Effect of Strain on the Carrier Mobility in Heavily Doped p-Type Si

Lucia Romano,* Alberto Maria Piro, and Maria Grazia Grimaldi
CNR-MATIS and Dipartimento di Fisica e Astronomia, Università di Catania, Via S. Sofia 64, I-95123 Catania, Italy

Gabriele Bisognin, Enrico Napolitani, and Davide De Salvador
CNR-MATIS and Dipartimento di Fisica, Università di Padova, Via Marzolo 8, I-35131 Padova, Italy
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We present an experiment that gives insight into the origin of the dependence of the hole mobility (μ) on the dopant species in heavily doped p-type Si under low electrical field. The Hall carrier concentration and mobility were measured in Si coimplanted with B and Ga in the $0.1–2 \times 10^{20}$ cm^{-3} concentration range. The strain induced by substitutional dopants, detected by high resolution x-ray diffraction, was varied by changing the relative B and Ga concentration. The effect of strain on mobility was disentangled and a linear relationship between $1/\mu$ and the perpendicular strain was found.

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Carrier mobility is a fundamental property of a semiconductor and is a characteristic parameter for device design and analysis. The carrier mobility in bulk Si has been deeply investigated since 1950 and, in a pioneering work by Morin and Maita [1], the dependence of the carrier mobility on temperature and impurity concentration was already explained in terms of scattering by phonons and ionized impurities. In the following years the model for carrier transport in bulk semiconductors was refined and the carrier mobility was related to the semiconductor band structure through the effective mass (m^*) and the relaxation time (τ). However, this model fails at high carrier concentration (above 10^{19} at./cm^3) since the average distance between the ionized impurities becomes comparable to the carrier wavelength and the scattering events cannot be considered independent. At high doping level, a dependence of the carrier mobility on the chemical dopant species becomes evident. In particular, the electron mobility is lower for As than P doped Si [2] and the hole mobility is lower for Ga than B doped Si [3,4]. Several authors attempted to explain the different mobility in P and As doped Si introducing impurity-core effect in the calculations [5–7]. However, the calculated mobility variation with chemical species did not fit the experimental observations. In a later approach the electronic charge distribution of the impurities calculated by the Thomas-Fermi theory using the energy functional formulation, the dispersive screening and pair scattering have been taken into account [8,9]. Monte Carlo simulations in a large range of concentrations ended up with a dependence of mobility on doping element too weak to account for the experimental results [9]. The hole mobility is a more complicated task, the effect of chemical species has not even been modeled and a limited amount of experimental data is available [3,4]. Therefore, although the huge effort devoted to characterize the properties of bulk Si, a comprehensive survey of the carrier mobility is still lacking in the high concentration regime. It must be considered that the electrical characterization of Si at high doping level is nowadays fundamental because of the high dopant concentration required for the device scaling down. In this Letter we will show that the strain induced by the dopant itself generates a variation of the effective mass and associated band/subband repopulation [10] that can account for the effect of chemical species on hole mobility.

The relevant point is that a high carrier mobility in either n- or p-type Si [2–4] is observed when the dopant has a covalent radius smaller than Si and that, an appreciable strain is generated in the doped layer at the concentration at which the chemical effect is detectable. The effect of strain on mobility has been largely debated and an enhanced mobility in tensile strained Si has been predicted [11] and detected in strained Si channels grown on virtual SiGe substrates [12]. However, these calculations (and measurements) refer to low dopant concentration and can not be applied to highly doped Si since (i) in heavily doped Si the mobility is limited by the ionized impurity scattering unlike in Si channels in which the dopant density is low and mobility is limited by the phonon scattering (ii) the strain due to substitutional dopants (at concentration higher than 10^{19} cm^{-3}) in Si is at least 1 order of magnitude less than that of strained Si channels.

In order to determine if the effect of chemical species on carrier mobility can be ascribed to the strain induced by substitutional atoms, we looked for a correlation between strain and mobility by measuring the carrier mobility (by Hall effect) and the strain [by high-resolution x-ray diffraction (HRXRD)] in Si doped with both B and Ga atoms (codoped) at high concentration ($1 \times 10^{19}–2 \times 10^{20}$ at./cm^3). Codoping allows us to vary the strain level apart from the carrier concentration by changing the relative fraction of B and Ga. In fact, B doping is associated to tensile strain since the B covalent radius ($r = 0.82$ Å) is smaller than Si ($r = 1.17$ Å), while Ga doping generates compressive strain being its covalent radius $r = 1.26$ Å.

