On the deformation field of bent crystals for channeling experiments

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SUMMARY. Anticlastic deformation (AD) is an established mechanical property of isotropic solid bodies, which has been recently used to steer particle beams through channeling in Silicon (Si) crystals. An analysis of AD in an anisotropic material such as Si has been worked out with particular emphasis to the cases used in channeling experiments. Both a theoretical model and finite element simulations were developed and compared to experimental data achieved by optical profilometry on bent Si crystals. A quantifier of the extent of anticlastic deformation, namely the ratio between primary and secondary curvature radii, has been found to be orientation dependent and determined analytically. The realistic case of Si crystal bending by a mechanical holder has been studied for applications. Crystals and the mechanical holder have been realized at the Sensors and Semiconductors Laboratory of the University of Ferrara.

1 INTRODUCTION

Elastic strips or tapes (wires) are commonly used in industrial applications. When such strips are bent, the longitudinal strains, which are purposely induced, are accompanied by lateral strains in the width direction of the strip. As a result, the strip takes the shape of a saddle, i.e., it bends to a surface in which the two principal curvatures are opposite in sign. This effect is referred to as anticlastic deformation (AD). For an amorphous material, if the longitudinal radius of curvature, i.e., the primary radius of curvature, R, into which the strip is being bent is large, the cross section is found to deform to an arc of a circle with secondary radius $R_A = R/\nu$, where ν is Poisson's ratio [1]. Thus, although the extent of AD is not large, it may cause practical difficulties. As an example, the edges of the magnetic tapes used in computer applications are found to wear because of it. Similar difficulties are encountered in the bending of the long metallic plates used to form the adjustable working sections of wind tunnels. The consequent AD of the plates is found to interfere with the air flow.

Although possible remedies to counteract anticlastic deformation do exist, e.g. by proper tapering of the edges on the concave sides of the tapes or plates, there are applications in which AD is desirable. For instance, mechanical bending of single-crystals can be used to produce deflection and diffraction of subatomic particles and channelling of positrons at high and ultrahigh energy level. Opportunely bent crystals find relevant applications in accelerators of particles, like

collimators and focuser of particles beams, and for measuring magnetic moments of electrical charges.
For example, properly deformed crystals can be used to extract and steer relativistic particles beams. In particular, during the last years, Silicon (Si) single-crystals have been intensively investigated to realize short bent crystals utilizable for highly efficient extraction and collimation of particles beams [2-4]. This represent a very important subject in modern technology and research.
A significant example is particle-beam steering through channeling in a crystal. Channeling is the confinement of charged particles within atomic planes in a crystal (planar channeling) or parallel to a crystalline string of atoms (axial channeling). Crystals in the form of a strip is used to bend a particle beam through AD as depicted in Figure 1. The advent of strip-like crystals in the field of channeling opened up the possibility to fabricate crystals with significantly shorter length than previously used configurations, e.g., the so-called O-shaped crystal [5].

