

Effects of doping on the elastic properties of silicon

Nicole Santen*, Reiner Vianden

Helmholtz - Institut für Strahlen- und Kernphysik, Nußallee 14-16, D-53115 Bonn, Germany

ARTICLE INFO

Article history:

Received 5 May 2008

Received in revised form 25 July 2008

Accepted 11 August 2008

Keywords:

Silicon

Strain

Elastic properties

PAC

Perturbed angular correlation

ABSTRACT

At present, the use of strained silicon in the design of high performance devices has been shown to be very successful. However, even if the method has found wide application many open questions still persist. A lot of interesting aspects in conjunction with the influence of dopant atoms on the elastic properties of silicon have not yet been fully understood or even studied. The influence of phosphorus and boron doping on the elastic properties of silicon is studied by means of the perturbed angular correlation (PAC) method using the acceptor ^{111}In as probe. It was found that the response of the silicon lattice to mechanical stress showed strong differences depending on the dopant species. Doping with donors leads to a significant reduction of the elastic constants of silicon whereas acceptors do not have any influence on them.

© 2008 Elsevier B.V. All rights reserved.

1. Introduction

Strained silicon is used widely nowadays in the production process of high performance devices [1]. It was found that strain increases the mobility of charge carriers considerably. For instance, the switching performance of n-MOSFETs is increased by 10% using tensile strain. In contrast, p-MOSFETs show an improved performance of about 25% under compressive strain [2].

The study of silicon doped with different donors by Tessema gave evidence that doping decreases the local elastic constants of silicon with a dependence on the type of implanted donor atom [3]. So the question arises if doping with acceptors also has an impact on the elastic properties of the silicon lattice. Hence, in this work we present a comparative study on boron- and phosphorus-doped silicon which is subjected to external uniaxial stress along a $\langle 110 \rangle$ crystal axis.

A further aspect must be taken into consideration. When only a small region of a Si wafer is doped, for instance by ion implantation, the mismatch of the lattice parameters leads to local strain, especially in the implanted region.

Cohen has measured the lattice constants of boron- and phosphorus-doped silicon using the X-ray double crystal spectrometer technique, and showed that the Si lattice constant decreases linearly with impurity concentration [4]. This is due to the smaller covalent radius of the impurities. Here we present a study of local lattice distortions due to the ion implantation of boron in various

concentrations, using the $\gamma\gamma$ perturbed angular correlation (PAC) technique, which is well suited for studying strain on an atomic scale.

2. Experimental details

The PAC method is a nuclear technique, based on the hyperfine interaction of the quadrupole moment Q of the radioactive probe nucleus with an electric field gradient (EFG) caused by the immediate lattice surrounding of the probe atom. The PAC technique does not rely on the prior orientation of the nuclei's spin. Instead, a $\gamma\text{--}\gamma$ cascade is required, where the two γ quanta are correlated via an intermediate state. Due to angular momentum conservation the emission direction of γ_2 with regard to γ_1 is no longer isotropic. The dependence of the emission probability on the angle included between γ_1 and γ_2 is called the radiation pattern. If an EFG is present, the hyperfine interaction causes a time-dependent perturbation of the anisotropic radiation pattern of the emitted γ -rays, which is called the PAC time spectrum $R(t)$. It can be calculated from spectra recorded in a planar detector geometry, with angles of 90° and 180° between them:

$$R(t) = 2 \frac{C(180^\circ, t) - C(90^\circ, t)}{C(180^\circ, t) + 2C(90^\circ, t)}$$

where the $C(\theta, t)$ are the geometric mean-values of the number of coincidences in spectra recorded at inter-detector-angles θ .

From angular correlation theory [5] it can be derived that for the probe ^{111}In $R(t)$ is equal to the product of the anisotropy coefficient

* Corresponding author. Tel.: +49 228 73 3000; fax: +49 228 73 2505.
E-mail address: santen@hiskp.uni-bonn.de (N. Santen).

A_{22} and the perturbation function $G_{22}(t)$:

$$R(t) = A_{22} G_{22}(t) = A_{22} \sum_i f_i G_{22}^i(t)$$

with fractional site populations f_i of the probe nuclei for different environments in the silicon lattice. The shape of the perturbation function is determined by the properties of the EFG present at the nuclear site and is given by:

$$G_{22}(t) = \sum_{n=0}^3 s_{2n} \cos(n\omega_0 t)$$

Here the primary frequency ω_0 is related to the hyperfine splitting of the intermediate nuclear level and depends on the nuclear quadrupole frequency $\omega_0 = 6eQV_{zz}/4I(2I-1)\hbar$. Generally, only the spin independent quadrupole interaction frequency $\nu_Q = eQV_{zz}/h$ is given, which is proportional to the quadrupole moment Q of the intermediate state of the cascade ($Q(5/2+) = 0.83(13)b$, [5]) and the principal component V_{zz} of the EFG tensor.

On lattice sites with cubic environment the EFG vanishes due to symmetry reasons. Since the EFG depends on the charge distribution of the microscopic lattice environment of the radioactive probe atom (usually $\sim r^{-3}$), the PAC technique is very sensitive to small lattice deformations caused for example by an applied external strain. A more detailed description of the PAC technique can be found in the literature [5].

