



# Effects of group-V impurities on the elastic properties of silicon

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## ABSTRACT

Besides reduction in device size the application of strained silicon in transistor design plays a crucial role in improving device speed and power consumption. Microscopic investigations are fundamental to understand the mechanical behaviour of strained Si layers, especially in combination with impurity atoms.

In the present work, the influence of group-V impurities on strain fields in silicon was studied by means of the perturbed angular correlation method using the acceptor <sup>111</sup>In as probe. This nuclear technique is well suited for studying strain on an atomic scale. After ion implantation of the group-V atoms and subsequent annealing the Si samples were bent along the  $\langle 110 \rangle$  crystal axis resulting in a uniaxial tensile strain.

For nitrogen-implanted silicon the response of the crystal lattice to mechanical stress shows no difference to undoped samples, which means that nitrogen has no influence on strain fields in silicon. However, after implantation of the donors P, As and Sb a significant strain relaxation is observed which is probably due to dislocations. We show that this relaxation caused by n-doping also extends to undoped areas which are adjacent to the implanted region.

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## 1. Introduction

In the last decades significant improvement of the performance of integrated circuits has been achieved by reducing device dimensions. However, further scaling is constrained since physical limits are approached; hence the application of new techniques is required. An alternative approach to further improve CMOS performance is the use of strained silicon [1–3]: By embedding lattice-mismatched materials such as SiGe and SiC in the source/drain region, tensile and compressive strain is induced in the transistor channel which enhances the mobility of charge carriers considerably [4]. This is attributed to the modification of the band structure of silicon due to strain. Additionally various effects of strain on silicon, especially in conjunction with dopant atoms are known, including the change of diffusion [5,6] and solubility of dopants [7]. Conversely, however, the implications of defects or dopants on strained systems are not well understood. Although it is known that defect formation such as dislocations relax the lattice strain, there are still many open questions concerning the mechanisms behind it [8]. In order to complete or verify these current models it is essential to have a good measure of strain.

In this study the  $\gamma$ - $\gamma$  perturbed angular correlation (PAC) technique was used to assess the impact of the group-V impurity atoms N, P, As and Sb on strained silicon. This method is well

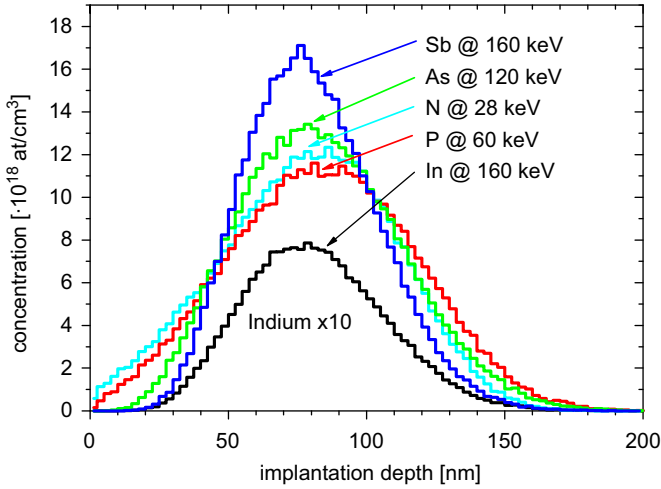
suitable to study strain on an atomic scale in the immediate surrounding of a radioactive probe atom.