Samples were prepared by implantation of $^{11}B^+$ and $^{69}Ga^+$ ions in Cz n-type Si (100) substrates (4–10 Ω cm) previously amorphized by Si implantation at low temperature (the thickness of the amorphous layer was 550 nm). Double energy implantation was performed in order to have smooth dopant concentration profiles confined in 250 nm thick surface layer. The energies were chosen in such a way to have similar concentration profiles for B and Ga impurities. For example, a peak concentration of 1×10^{20} B/cm^3 was realized by implantation of 17 keV B^+ (fluence 0.25×10^{15} cm^{-2}) and 29 keV B^+ (fluence 0.95×10^{15} cm^{-2}). A peak concentration of 1×10^{20} Ga/cm^3 was realized by implantation of 90 keV Ga^+ (fluence 0.20×10^{15} cm^{-2}) and 160 keV Ga^+ (fluence 1.14×10^{15} cm^{-2}). Several samples were prepared with peak concentration ranging between $0.1–2 \times 10^{20}$ at./cm^3. Some samples were codoped with B and Ga. The overlap of B and Ga concentration profiles is confirmed by secondary ion mass spectrometry analyses. Samples were then annealed at 580 °C for 1 h in N_2, to recrystallize Si by solid phase epitaxy (SPE) and to activate the implanted dopants at concentration above the solid solubility [13,14]. The strain in the regrown layer was measured by HRXRD using a Philips X'PERTTM PRO MRD Diffractometer (at the Cu $K\alpha_1$ wavelength). The perpendicular strain ($\varepsilon_\perp$) profile was extracted by a fitting procedure [15]. Channeling analyses [16] using 2.0 MeV He^+ and a 650 keV H^+ beam for Ga and B, respectively, indicated that the implanted atoms were substitutional after SPE. Van der Paw and Hall effect measurements indicated a complete electrical activation of the implanted ions. The carrier concentration in codoped samples was equal to the sum of those relative to single B and Ga doping, so that the formation of not active B-Ga complexes is ruled out.

The Hall mobility, measured at room temperature, is reported in Fig. 1 as a function of the carrier fluence for B doped Si (full circles), Ga doped Si (full triangles) and codoped Si (empty symbols). The top axis indicates the corresponding peak concentration. At a given concentration the carrier mobility of Ga doped samples is about a factor of 2 smaller than that of B doped Si, in agreement with the literature [1,3]. Codoped samples were prepared by implanting Ga in a substrate previously implanted with B. Therefore, the data points relative to codoped samples (empty squares) read as follows: the carrier concentration at the beginning of the dashed line is due only to B doping, the successive increase of carrier concentration results from Ga doping. The mobility of codoped Si is intermediate between that of B and Ga doped Si. It should be noted that, at a given Ga concentration the mobility can be enhanced by the addition of a comparable concentration of electrically active B despite the greater concentration of ionized impurities. In other words, the Ga scattering efficiency decreases in the presence of B, therefore the scattering probability by the different impurities cannot be summed with the Mathiessen's rule [17] and an additional term must be entered in the mobility calculation. Such a term is likely to depend on strain that can be of the order of $\sim 1‰$ at this concentration. In order to disentangle the effect of strain we prepared a set of samples with constant impurity concentration $C_{Ga} + C_B = 1.2 \times 10^{20}$ at./cm^3 (where C_{Ga} and C_B are the Ga and B concentration, respectively) varying the relative amount of B and Ga impurities. The fraction of Ga is quantified by the parameter χ: $\chi_{Ga} = C_{Ga}/(C_{Ga} + C_B)$. The Hall mobility (empty circles) as a function of χ_{Ga}, reported in the inset of Fig. 1, shows a progressive decrease from 41 cm^2/Vs for B to 20 cm^2/Vs for Ga doped Si. The corresponding strain profile $\varepsilon_\perp$ is reported in Fig. 2: it changes progressively from tensile (negative value) in B doped layer ($\chi_{Ga} = 0\%$) to compressive (positive value) in Ga doped layer ($\chi_{Ga} = 100\%$) and depends on the relative B and Ga concentrations. The experimental values of $\varepsilon_\perp$ are in good agreement with those calculated for a pseudomorphically grown Si-dopant solid solution. Balance over the entire layer occurs for $\chi_{Ga} \sim 80\%$.