For the experiments, 100 μm thick CZ-silicon wafers were cut into 7 mm \times 20 mm samples. Hereby the long edge was aligned with the $\langle 110 \rangle$ crystal axis so that the stress could be applied along this direction. The radioactive probe atom ^{111}In (^{111}Cd) was implanted with an energy of 160 keV and a typical fluence of $\sim 10^{13}$ at cm^{-2} . In order to create an overlap with the implantation profile of the ^{111}In probes (SRIM2003: range and straggling $\sim 80 \pm 25$ nm, [6]) the co-implantations of phosphorus (dose: 1×10^{14} P cm^{-2}) and boron (5×10^{13} B cm^{-2}) were performed with an energy of 60 and 21 keV, respectively. 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 specially designed sample holders with a defined curvature radius (47–110 mm) [7]. The resulting stress can be calculated by using Hooke's law:

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

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:

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

where 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 [8], stress values ranging from 77 to 180 MPa could be achieved.

3. Results and discussion

A typical PAC spectrum of a boron-doped silicon sample (dose 1×10^{14} B cm^{-2}) bent along a $\langle 110 \rangle$ crystal axis is shown in Fig. 1(top). Two fractions are necessary to describe the data: a strain sensitive fraction f_0 of probe atoms, 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.

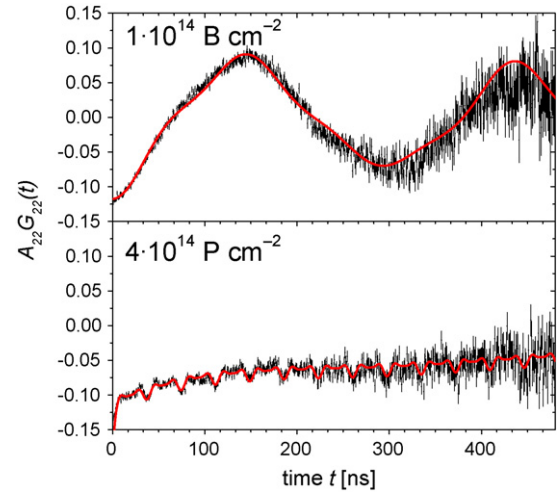


Fig. 1. PAC-spectra for boron- (top) and phosphorus- (bottom) doped silicon measured with the probe ^{111}In . The implanted dose was 1×10^{14} B cm^{-2} and 4×10^{14} P cm^{-2} , respectively. A stress of 180 MPa was applied along a $\langle 110 \rangle$ direction (calculated by using the elastic modulus of intrinsic silicon, see text). The slow, distinct QI frequency is induced by the mechanical stress, whereas the fast oscillation in the P-doped sample spectrum is due to In–P pairs.

For the first fraction the quadrupole interaction frequency (QIF) due to the applied stress of 180 MPa is found to be $\nu_{Q,0} = 22.8(2)$ MHz. The corresponding electric field gradient (EFG) results from the deformation of the Si-lattice around the ^{111}In probe due to the external stress and increases continuously with the induced strain (Fig. 2).

A PAC spectrum of a silicon sample doped with 4×10^{14} P cm^{-2} is shown in Fig. 1(bottom). This sample is also exposed to tensile stress along a $\langle 110 \rangle$ axis. Here, the amplitude of the strain induced frequency f_0 compared to the boron-doped sample is smaller indicating that less probe atoms sense the strain in this sample.

For P-doped silicon a further fraction f_1 arises from substitutional probe atoms that have formed pairs with adjacent substitutional P-atoms, which are expected to be attracted to probes due to the Coulomb interaction. These In–P complexes are characterised by a well-defined QI frequency of 179(1) MHz (fast oscillation) [9]. This QI frequency is not affected by stress applied externally [10].

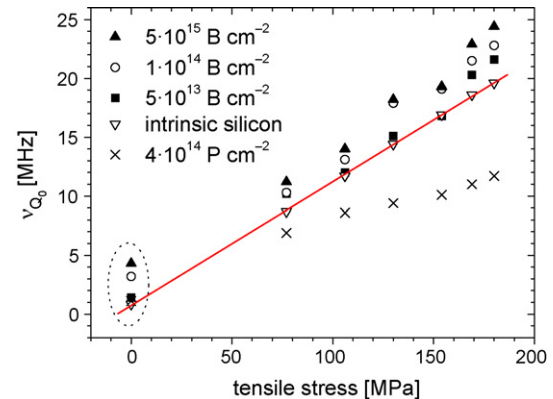


Fig. 2. Dependence of the strain induced QI frequency on stress along a $\langle 110 \rangle$ direction for undoped, phosphorus- and boron-doped silicon. The impurity doses are given in the figure. The straight line is a linear fit to the data for the undoped silicon sample. Encircled are the results found in the unbent samples. The error bars are smaller than the symbols.