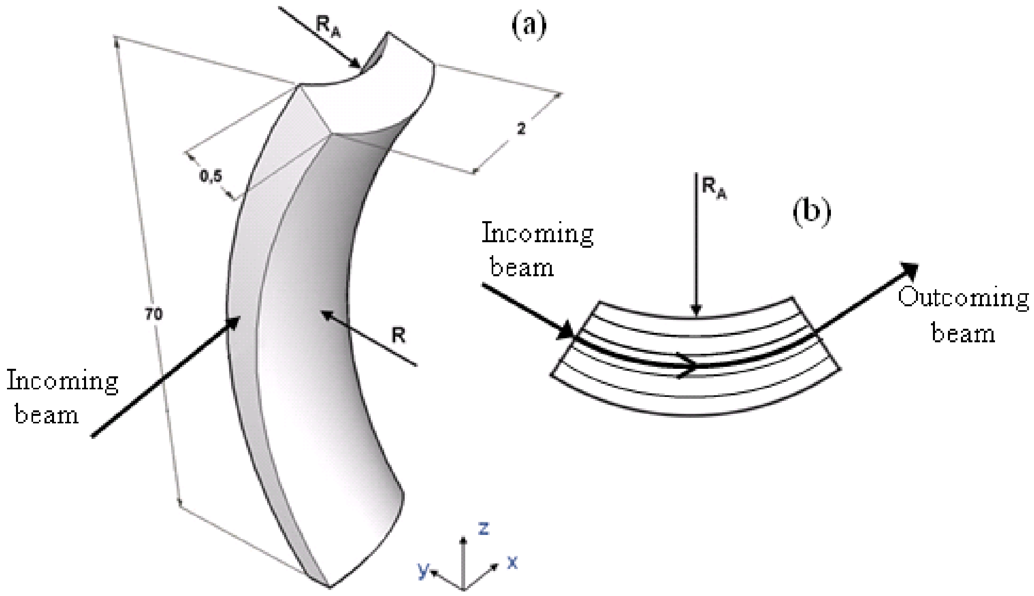

Figure 1: (a) Sketch of a bent silicon strip for channeling experiments (quotes are expressed in mm). (b) Cross-section of the crystal; the incoming particles are captured by the potential of atomic planes and the beam is being deflected.

Crystals in the shape of a strip with the anticlastic curvature to steer the particles were used to optimize the thickness of material traversed by the particles, which is an increasing function of beam energy. An experiment carried out with a strip crystal allowed to attain the top efficiency of 85% for extraction of a 70 GeV proton beam out of a synchrotron [5]. Secondly, the holder used to impart the primary strain can set far apart from the particles and hence it reduces any unwanted interaction with the beam. As one might expect, AD of an anisotropic material, as needed for channeling experiments, would lead to significant dependence of the curvature ratio R/R_A on the chosen crystallographic direction. This work is a study of the deformation properties in anisotropic materials with the shape of a strip. Special attention is given to the curvature ratio R/R_A, whose knowledge is essential to design properly shaped crystals for channeling experiments.

2 ANTICLASTIC DEFORMATION IN A SILICON STRIP

We herewith review some concepts of anticlastic deformation in a isotropic material that are necessary for understanding further modelling and experiments. Channeling of particles with energy from tens to hundreds GeV occurs in strip-like crystals, i.e., in a crystal with one dimension much longer than the other two sizes. As an example, a Si strip which was recently used in experiment [6] at CERN with 400 GeV protons was l = 70 mm long with rectangular 2 x 0.5 mm^2 cross section (see Fig. 1). Thereby, the shape of the crystal is such that the theory of a mechanical beam can be worked out extensively.

Crystalline silicon exhibits FCC cubic symmetry and diamond lattice with each atom on the centre of a tetrahedron with four nearest-neighbour atoms at the four vertexes. Thereby, Young's modulus and Poisson's ratio are direction dependent [7]. As for any FCC symmetry, the elastic properties are completely characterized by only 3 independent constants. For Si, the compliance matrix, $\boldsymbol{S}$, referred to the canonical base **<e>** = {<100>, <010>, <001>}, (where <100>, <010>, <001> are main crystalline axes of the cubic cell), takes the form:

$$\mathbf{S}^{<e>} = \begin{pmatrix} 7.678 & -2.144 & -2.144 & 0 & 0 & 0 \\ & 7.678 & -2.144 & 0 & 0 & 0 \\ & & 7.678 & 0 & 0 & 0 \\ & & & 12.531 & 0 & 0 \\ & Sym & & & 12.531 & 0 \\ & & & & & 12.531 \end{pmatrix} 10^{-3}\ MPa^{-1} \tag{1}$$

In channelling experiments, the crystal is bent to a relatively modest curvature and the primary deformation is imparted at the edges of the strip through a mechanical couple of moment $\boldsymbol{M}$ by clamping onto a rigid holder. Such a system can be modelled as a homogeneous and anisotropic bar under infinitesimal deformations and small displacement, supported at its ends by kinematics and concentrated supports and bent by a point-like couple of forces at its edges, as shown in Figure 2. The displacement of the strip along y direction is given by [8]:

$$v(x,y,z) = \frac{1}{2\,a_{33}R}\left(-a_{13}x^2 + a_{23}y^2 + a_{33}(lz - z^2) - a_{35}xz\right) \tag{2}$$