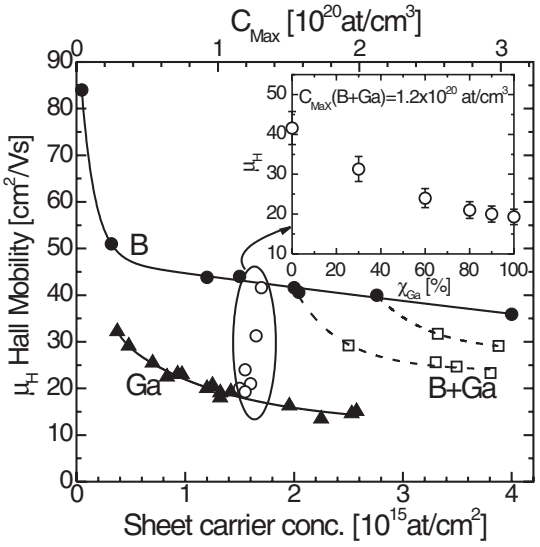

FIG. 1. Hall mobility as function of the sheet carrier concentration measured in B (full circles), Ga (full triangles), and B + Ga (empty symbols) doped Si. The inset shows the Hall mobility as a function of the χ_{Ga} (see the text) for a fixed carrier concentration (empty circles indicated by the arrow) and total impurity (maximum) concentration of about 1.2×10^{20} at./cm^3. Solid and dashed lines are guides for the eye.

The inverse of mobility is plotted in Fig. 3 as a function of the perpendicular strain $\varepsilon_\perp$ at the dopant peak concentration. The inverse of mobility decreases in tensile strained Si and its dependence on $\varepsilon_\perp$ can be fitted by a straight line. Therefore, at a fixed concentration of ionized impurity the strain effect is evident and we claim that the high mobility in B doped Si has to be ascribed to the tensile strain induced by substitutional B. A phenomenological

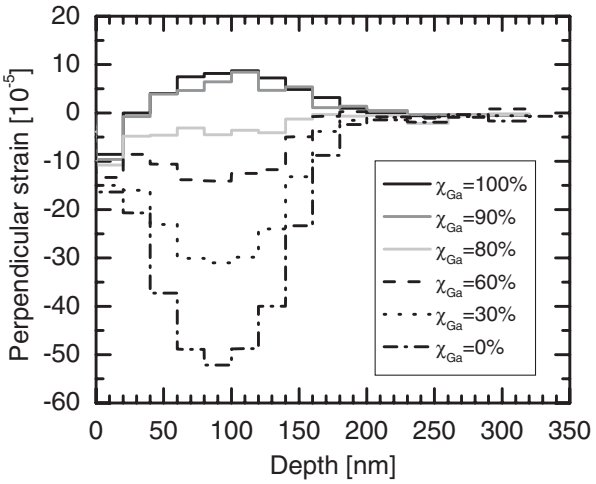

FIG. 2. Perpendicular strain vs depth obtained by HRXRD analyses of B and Ga codoped samples at a fixed impurity concentration of 1.2×10^{20} at./cm^3. χ_{Ga} (see the text) represents the Ga percentage with respect to total impurities (B + Ga) concentration.

approach is to regard the inverse of mobility as the sum of two terms taking into account the scattering by ionized impurities and the strain, respectively. If the linear dependence of mobility on strain reported in Fig. 3 holds all over the investigated concentration range, it can be used to correct the measured mobility ($\mu_{strained}$). Under these assumptions the mobility of unstrained Si $\mu_{unstrained}$ is:

$$\frac{1}{\mu_{unstrained}} = \frac{1}{\mu_{strained}} - \beta \cdot \varepsilon_{\perp}(C_B, C_{Ga}), \qquad (1)$$

where β is the slope of the fit shown in Fig. 3, $\varepsilon_{\perp}$ depends

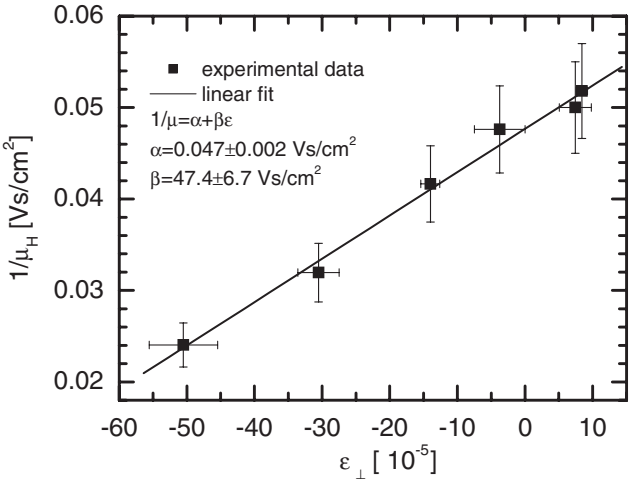

FIG. 3. Inverse of the Hall mobility (reported in the inset of Fig. 1) of codoped samples at a fixed carrier concentration of 1.2×10^{20} at./cm^3 as a function of the perpendicular strain measured at a depth of ~100 nm (Fig. 2). The linear fit ($1/\mu = \alpha + \beta\varepsilon_{\perp}$) parameters are $\alpha = 0.047$ Vs/cm^2 and $\beta = 47.4$ Vs/cm^2.

on B and Ga concentrations. The data reported in Fig. 1 have been corrected according to the Eq. (1) and plotted in Fig. 4. It is remarkable that all the data points collapse on a unique curve regardless of the dopant species. This finding strongly supports that the effect of chemical species on carrier mobility derives from the strain induced by the substitutional impurities.