## 2. Experimental details

The  $\gamma$ - $\gamma$  perturbed angular correlation (PAC) method is a nuclear technique, based on the hyperfine interaction of the quadrupole moment  $Q$  of a radioactive probe nucleus with an electric field gradient (EFG) caused by the immediate lattice surrounding of the probe atom. The radioactive probe has to decay via a  $\gamma$ - $\gamma$  cascade to the ground state through an intermediate state. Due to angular momentum conservation the emission direction of  $\gamma_2$  with regard to  $\gamma_1$  is not isotropic. The dependence of the emission probability on the angle between  $\gamma_1$  and  $\gamma_2$  is called radiation pattern. If an EFG is present at the site of the probe, the hyperfine interaction causes a time-dependent perturbation of the anisotropic radiation pattern of the emitted  $\gamma$ -rays, which is called the PAC time spectrum. The time modulation of the angular correlation coefficients  $A_{kk}$  ( $k = 2, 4$ ) can be described by a perturbation factor  $G_{kk}(t)$  from which the parameters of the quadrupole interaction (QI) can be derived. The strength of the interaction is usually given by the quadrupole coupling constant  $\nu_Q = eQV_{zz}/h$ , which is proportional to the quadrupole moment  $Q$  of the intermediate state of the cascade (for the probe nucleus <sup>111</sup>In:  $Q(5/2^+) = 0.83(13)$ b, [9]) and the principal component  $V_{zz}$  of the EFG tensor. On lattice sites with cubic environment the EFG

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**Fig. 1.** SRIM-simulations of the implantation profiles for different group-V impurities (fluence  $1 \times 10^{14}$  at  $\text{cm}^{-2}$  in each case) as well as for the  $^{111}\text{In}$  probe atoms ( $5 \times 10^{12}$  at  $\text{cm}^{-2}$ ) in silicon.

vanishes due to symmetry reasons. Since the EFG depends on the charge distribution in the microscopic lattice surrounding of the radioactive probe atom (usually  $\sim r^{-3}$ ), the PAC technique is very sensitive to small lattice deformations caused, for example, by applied external stress. When bending a crystal an electric field gradient is induced at the probes site. From the corresponding quadrupole interaction frequency the resulting strain can be determined. A more detailed description of the PAC technique can be found in the literature [9].

For the experiments,  $100 \mu\text{m}$  thick CZ-silicon wafers were cut into  $7 \times 20 \text{ mm}^2$  samples. Hereby, the long edge was aligned with the  $\langle 110 \rangle$  crystal axis so that the stress could be applied along this direction. For the main measurements presented here, the radioactive probe atom  $^{111}\text{In}$  ( $^{111}\text{Cd}$ ) was implanted with an energy of 160 keV and a typical fluence of  $\sim 10^{13}$  at  $\text{cm}^{-2}$ . In order to create an overlap with the implantation profile of the  $^{111}\text{In}$  probes (SRIM 2008: range and straggling  $\sim 80 \pm 25$  nm, [10]) the co-implantations of nitrogen, phosphorus, arsenic and antimony were performed with an energy of 28, 60, 120 and 160 keV, respectively, with a fluence of  $1 \times 10^{14}$  at  $\text{cm}^{-2}$  in each case (see Fig. 1). After implantation, the samples were subjected to rapid thermal annealing for 120 s at 1173 K under flowing nitrogen.

Uniaxial tensile strain was induced by mounting the samples on sample holders with a defined curvature radius (47–110 mm) [11]. The resulting stress can be calculated by using Hooke's law