where a_{ij} are the 6x6 coefficients of $\mathbf{S}^{<e>}$. Presence of the z^2 term is related to the imposed principal bending while the x^2 term shows that x-y cross section is deformed as a parabola, giving rise to anticlastic bending, whose magnitude is linearly proportional to the imposed bending. The mostly direct observable physical quantity is the principal curvature while anticlastic deformation is quantified by the secondary curvature. Thus, the ratio R_A/R determines the extent of anticlastic deformation in dimensionless units. Differently from the case of an isotropic material, the ratio between anticlastic and principal bendings is determined by the two components of the elastic compliance tensor. For the channeling applications, the region of interest is the central part of the crystal so that R_A/R is calculated at $x = 0$, $y = 0$, $z = l/2$:

$$\frac{R_A}{R} = -\frac{a_{33}}{a_{13}} \tag{3}$$

It should be remarked that a_{33} cannot vanish, thereby it is impossible to find a bent Si crystal without anticlastic deformation. Moreover, R and R_A have opposite signs, i.e., the crystal takes the shape of a saddle.

The ratio in Eq. (3) is orientation dependent so that designing a bent crystal for channeling and volume reflection experiments demands its knowledge for any orientation of the strip. For planar channeling and volume reflection the (110) planes were found to be best efficient, namely the crystal is to be oriented with such axis along y axis in Figure 2. The remaining two directions are to be chosen and R/R_A should be studied as a function of the base, **<m>**, with the vectors parallel to the sides of the crystal. Thereby, the compliance tensor in the base **<m>** is linked to $\mathbf{S}^{<e>}$ through a similarity transformation:

$$\boldsymbol{S}^{<m>} = \boldsymbol{K}\,\boldsymbol{S}^{<e>}\boldsymbol{K}^T \tag{4}$$

$\boldsymbol{K}$ being the rotation matrix connecting the **<e>** base to the **<m>** base.

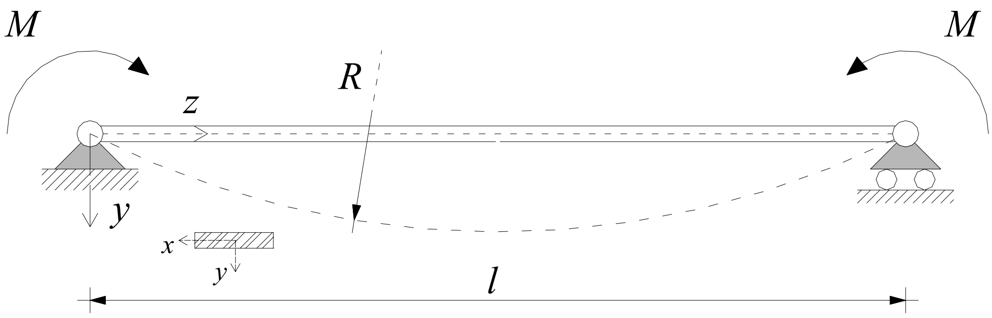

Figure 2: Schematic representation of bending of a beam of length l under the action of a couple of moments M applied at its ends.

3 SIMULATION AND EXPERIMENT

In order to study the orientation dependence of strained silicon strips, several crystals of size 2x0.5x70 mm^3 were diced from a 0.5 mm thick (110) Si circular wafer according to the procedure described in [9]. Si strips have been realized at the Sensors and Semiconductors Laboratory of the University of Ferrara.

The wafer's "flat", i.e., the cut done by the manufacturer for better usage of the wafer was parallel to the $(1\bar{1}0)$ plane. The crystals were cut at some inclination, θ, with respect to the flat (see Figure 3 and Table I) and all of them were oriented with the <110> direction along y axis.

The ratio R_A/R was studied by bending the crystal through a specifically designed holder, realized at the Sensors and Semiconductors Laboratory of the University of Ferrara, borrowed by the instrumentation used in high energy channelling experiments [10], see Figure 4. The principal and anticlastic radii were measured by means of a white-light profilometer (Veeco NT1100) capable of recording the profiles of the bent crystal with height resolution of 3 nm. In order to make the surface orientation independent of the alignment with respect to the profilometer objective, tilt and piston terms were removed via software.

