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Abstract

Group-IV based light sources are one of the missing links towards fully CMOS compatible photonic circuits. Combining both silicon process compatibility and a pseudo-direct band gap, germanium is one of the most viable candidates. To overcome the limitation of the indirect band gap and turning germanium in an efficient light emitting material, the application of strain has been proven as a promising approach. So far the experimental verification of strain induced band gap modifications were based on optical measurements and restricted to moderate strain levels. In this work, we demonstrate a methodology enabling to apply tunable tensile strain to intrinsic germanium \(\{111\} \) nanowires and simultaneously perform \textit{in situ} optical as well as electrical characterization. Combining \(I/V\) measurements and \(\mu\)-Raman spectroscopy at various strain levels, we determined a decrease of the resistivity by almost three orders of magnitude for strain levels of \(\sim 5\%\). Thereof, we calculated the strain induced band gap narrowing in remarkable accordance to recently published simulation results for moderate strain levels up to 3.6\%. Deviations for ultrahigh strain values are discussed with respect to surface reconstruction and reduced charge carrier scattering time.

Supplementary material for this article is available online

Keywords: germanium, nanowire, strain, band gap narrowing

(Some figures may appear in colour only in the online journal)

The convergence of photonics into a CMOS compatible platform remains a key challenge for the development of future microelectronics technology. Improved functionality and performance such as low-latency and high-bandwidth communication are among the promising outcomes driving this technology. Although great efforts have been invested, a key bottleneck for on-chip photonics is a CMOS-compatible light source \[1\]. While effective light emitters are natively based on III–V compound semiconductors, the integration of these materials into mature silicon (Si) platform technology requires costly and elaborate heterogenic processing techniques \[2\]. In contrast, germanium (Ge) can be monolithically integrated in the Si process flow \[3, 4\] and exhibits a pseudo-direct band gap with a difference in energy of only 136 meV between the direct gap at the \(\Gamma\)-valley \( (E_{\text{\text{\Gamma}}}^\text{\text{dir}} = 0.80 \text{ eV})\) and the fundamental indirect gap close to the \(L\)-valley \( (E_{\text{\text{L}}}^\text{\text{ind}} = 0.66 \text{ eV})\) \[5\]. To overcome the indirect behavior of Ge and thus inefficient photon emission, several approaches have been explored such as modifying the band structure by quantum confinement \[6\], alloying \[7\], or strain engineering. Regarding the latter approach, the predicted transformation of Ge to a...
the strain applied to individual Ge NWs integrated in a growth direction of Ge NWs for tensile strain up to 5.1%. Among the manifold techniques, applying uniaxial strain to a perfect candidate for strain induced band gap tuning enabling the predicted high strain levels for indirect-direct transition of approximately 5.3% [8, 9], and 5.7% [8], along the ⟨111⟩ and ⟨001⟩ growth directions, respectively. In this context, experimental works on the measurement of strain induced band gap modifications in Ge were restricted to optical techniques [5, 13, 15, 23] or electrical measurements up to ≈3.5% [14].

In this work, we present an approach enabling to investigate the electrical behavior for VLS grown along the ⟨111⟩ growth direction of Ge NWs for tensile strain up to 5.1%. The uniaxial strain is applied to individual Ge NWs integrated in a micromechanical straining device (MSD) as displayed in figure 1(a). The MSD is based on a silicon on insulator wafer with a handle wafer and device layer thickness of 500 μm and 3 μm respectively. In a first step, trenches about w = 1.5 μm wide were patterned in the device layer using optical lithography and reactive ion etching. Subsequently, the underlying 1 μm thick buried oxide was selectively etched using hydrofluoric acid resulting in freestanding Si beams with an undercut of about u = 120 μm. To ensure electrical isolation of the MSD, wet thermal oxidation was carried out forming a SiO2 passivation layer with a thickness of 300 nm resulting in a final trench width of w = 1 μm. To complete the device, about 120 nm thick Ge NWs are deposited across the trenches by drop casting. Subsequently, the NWs are fixed by sputter deposited Ti/Au metallic contact pads with a thickness of 200 nm. Figure 1(a) shows the schematic view and the SEM image in the inset of a fully featured MSD with the integrated Ge NW. For the actual investigations, NWs aligned 90° with respect to the trenches were selected to guaranty uniaxial straining and to minimize shear forces in the NW. Finally, the MSD was inserted in a 3-point bending device below a multifunctional confocal µ-Raman setup. Figure 1(b) shows the basic working principle of the MSD: deformation of the MSD as indicated by a 3-point bending (red arrows) exerts tensile strain above the neutral axis (red line) and compressive strain beneath, thus increasing the width of the gap (w'). By controlling the applied force and therefore the degree of bending, the MSD allows for continuous strain tuning of an integrated NW. Based on vector analysis (see supplementary material (available online at stacks.iop.org/NANO/32/145711/mmedia)) the gap width increases with increasing underetch and thus allows the application of amplified strain values compared to a common planar three point bending device.