It is known that the strain modifies the band shape and several authors calculated the variation of the hole effective mass in strained Si [11]. However, such calculations refer to strain higher than 1%, well above the region investigated here. At high strain in the 10^{-2} range the hole mobility is expected to increase for both compressive and tensile strain, however, a linearization for small strain predicts that the mobility should decrease for one type of strain, increase when the opposite stress is applied [10], and large quantitative and even qualitative differences should be expected between the two regimes.

A general expression for the mobility is

$$\mu(N, \varepsilon) = \frac{e\langle\langle \tau(N) \rangle\rangle}{m^*(\varepsilon)}, \qquad (2)$$

where N and ε between brackets indicates the generic functional dependence on carrier concentration and strain, respectively. The relaxation time $\langle\langle r \rangle\rangle$ takes into account all the scattering process involved, but no analytical expression is available in this regime. In first approximation we assume that the effect of strain is enfolded in the effective mass m^*. For small strain, using a first order approximation for $m^*(\varepsilon)$ and the linear dependence

$$\frac{1}{\mu} = \alpha + \beta\varepsilon_{\perp} \qquad (3)$$

reported in Fig. 3, we can evaluate the variation of the hole effective mass with the strain

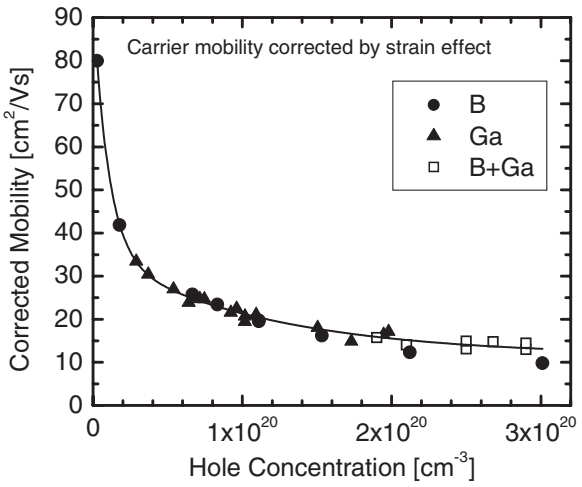

FIG. 4. Hall mobility versus carrier concentration in unstrained material, obtained by the measured Hall mobility corrected by the strain effect. The solid line is a guide to the eye.

$$\frac{\Delta m^*}{m_0^*} \approx \frac{\beta}{\alpha}\varepsilon, \tag{4}$$

where m_0^* is the effective mass at zero strain and the ratio $\beta/\alpha \sim 10^3$ was obtained by the fit of Fig. 3. The large value of the β/α ratio indicates that the effective mass is very sensitive to the strain and, for example, a 10% variation of the hole effective mass is expected for a $\sim 10^{-4}$ strain. Calculations of the hole effective mass in strained Si [11] have been reported for strain greater than that involved in the present experiment and they predicted $\Delta m/m \sim 30\%$ for $\varepsilon_\perp \sim 1\%$. These calculations can not be directly compared to our results because of the different range of strain investigated, however the merging of experimental and theoretical results suggests that the variation of the effective mass with strain is greater at low strain level. It should be noted that the interpretation of our results within this framework is not straightforward since in our samples the strain is not uniform as in the ideal case or in Si grown on virtual SiGe. In fact, we expect to have a highly strained region (close to the impurity) separated by a slightly deformed region and the mobility, that we have correlated to the average strain, could be mainly determined by the highly strained Si.

In conclusion we have shown that, in heavily doped Si, the substitutional dopant atoms induce strain that determines a variation of the hole mobility. This variation is detectable as the strain becomes greater than 10^{-4} and the well-known effect of chemical species on carrier mobility can be completely explained on the basis of the strain induced by dopant itself. The mobility versus carrier concentration for unstrained Si has been calculated using the $\mu(\varepsilon)$ function, determined by the Si codoping experiment, to correct the measured values.

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*Electronic address: lucia.romano@ct.infn.it

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