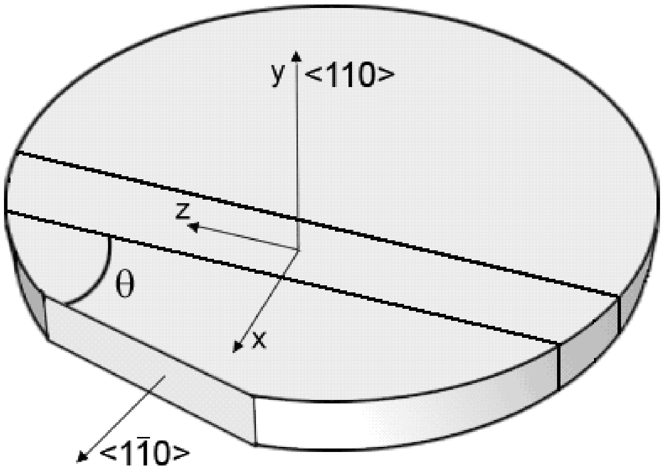

Figure 3: Silicon crystals are diced from a (110) wafer. The length of 70 mm is achieved at several angles θ with respect to the wafer's flat. The *Y* axis is always the <110> direction, while *x* and *z* vary as function of θ.

θ (deg)	$\lvert R_A/R \rvert$ (measured)	$\lvert R_A/R \rvert$ (theoretical)	$\lvert R_A/R \rvert$ (FEM)
0	3.52	3.59	3.58
15	3.98	4.00	4.00
35.26	6.31	6.20	6.15
45	6.82	6.80	6.73
60	4.72	4.70	4.67
75	3.16	3.15	3.14
90	2.75	2.76	2.75

Table 1: Ratio between anticlastic and principal bending radii as a function of θ: comparison between theoretical model, measurements and FEM simulations.

Figure 5 shows a typical profile of the strip taken in a central region 2x2 mm^2 wide, which exhibits a saddle-like surface as predicted by elasticity theory. Figure 6 illustrates the experimentally recorded levels of R_A/R for the values of θ in Table I. Clear signature of orientation dependence is observed with the ratio R_A/R attaining its maximum for the direction <1/√2 1/√2 1> and its minimum for the direction <100>. Such trend reflects the behaviour of Poisson coefficient for a

(110) plane [7]. Moreover, it should be noted that the crystalline orientation θ = 35.26° corresponds to a crystal with the <111> axis along the beam direction, i.e., the most favourable condition to study axial channeling [11].

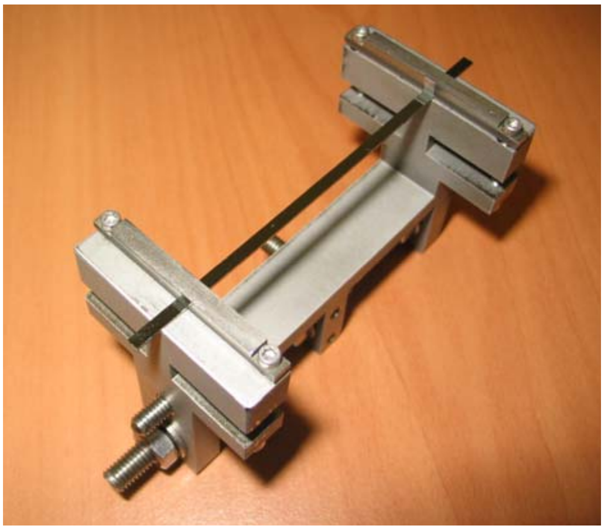

Figure 4: A silicon strip-like crystal bent by a mechanical holder.

The expected ratio of $|R_A/R|$ versus the angle θ, reported in Figure 6, has been obtained analytically by calculating the ratio $|a_{33}/a_{13}|$ which, as known by classical mechanical beam theory, is the Poisson ratios for the corresponding crystalline direction. A good agreement between experimental and theoretical values of ratio $|R_A/R|$ occurs for each crystalline direction.