In-situ strain monitoring was performed by confocal µ-Raman spectroscopy using a green laser (λ = 532 nm) which was focused on the suspended NW. The application of uniaxial strain along the ⟨111⟩ direction of the Ge NWs causes a redshift of the Ge LO phonon mode [24, 25] which is given by:

$$\Delta \Omega \cong - k * \epsilon_L$$

(1)

with ΔΩ representing the measured redshift of the Raman LO peak with respect to the unstrained NW, k a crystal orientation dependent material constant [13, 25] and ⃗{ε}L the strain applied along the Ge ⟨111⟩ NW growth axis. The proportional constant k for uniaxial strain along the ⟨111⟩ direction in Ge NWs was determined by Greil et al [13] with k = 4.34 cm⁻¹. At this point we want to note, that a strain dependent nonlinearities in Raman shift have been found for strain levels >3% [25]. However, according to the mechanical response of our MSD, we observed no significant nonlinear Raman strain behavior within the investigated strain regime.
shift is in accordance with bulk Ge with the main LO peak position increasing uniaxial tensile strain. For the unstrained NW, the raman levels characteristics of the suspended NW for various strain electrical characterization was performed by measuring the $I/\rho$ with the carrier concentration $n_i$ extracted from the resistivity values according to

$$E_g = \ln \left( \frac{n_i^2}{N_{NC} N_{NV}} \right) k_B T$$

with the carrier concentration $n_i$ extracted from the resistivity

$$E_g = \frac{\epsilon}{h^2} \ln \left( \frac{n_i^2}{N_{NC} N_{NV}} \right) k_B T$$

with the carrier concentration $n_i$ extracted from the resistivity

$$n_i = \frac{1}{\rho q (\mu_n + \mu_\rho)}$$

with $\rho$ the resistivity, $k_B$ the Boltzmann constant, $T$ the temperature, and $q$ the elementary charge. The effective densities of states $N_C$ and $N_V$ in the conduction and valence band, respectively as well as the mobility of electrons ($\mu_n$)
and holes ($\mu_p$) were assumed to be the same as for bulk Ge [14].

The band gap $E_g$ as a function of the applied strain is displayed on the right green y-axis in figure 3, together with the recently simulated data from J M Escalante [8]. Strikingly the experimental data are systematically downshifted. The reason therefore is the above mentioned lower resistivity of intrinsic NWs compared to their bulk counterparts, due to accumulation of charge carriers induced by surface traps [34]. However for strain levels from 0.9% to 3.6% the calculated band gap narrowing of $\approx -107$ meV %$^{-1}$ extracted by a linear fit, is in perfect agreement with J M Escalante.6 For even higher strain values $>3.6\%$ in contradiction to the simulation we observed a flattening of the band gap narrowing with increasing strain. We assume that for such high strain, a modification of the mobility has to be taken into account. The mobility for charge carriers in semiconductors is defined as [28]

$$\mu = \frac{q\tau}{m^*} \quad (4)$$

with $\tau$ the scattering time of charge carriers and $m^*$ the respective effective mass. Murphy-Armando et al. [37] reported, that an uniaxial strain of 4.7% along (111) in Ge nanowires will lead to an overall electron mobility enhancement by a factor of 5, further increasing with strain. This is mainly governed by an effective electron population of the $\Gamma$ valley as the distance between $L$ and $\Gamma$ valley decreases [37]. However, a higher mobility results in a reduced resistivity, which is in the opposite of the experimentally observed behavior.

A possible explanation for this counterintuitive behavior is related to the fact that the application of high strain to NWs result in a reconfiguration of surface states, due to the stress induced modulation of the surface potential [38–40]. This will further result in a redistribution of trap states. According to Winkler et al [38], this can overcompensate the mobility improvement due to strain.

Further, it is well known that the scattering time of charge carriers in NWs can be altered by the application of strain [37, 41]. This includes phonon [37, 41, 42], coulomb [41, 42, 44] as well as surface roughness scattering [41, 42, 44]. Consequently, an increased scattering time could additionally counteract the mobility increase by an intervalley scattering induced effective mass reduction.

Conclusions

In conclusion, we demonstrated an MSD enabling the application of uniaxial tensile strain to quasi-1D nanostructures and simultaneous optical and electrical characterization. For VLS grown (111) oriented Ge NWs we extracted a resistivity change of almost three orders of magnitude for the maximum achievable strain of 5.1% before rupture. In excellent agreement with a very recent theoretical study, we calculated a narrowing of the electronic band gap at the $L$-point of $\approx -107$ meV%$^{-1}$ from a resistivity dependent model. For strain values above 3.5%, increased strain induced surface reconfiguration and altered scattering time of charge carriers appear to be the most reasonable candidates for the observed strong deviation from the applied model. As this approach is not limited to Ge it may in general contribute to a better understanding of highly strained nanostructures complementary to optical investigations.

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Author’s contributions

M G B and M S contributed equally to this work. M G B wrote the manuscript, M G B, M S and S G performed the fabrication of the samples and conducted the electrical and optical measurements. B S, T B and P G synthesized the Ge NWs. J S provided expertise on experimental and theoretical interpretations. A L conceived the project and contributed essentially to the experimental design.

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