It was argued that this enhanced electrical conductivities of the NWs come from the current conduction through their surface states and the Ge or Si/SiGe NWs are more strongly influenced by the surface than the Si ones.

Axial $Si/Si_{1-x}Ge_x$ heterostructure nanowires (NWs) are attractive candidates for nanoelectronic, optoelectronic and thermoelectric devices [1] because of the possibilities of strain-induced enhancement of carrier mobility [2], embedding quantum well structures by modulated doping [3] and lower thermal conductivity [4]. Such heterostructure NWs have already been fabricated by molecular beam epitaxy (MBE) [5], chemical vapor deposition (CVD) [6] and hybrid pulsed laser ablation/chemical vapor deposition (PLA–CVD) [7] techniques. It is possible to incorporate single, as well as multiple SiGe segments in the Si NWs by all of the above growth techniques. Although the thermal conductivity of the PLA–CVD-grown Si/SiGe supper-lattice NWs has been reported [8] and the effect of elastic strain relaxation in the MBE-grown Si/SiGe NWs has been investigated [9], there is no report on the electrical properties of such heterostructure NWs until now. In this communication, we report on the electrical measurements of individual Si/SiGe NWs and compare them with that of pure Si and Ge NWs.

The growth of Si/SiGe NWs by MBE has already been reported earlier [5]. In the previous work, the $Si_{1-x}Ge_x$ segment of the NW was compositionally graded with the maximum Ge concentration at 10%. For the current NWs, the maximum Ge concentration was increased to 26% by optimizing the growth parameters. RCA-cleaned n-type (P doped, 5–10 Ω cm) 5″ Si⟨111⟩ wafers were used as the growth substrate. First a 200-nm Si buffer layer was grown followed by *in situ* Au (catalyst) deposition and subsequent growth of the first Si segment of the Si/SiGe heterostructure NWs at 545 °C. The growth temperature was lowered to 300 °C in steps and the SiGe segment was grown by diffusing Ge into the NWs through Au. The temperature was subsequently increased to 545 °C to grow the top Si segment. In order to compare the electrical properties of the heterostructure NWs, pure Si and Ge NWs were also grown following the exactly same temperature profile. Details of the growth process will be discussed elsewhere.

The NWs were single crystalline as revealed by the transmission electron microscopy (TEM) investigation (Fig. 1(a)). The Ge concentration along the length of the NWs was measured by many-beam TEM bright field imaging. For a typical NW in Fig. 1(a), the Ge concentration (x) showed a Gaussian profile with a peak value of 26% and FWHM of 7 nm (Fig. 1(b)).

Electrical measurements of individual NWs were performed by the technique already described in details earlier [10]. Small pieces were cleaved from the wafers and mounted on a copper stage of an scanning electron microscope (SEM) (JEOL, JSM6400) by making a back contact with silver paste. Silver gives a rather good Ohmic contact with Si. The measured contact resistance was around 3 kΩ. Tips of the individual NWs were contacted with Pt/Ir tips (Fig. 2(a)) of diameter 100–300 nm, etched electrochemically [11] from 250-μm-thick wires (Pt/Ir 80:20, Goodfellow) and attached to a micro-manipulator (Kliendiek, MM3A-EM). The micro-manipulator was connected to a pico-ammeter with an internal voltage source (Keithley 6487, <2 fA noise) to measure the *I–V* characteristics. Prior to every measurement, an SEM image was taken (Fig. 2(b)), and during the measurement the electron beam was blanked to avoid its influence. The gold caps on top of

* Corresponding author.
E-mail address: kanungo@mpi-halle.de (P. Das Kanungo).