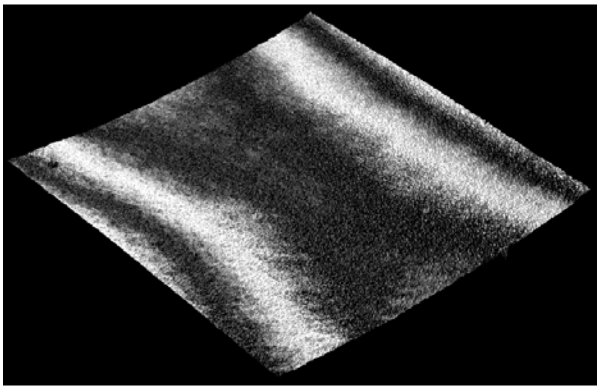

Figure 5: Deformation of the crystal surface when bent by the holder. The crystal is diced at θ= 35.26°. A saddle deformation is visible thanks to interference fringes.

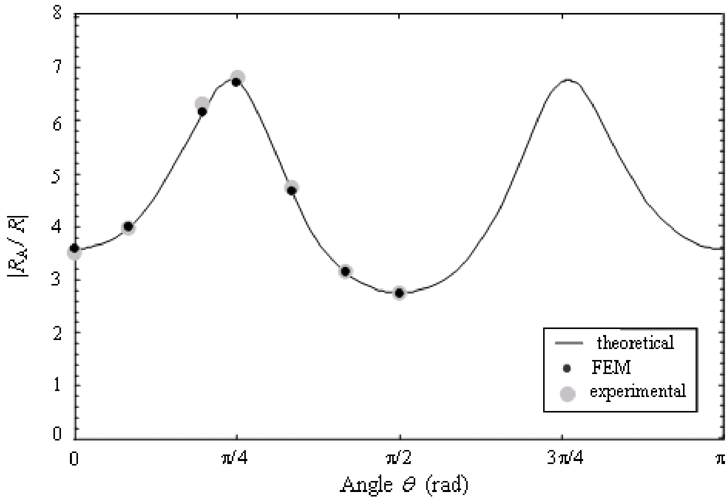

Figure 6: Ratio $|R_A/R|$ as function of θ (for its definition see Fig. 3). Experimental data are compared with FEM simulation and with the model. The figure shows that the ratio $|R_A/R|$ is direction dependent as expected from a crystal.

It should be remarked that Eq. (2) holds true for the ideal case of concentrated supports at the edges of the strip but, in practice, clamping of the crystal mounted on the holder occurs over a finite region. Due to this, distortion of the shape of the bent crystal from a saddle is expected, particularly in proximity of the holder jaws. Analytical formulations including a non point-like constrain does not exist in the literature. Thus, with the purpose to take into account a more realistic condition of the constrains and, in turn, information about the portion of crystal not influenced by the presence of holder jaws, Finite Element Method (FEM) simulations based on STRAUS7 software (release 2.3.3) have been worked out for the purpose. A sketch of the FEM mesh is given in Figure 7.