$$\sigma = E \cdot \frac{\Delta L}{L} \quad (1)$$

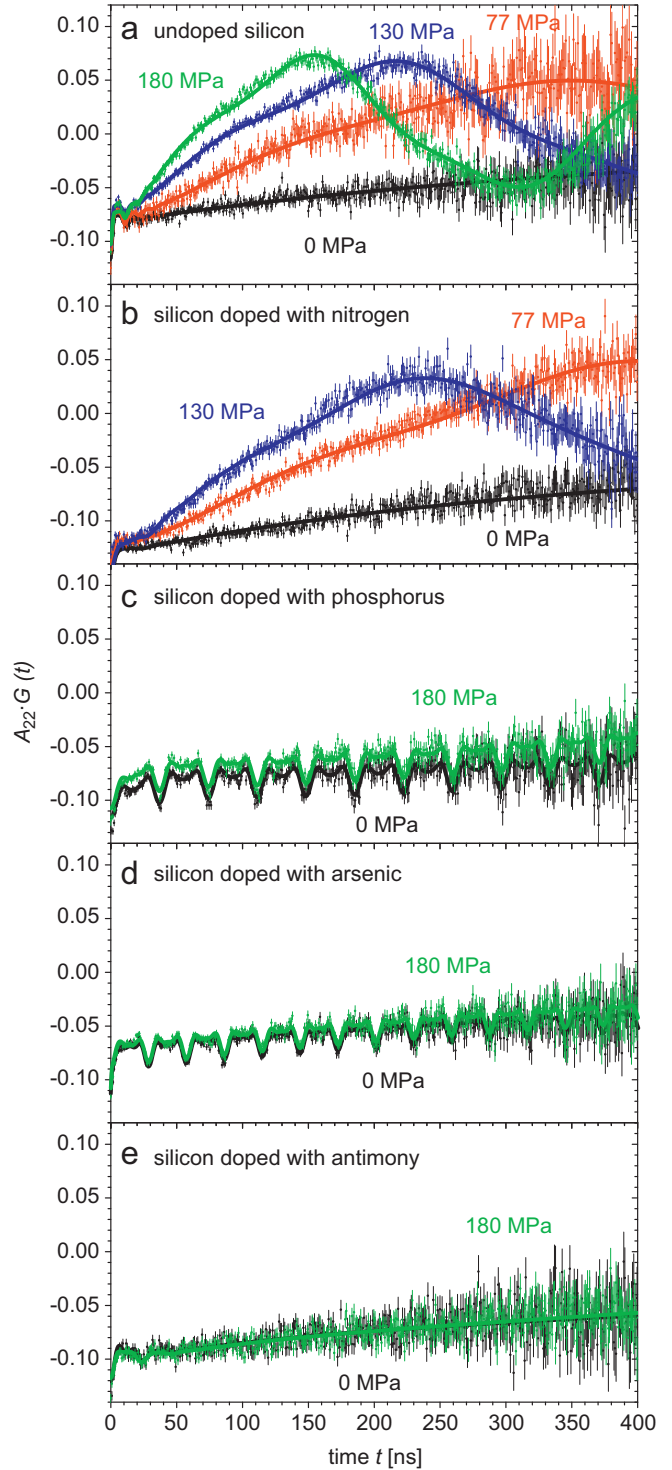
where  $E$  is the elastic modulus and  $\Delta L/L$  is the relative change of length in the implanted region close to the sample surface. It can be calculated using the relation

$$\frac{\Delta L}{L} = \frac{D}{2R + D} \quad (2)$$

$D$  and  $R$  are the thickness and radius of curvature of the sample, respectively. Thus, using the elastic modulus of intrinsic silicon for a  $\langle 110 \rangle$  stress direction with  $E = 169$  GPa [12], stress values ranging from 77 to 180 MPa could be achieved.

### 3. Results and discussion

In Fig. 2 at the top, PAC spectra of undoped silicon (i.e. here just implanted with the indium probe atoms) are shown. Two



**Fig. 2.** PAC spectra for  $^{111}\text{In}$  in undoped silicon (a) and silicon doped with N (b), P (c), As (d) and Sb (e) with a fluence of  $1 \times 10^{14}$  at  $\text{cm}^{-2}$  in each case. For each sample, spectra are shown for unstrained silicon as well as after bending the crystal along a  $\langle 110 \rangle$  axis. The applied stress is indicated in the frames. The solid lines represent fits to the experimental data.

fractions of probe atoms for different environments in the silicon lattice are necessary to describe the data: a strain sensitive fraction  $f_0$  of probes which occupy substitutional lattice sites where the In-atom is surrounded by Si-atoms only. The second fraction describes probe atoms in a heavily disturbed environment. In the case of unstrained silicon a nearly straight

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