0026-2692/$ - see front matter © 2008 Elsevier Ltd. All rights reserved.
doi:10.1016/j.mejo.2008.06.021

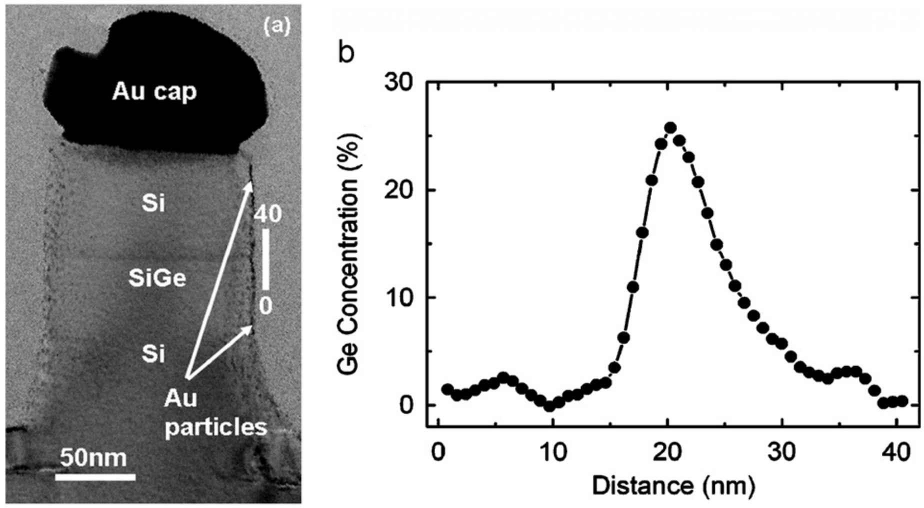

Fig. 1. (a) TEM image of a $Si/Si_{1-x}Ge_x$ heterostructure NW. (b) Ge concentration (x) profile of the NW in part (a) along the NW length.

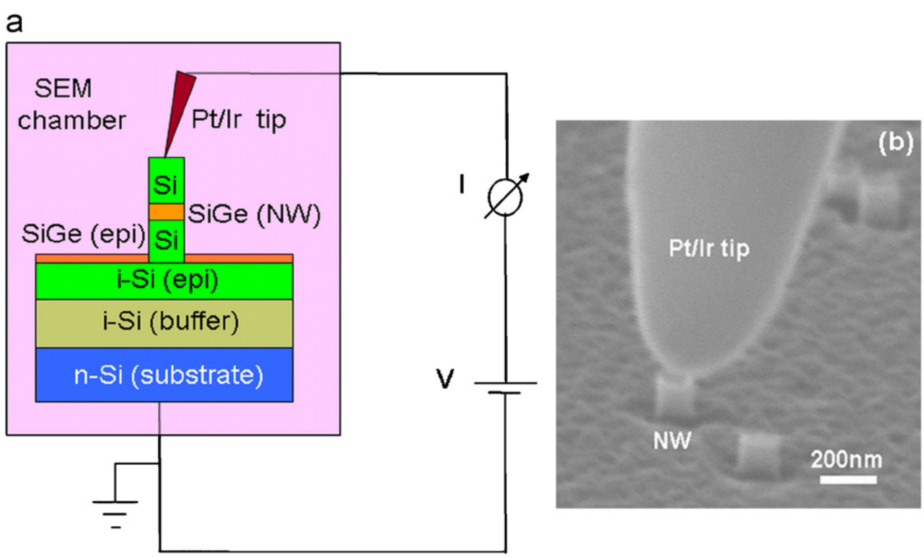

Fig. 2. (a) Schematic of the electrical measurement setup. (b) SEM image of a contacted NW.

the NWs were removed by a 5 min dip in an aqueous solution of KI and I_2 (4:1), a standard gold etchant, so that the Pt/Ir tip could make direct contacts with the NWs. The Au–Si contact is generally Schottky, whereas the Pt/Ir–Si contact is generally Ohmic due to the reduced barrier height [12].