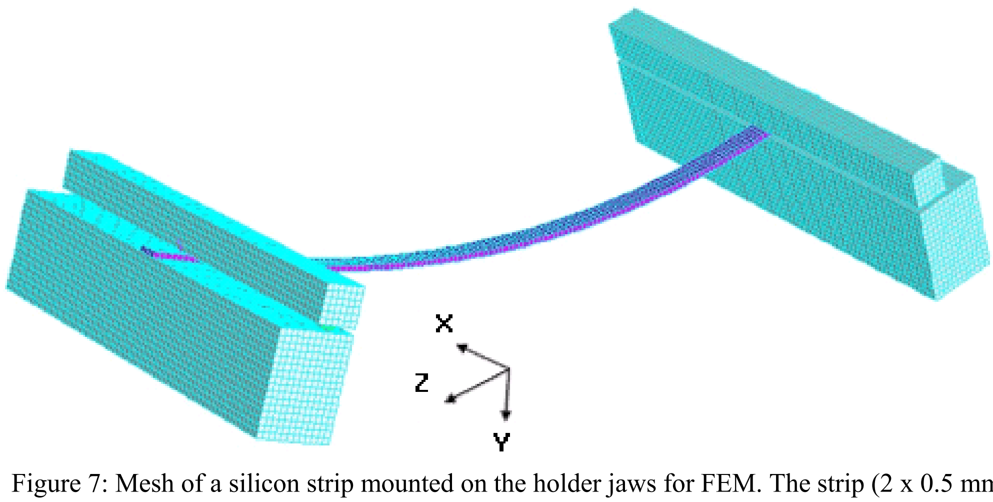

Figure 7: Mesh of a silicon strip mounted on the holder jaws for FEM. The strip (2 x 0.5 mm^2) is simulated by 528 bricks elements, whereas 36496 bricks elements model the holder supports.

Since the deformation of the crystal is expected to be not appreciably affected by the whole holder structure, only the jaws of the holder have been modelled in our numerical simulation. The silicon crystal was modelled as 3D anisotropic cubic bricks elements, whereas the aluminium supports of the holder were modelled as isotropic 3D elements. Both the strip and the holder were considered homogeneous elastic bodies under small strains. The strip was assumed to be perfectly bonded to the holder supports. Bending of the silicon strip is achieved by imposing rotations of both the lower aluminium jaws along the x axis, obtaining a symmetric flexure of the crystal in the yz plane. Figure 8 shows the dependence of $|R_A/R|$ as a function of coordinate z for the first half of the strip at R = 12 m and θ = 35.26°. As expected, for most of the crystal it holds $|R_A/R|$ = 6.2, according to the simulations and measurements in Figure 6. The ratio $|R_A/R|$ is distorted only in proximity of the jaws within an extension estimated to be about $l/8$ on each side. This achievement is consistent with the experimentally gained criterion for which the central third of the crystal can safely be used for channeling experiments. FEM analysis has shown that this is in fact a prudent criterion.

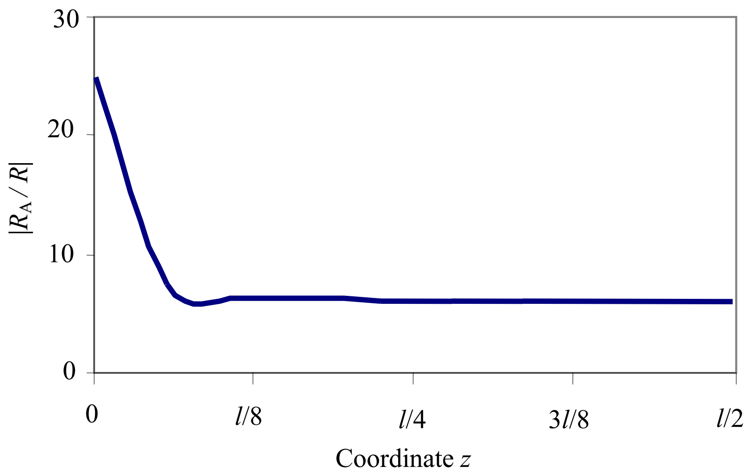

Figure 8: FEM-simulated values of $|R_A/R|$ along the length of a bent crystal cut at θ = 35.26° and R_A = 12 m. The numerical values largely agree with the theoretical prediction $|R_A/R|$ = 6.2 except for a small region of the crystal close to the jaws of the holder.

4 CONCLUSIONS

An analysis about anticlastic deformation for bent strip crystals for channeling experiments has been worked out through an analytical approach and FEM simulations. Both methods were validated by an experimental observation of the deformation profile via optical profilometry. The quantifying parameter of the deformation for channeling experiments, i.e., the ratio $|R_A/R|$, has been determined as a function of the crystal orientation.

This is useful information to design properly bent crystals relying on a measurement of the primary curvature. As an example, the knowledge of the consistency of the ratio $|R_A/R|$ for most of the crystal envisages a tool for online monitoring of the crystal curvature based on direct measurement of R. Here, the determination of R_A can be inferred indirectly with a better precision than for a direct measurement and this fact can be employed under harsh conditions such as a measurement of the crystal curvature through a window in the under-vacuum environment of an accelerator.

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