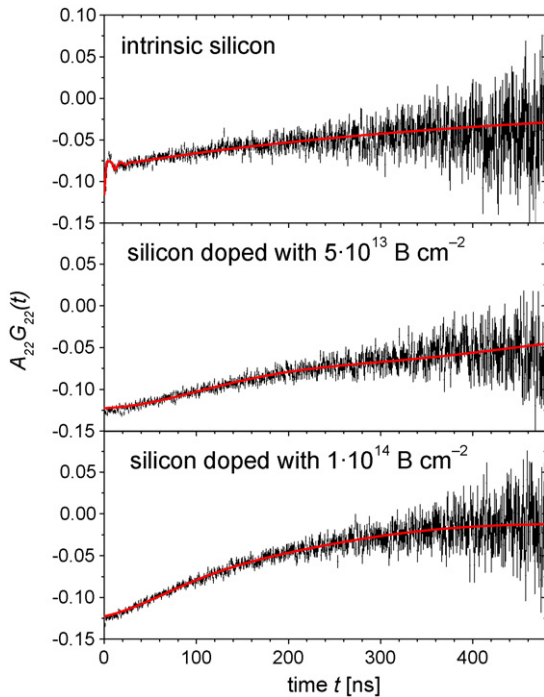


Fig. 3. PAC-spectra for unbenet silicon samples, undoped (top) and boron-doped (doses 5×10^{13} and $1 \times 10^{14} \text{ B cm}^{-2}$), measured with the probe ^{111}In . The internal strain due to the ion implantation increases with the boron concentration.

In Fig. 2 the dependence of the strain induced frequency on stress along a $\langle 110 \rangle$ direction for phosphorus- and boron-doped silicon is shown. For comparison, the results for an undoped silicon sample are included. The stress was calculated using Eqs. (1) and (2) with the elastic modulus of intrinsic silicon. The experiments reveal that the QI frequency of the P-doped sample is only $\sim 50\%$ of the value reached in undoped silicon when both samples are bent to the same radius. This means that locally (i.e., in the implanted region) there is less stress in the sample since the strain-induced frequency is proportional to the stress. From this we conclude that P-doping reduces the elastic modulus of silicon similar to other donors [10]. In the case of doping with boron, which acts as an acceptor in silicon, it is found that the QI frequencies are generally larger as compared to undoped silicon. This seems to indicate that B-doping enhances the elasticity of the silicon lattice. However, a closer examination reveals that it is rather an offset since a non-zero QI frequency is also observed in unbenet samples (Fig. 2, encircled).

Most probably, this is due to internal strain at the In site caused by the implantation of the smaller B-atoms into the Si-crystal. To verify this experimentally, we implanted different boron doses and measured the QI frequency in dependence on the applied strain. We infer from Fig. 2, that the higher the amount of implanted boron atoms the larger is the QIF offset as compared to the undoped sample. Fig. 3 shows the PAC spectra of unbenet silicon samples with different boron doses where it can be seen that the strain induced frequency increases with the boron concentration. Thus, we conclude that indeed internal tensile strain is brought into the silicon lattice by boron implantation explaining the observed offset.

In XRD experiments an average reduction of the lattice constant with increasing B concentration was observed [4]. However, since the PAC method measures the local lattice distortion at the In probe, the discrepancy is not astonishing.

4. Conclusions

The impact of dopants on the elastic properties of silicon was studied by means of the PAC technique. It turned out that the reaction of the silicon lattice to mechanical stress shows strong differences, depending on the dopant species. In the case of the implantation of the donor phosphorus a significant reduction of the elastic constants of the silicon lattice could be observed. Here it is assumed that the change in the binding energy by replacing a large fraction of Si–Si bonds by Si–P bonds is responsible for this behaviour. Doping with the acceptor boron did not change the elastic properties of silicon. Instead, boron doping introduces tensile strain in the silicon lattice which increases with its concentration.

References

- [1] M.L. Lee, E.A. Fitzgerald, M.T. Bulsara, M.T. Currie, A. Lochtefeld, *J. Appl. Phys.* 97 (2005) 11101.
- [2] S.E. Thompson, M. Armstrong, C. Auth, et al., *IEEE Electr. Device Lett.* 25 (2004) 191.
- [3] G. Tessema, Indium–impurity pairs in semiconductors and the study of the influence of uniaxial stress on defect complexes in silicon, PhD Thesis, Universität Bonn, 2003.
- [4] B.G. Cohen, *Solid State Electron.* 10 (1967) 33.
- [5] G. Schatz, A. Weidinger, *Nuclear Condensed Matter*, John Wiley and Sons, Chichester, 1996.
- [6] J.F. Ziegler, J.P. Biersack, U. Littmark, *The Stopping and Range of Ions in Solids*, Pergamon, New York, 1985.
- [7] N. Santen, PAC–Untersuchungen von dotiertem Silizium unter uniaxialer Zugspannung, Diploma Thesis, Universität Bonn, 2006.
- [8] W.A. Brantley, *J. Appl. Phys.* 44 (1973) 534.
- [9] T. Wichert, M.L. Swanson, *J. Appl. Phys.* 66 (1989) 3026.
- [10] G. Tessema, R. Vianden, *Appl. Surf. Sci.* 240 (2005) 146.