There is a systematic uncertainty in our results because of the unknown real contact area and contact pressure at the top of the NWs with the Pt/Ir tip, which can change the measured current. In order to minimize this, we relied only on the repeatable data. To make a meaningful comparison, we picked Si/SiGe, Si and Ge NWs of comparable dimensions, i.e., of diameter 155 nm and length 200 nm. All the *I–V* curves were measured between −500 and 500 mV. The *I–V* curve of the Si/SiGe NW showed Ohmic/linear behavior (Fig. 3(a)) with a current in the range of 1 μA at 500 mV. The calculated resistance was 470 kΩ and resistivity 4 Ω cm. This value would correspond to a carrier concentration of $1\times10^{15}\,cm^{-3}$ for n-type and $3\times10^{15}\,cm^{-3}$ for p-type Si if we use bulk mobility values [12]. We also estimated the carrier concentration of this NW by making a simulation of its band structure based on the 'finite difference method' (Fig. 3(b)) at zero applied bias with the simulation tool Next-Nano[3]. The NW was treated as a line (one dimensional) with the Gaussian Ge concentration (x) profile of Fig. 1(b). The band gap was treated as a linear function of x [13]. The band structure showed strain-induced splitting of X conduction band (X1, X2) and light hole (LH) and heavy hole (HH) valence bands in the SiGe segment as expected. A 'Type II' band alignment led to the Fermi level (E_F) pinning at 0.58 eV above the valence band. This would result an electron (n) concentration of 5×10^{10} cm^{-3} and a hole (p) concentration of $2\times10^{9}\,cm^{-3}$ following the Fermi Dirac distribution statistics. These values are 6 orders of magnitude less than that obtained from our *I–V* curve (Fig. 3(a)). The pure Ge NW also showed Ohmic behavior (Fig. 4(a)) with significantly higher conductivity as well. The extracted resistivity was 0.2 Ω cm, which corresponds to a carrier concentration of $1\times10^{16}\,cm^{-3}$ for n-type and $4\times10^{16}\,cm^{-3}$ for p-type Ge. Both of them are 3 orders of magnitude higher than that of intrinsic carrier concentration in Ge ($2\times10^{13}\,cm^{-3}$). The pure Si NW showed rectifying characteristic (Fig. 4(b)), which agreed with our previous observation [10]. As demonstrated earlier, the rectification in this case comes from the space charge region at the base of

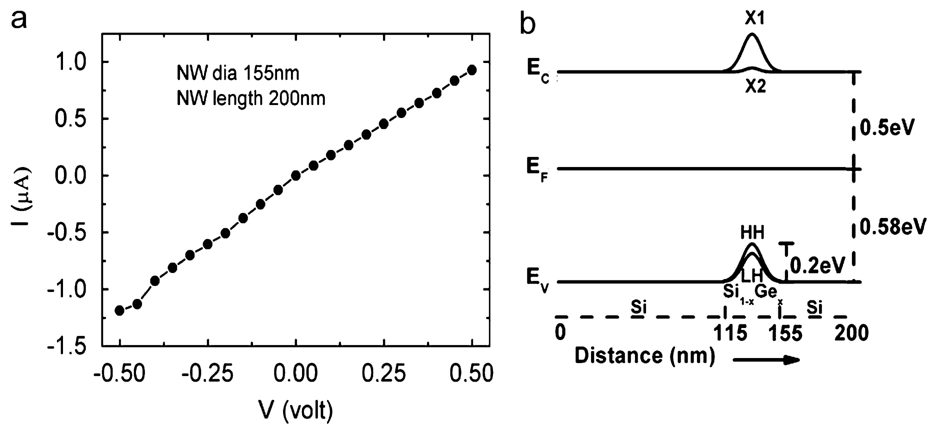

Fig. 3. (a) *I–V* characteristic of a Si/SiGe heterostructure NW. (b) Simulated band diagram of a Si/SiGe NW at zero bias using the Ge concentration profile in Fig. 1(b).

