Investigation of non-decorated glide dislocations by infra-red light scattering tomography

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Abstract. The laser scattering tomography technique enables the observation of non-decorated dislocations in Si crystals. In polarization and tomography measurements, changes in the dislocation scattering intensity are observed. A study of the light scattering by a dislocation was then developed and described in this paper. Based on theoretical results and experimental observations, slip system of a non-decorated mixed dislocation can be totally determined.

1. Introduction
Laser Scattering Tomography (LST) has been used to study oxygen precipitates in Si wafers for many years [1,2]. This technique is able to measure densities in the range of $10^5$–$10^{10}$ cm$^{-3}$, and sizes down to 20 nm [3]. Such defects fulfill the approximations of Rayleigh scattering (size < wave length) for which the scattered intensity can be easily calculated. The ability to image extended defects by LST has also been demonstrated in various materials (quartz, sapphire, III-V, Si) [1,4-7]. All works on Si has addressed dislocations introduced during long high temperature annealing, which necessarily leads to decoration of dislocations by oxygen atoms and precipitates. No non-decorated dislocations in Si were investigated so far. Dislocations cannot be considered as point-like scatterers and their scattering must be evaluated from the Maxwell equations as done by Moriya [4].

In this paper, we focus on the study of oxygen-free mixed dislocations in Si by the IR-LST technique. After discussing the theory of light scattering by dislocations, we demonstrate the possibility to image non-decorated glide dislocations. Using polarized light, we were able to identify the dislocation slip plane and Burgers vector using scattering simulation developed from [4]. Finally we show that it is possible to discriminate between non-decorated and decorated glide dislocations by LST.

2. Simulation of 90° light scattering from a dislocation in silicon
For non-decorated dislocations, the LST scattering contrast arises from photo-elastic effect [4,6], that is changes in the refractive index originated by the stress field surrounding the dislocation. The electric field scattered by the dislocation is [8]:

$$
\mathbf{E}_s(R) = \frac{\exp(iKR)}{R} \left( \mathbf{\hat{s}} \times \mathbf{\mathbf{\hat{s}}} \times \mathbf{F}(\mathbf{g}) \right) \mathbf{E}_i
$$

(1)

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with $R$ the position where the field is measured, $k$ the wave number, $\vec{g}$ the scattering vector defined as $\vec{g} \equiv \vec{s} - \vec{s}_0$, $\vec{s}_0$ being the direction of the incoming light, $\vec{s}$ the scattering direction and $\vec{E}_i$ the incident electric field in the case of incoming plane wave. The scattering factor $\vec{F}$ is defined as the Fourier transform of the tensor of the inverse dielectric constant variation $\Delta \varepsilon^{-1}(\vec{r})$:

$$\vec{F}(\vec{g}) = FT(\Delta \varepsilon^{-1}(\vec{r})) \quad \text{where} \quad \Delta \varepsilon^{-1}(\vec{r}) = p \times \vec{s} \quad \text{and thus} \quad \vec{F}(\vec{g}) = p \times \vec{S}$$

with $\vec{S}$ the strain tensor of the dislocation, $\vec{S}$ the Fourier transform of $\vec{S}$ and $p$ the strain-optic 4 rank tensor with in the case of silicon reduces to only 3 non-zero coefficients $[9] (p_{11}, p_{12} \text{ and } p_{44})$.

If one considers dislocations in silicon, provided they are not produced at too high temperature, it is well known that their lines are parallel to the three $<110>$ Peierls valleys in the glide plane. So we will consider a hexagonal dislocation loop in the $\{111\}$ planes.

The strain field tensor of such a loop is complex and has been simplified as follows:

i.) the loop is considered as the sum of linear straight segments

ii.) the strain field tensor is evaluated in a position close enough to the dislocation segment, so the latter can be considered to have infinite length.

The calculation of the strain field tensor is developed in the dislocation coordinate system ($x,y,z$). This coordinate system is built to have the dislocation line along the $x$-axis. The $x$-$y$ plane corresponds then to the $\{111\}$ glide plane and the Burgers vector of the dislocation forms an angle $\phi$ with the $x$-axis. By means of $\phi$, the mixed dislocation can be introduced in the calculation. In this coordinate system, the Fourier transform of the strain field components $[10]$ can be expressed as:

$$\hat{S}_{xx} = 0 \quad \hat{S}_{yy} = \frac{q}{ik(g_y^2 + g_z^2)^{1/2}} \frac{b \sin \phi}{4(1-\nu)} \left( \cos 3B + (3-4\nu)\cos B \right)$$

$$\hat{S}_{zz} = \frac{q}{ik(g_y^2 + g_z^2)^{1/2}} \frac{b \sin \phi}{4(1-\nu)} \left( \cos 3B + (4\nu - 1)\cos B \right) \quad \hat{S}_{xy} = \frac{q}{ik(g_y^2 + g_z^2)^{1/2}} \frac{b \cos \phi}{2} \cos B$$

$$\hat{S}_{yz} = \frac{q}{ik(g_y^2 + g_z^2)^{1/2}} \frac{b \sin \phi}{4(1-\nu)} \left( \sin 3B + \sin B \right) \quad \hat{S}_{xz} = \frac{q}{ik(g_y^2 + g_z^2)^{1/2}} \frac{b \cos \phi}{2} \sin B$$

Here, $B$ is defined by $\tan B = -\frac{g_y}{g_z}$ and $q = \frac{2 \sin(kg_s x_0)}{kg_s}$

where $b$ is the modulus of Burgers vector, $g_y$ and $g_z$ are the scattering vector components, $\nu$ the Poisson’s ratio. Here $2x_0$ is the length of the dislocation line visible by the objective lens taking into account the numerical aperture of the objective.