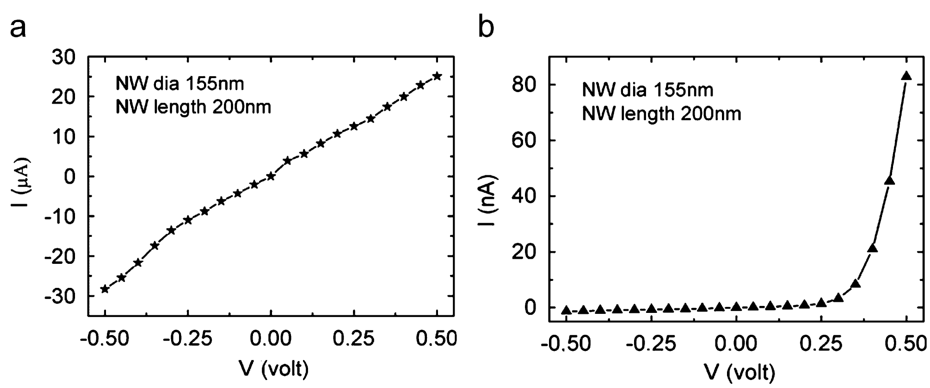

Fig. 4. (a) *I–V* characteristic of a pure Ge NW. (b) *I–V* characteristic of a pure Si NW.

the NW between the NW and the underlying epi-layer that grows in parallel with it [5]. The series resistance calculated from the diode-like curve of Fig. 4(b) was 1.61 MΩ. This corresponds to a resistivity of 15 Ω cm and a carrier concentration of $3 \times 10^{14}\,\mathrm{cm^{-3}}$ for n-type or $1 \times 10^{15}\,\mathrm{cm^{-3}}$ for p-type Si, which are 4–5 orders of magnitude higher than the intrinsic carrier concentration in Si ($1 \times 10^{10}\,\mathrm{cm^{-3}}$).

We observed a consistent enhancement of electrical conductivities in Si/SiGe, Ge and Si NWs. As calculated earlier, the carrier concentration in all of them is much higher than the corresponding intrinsic values. Owing to the cylindrical geometry and nanometric diameter, the NWs have a high surface-to-volume ratio. Their surfaces are invariably covered with a very thin (1–2 nm) layer of native oxide decorated with Au nanoparticles (Fig. 1(a)) that are remnants of the Au catalyst initiating the growth. These Au nanoparticles can add to the oxide charges or surface states at the NW–native oxide interface. In general, they deplete the volume of the NWs by trapping the free carriers. Unless the NWs are highly doped with the free carrier concentration at least in the range of $10^{18}\,\mathrm{cm^{-3}}$ [14], the surface states with a nominal density of $10^{11}\,\mathrm{cm^{-2}}$ should be able to fully deplete them. As a result, there should be no volume conductivity. However, the surface states can enhance the surface conductivities of both Si and Ge NWs, as observed earlier [15,16]. We think that the observed enhanced conductivity of our NWs is due to the surface states as well. The oxide charges including the Au nanoparticles probably offer an alternative conduction path to the electrons/holes. The exact nature of this conduction is still unknown, but it can be hopping as argued earlier [8] or simple leakage. In case of Si/SiGe or Ge NWs, the conductivity enhancement is much larger than that in Si NWs and no current rectification is observed. This suggests that the Ge incorporation in the NWs makes them more sensitive to the surface and even the space charge region at the base of the NW is removed. Low temperature *I–V* measurements of these NWs will be performed next to study the temperature dependence of the electrical conductivity and the carrier transport will be modeled accordingly.

In conclusion, we have reported a systematic study of the electrical properties of the Si/SiGe heterostructure NWs and found them much more conductive than expected. The same trend was observed in pure Si and Ge NWs, and we attributed it to the surface states on the NWs.

The authors thank Mr. Andreas Frommfeld and Mr. Kai-Uwe Assmann for the technical support for MBE and SEM, respectively, and Mrs. Sigrid Hopfe for the TEM sample preparations.

References

[1] L.J. Lauhon, M.S. Gudiksen, C.M. Lieber, Semiconductor nanowire heterostructures, Philos. Trans. R. Soc. Lond. A 362 (2004) 1247–1260.
[2] F. Schaeffler, High-mobility Si and Ge structures, Semicond. Sci. Technol. 12 (1997) 1515–1549.
[3] K. Ismail, B.S. Meyerson, Si/SiGe quantum wells: fundamentals to technology, J. Mater. Sci.: Mater. Electron. 6 (1995) 306–310.
[4] S.T. Huxtable, A.R. Abramson, C.L. Tien, A. Majumdar, C. LaBounty, X. Fan, G. Zeng, J.E. Bowers, A. Shakouri, E.T. Croke, Thermal conductivity of Si/SiGe and SiGe/SiGe superlattices, Appl. Phys. Lett. 80 (2002) 1737–1739.
[5] N.D. Zakharov, P. Werner, G. Gerth, L. Schubert, L. Sokolov, U. Goesele, Growth phenomena of Si and Si/Ge nanowires on Si (111) by molecular beam epitaxy, J. Cryst. Growth 29 (2006) 6–10.

[6] T.E. Clark, P. Nimmatoori, K.K. Lew, L. Pan, J.M. Redwing, E.C. Dickey, Diameter dependent growth rate and interfacial abruptness in vapor–liquid–solid Si/$Si_{1-x}Ge_x$ heterostructure nanowires, Nano Lett. 8 (2008) 1246–1252.
[7] Y. Wu, R. Fan, P. Yang, Block-by-block growth of single-crystalline Si/SiGe superlattice nanowires, Nano Lett. 2 (2002) 83–86.
[8] D. Li, Y. Wu, R. Fan, P. Yang, A. Majumdar, Thermal conductivity of Si/SiGe superlattice nanowires, Appl. Phys. Lett. 83 (2003) 3186–3188.
[9] M. Hanke, C. Eisenschmidt, P. Werner, N.D. Zakharov, F. Syrowatka, F. Heyroth, P. Schäfer, O. Konovalov, Elastic strain relaxation in axial Si/Ge whisker heterostructures, Phys. Rev. B 75 (2007) 161303-1–161303-4.
[10] J. Bauer, F. Fleischer, O. Breitenstein, L. Schubert, P. Werner, U. Gösele, M. Zacharias, Electrical properties of nominally undoped silicon nanowires grown by molecular-beam epitaxy, Appl. Phys. Lett. 90 (2007) 012105–012107.
[11] L. Libioulle, Y. Houbion, J.M. Gilles, Very sharp platinum tips for scanning tunneling microscopy, Rev. Sci. Instrum. 66 (1995) 97–100.
[12] S.M. Sze, Physics of Semiconductor Devices, second ed., Wiley, New York, 1981.
[13] T. Ebner, K. Thonke, R. Sauer, F. Schaeffler, H.J. Herzog, Electroreflectance spectroscopy of strained $Si_{1-x}Ge_x$ layers on silicon, Phys. Rev. B 57 (1998) 15448–15453.
[14] P.D. Kanungo, N. Zakharov, J. Bauer, O. Breitenstein, P. Werner, U. Gösele, Controlled *in situ* boron doping of short silicon nanowires grown by molecular beam epitaxy, Appl. Phys. Lett. 92 (2008) 263107.
[15] J.Y. Yu, S.W. Chung, J.R. Heath, Silicon nanowires: preparation, device fabrication, and transport properties, J. Phys. Chem. B 104 (2000) 11864–11870.
[16] G. Gu, M. Burghard, G.T. Kim, G.S. Duesberg, P.W. Chiu, V. Krstic, S. Roth, W.Q. Han, Growth and electrical transport of germanium nanowires, J. Appl. Phys. 90 (2001) 5747–5751.