**Figure 1.** Scheme of the LST geometry and of the relative orientations of coordinate systems attached to Si and observation set-up.
The calculation of the scattering factor in the observation coordinate system \((\xi, \eta, \zeta)\) can then be obtained by an additional matrix transformation. If \(M\) is the transformation matrix between the Si coordinate system \((X,Y,Z)\) and the dislocation coordinate system \((x,y,z)\), and \(P\) is the matrix transformation between the observation coordinate system \((\xi, \eta, \zeta)\) and the Si coordinate system \((X,Y,Z)\), then one can obtain as a final result:

\[
\hat{S}_{(X,Y,Z)} = M^{-1} \times \hat{S}_{(x,y,z)} \times M \quad \tilde{F}(\hat{g})_{(X,Y,Z)} = P \times \hat{S}_{(x,y,z)} \quad \tilde{F}(\hat{g})_{(\xi, \eta, \zeta)} = P^{-1} \times \tilde{F}(\hat{g})_{(X,Y,Z)} \times P
\]

Perfect 90° scattering corresponds to the case where incoming and scattered lights have fixed directions and are strictly perpendicular to each other. Hence, Eq. (1) can be written as:

\[
\tilde{E}_x(R) = \frac{\exp(ikR)}{R} \begin{pmatrix} 0 & F_{12} & F_{32} \\ 0 & 0 & 0 \\ 0 & F_{13} & F_{33} \end{pmatrix} \begin{pmatrix} \hat{E}_x \\ \hat{E}_y \\ \hat{E}_z \end{pmatrix} \quad \text{and} \quad \tilde{E}_y(R) = \begin{pmatrix} E_\eta \\ \eta \end{pmatrix}
\]

\(F_{ij}\) being the coefficients of the scattering factor matrix. Introducing the polarization angle \(\beta\) of the incoming light as the projection of incident electric field in the observation coordinate system gives:

\[
\tilde{E}_x(R) = \frac{\exp(ikR)}{R} \begin{pmatrix} 0 & F_{12} \sin \beta & F_{32} \cos \beta \\ 0 & 0 & 0 \\ 0 & F_{13} \sin \beta & F_{33} \cos \beta \end{pmatrix} E_0
\]

with \(E_0\) the amplitude of the incident electric field. Finally, the scattered intensity can be written as:

\[
I_R = \left| \frac{\tilde{E}_x(R)}{\tilde{E}_y(R)} \right|^2 = \frac{1}{R^2} \left( (F_{12} \sin \beta + F_{32} \cos \beta)^2 + (F_{13} \sin \beta + F_{33} \cos \beta)^2 \right) E_0^2
\]

Based on these calculations, the theoretical scattering intensity of a non-decorated glide dislocation in Si can be determined as a function of the polarization angle \(\beta\), the Burgers vector being introduced via the angle \(\varphi\) and the dislocation line orientation in the coordinate system \((x,y,z)\).

In a real optical system, the 90° scattering equations remain valid but the incoming and scattered lights spread out within a cone which numerical aperture depends on the system. In order to simulate more completely the measured signal, this experimental feature must be included in the calculations. In our specific case, the light is considered to be collected within a cone of 11° surrounding the scattering vector \(\hat{g}\) parallel to the [111] direction.

Applying the method detailed above, we implemented in Matlab software a numerical simulation of the intensity scattered by a dislocation described by \(\varphi\) and its coordinates \((x,y,z)\) as the function of the light polarization angle \(\beta\). This enables a direct comparison between the scattered intensity measured by our LST tool and the calculated intensity.

3. Observation and simulation of scattered intensity from non-decorated dislocation

3.1 Experimental procedure

300 mm wafers free of COP (crystal originated particle, which are in fact voids due to vacancy agglomeration) and without detectable LST defects were annealed at 1150°C for 2 min in H\(_2\) in a clean CVD epitaxial reactor. This setup allows a large temperature gradient between the wafer centre and edge to be introduced intentionally generating glide dislocations. Wafers were analyzed by LST 300A from Semilab using the standard configuration, and the tomography options developed for individual defect measurement and polarization options. Details were described previously [11,12].

In the wafers, we analyzed several dislocation half loops exhibiting various contrasts. Sizes of these half loops vary from 50 to 500 µm and their density can reach 10\(^7\) cm\(^{-3}\). We will show here, as an example, how the full characterization of such a half loop can be obtained from its scattered intensity.
3.2 Glide plane determination

Depending on the orientation of the glide plane, the dislocation half loop can result in different images on the CCD camera (110) plane. In our experimental set-up, if the dislocation lies in (111) or (11-1) planes, as shown in figure 2a, the half loop image is a facetted or curved line. Such an image is shown in figure 2b, where the longest segment (e.g. b in figure 2b) is almost parallel to [-110]. Only a short oblique straight line would be visible if the dislocation lies in the (-111) or (1-11) planes. Oblique lines were observed, but here we will concentrate on the first configuration: the half loop.

![Diagram](https://example.com/diagram.png)

**Figure 2.** (a) Experimental set-up with crystallographic orientations. (b) Dislocation half loop observed in (110) plane, with polarization direction at 90° and 0°. Three intensity profiles were measured on the left side a, on the centre b and on the right side c of the dislocation.

Using the tomography option we investigated the relative position of the maximum of the scattered intensity (MSI) along the [110] direction for the different branches of the image (a, b and c in figure 2b). It is clear from figure 2a that if the MSI of branch b appears after the MSI of branches a and e by moving the beam in [110] direction, the half loop belongs to the (111) plane and it belongs to (11-1) if the MSI of branch b arises before that of branches a and c. The output of such measurement is shown in figure 3, where the relative position of the MSIs corresponds to a dislocation belonging to the (11-1) plane.

![Graph](https://example.com/graph.png)

**Figure 3.** Scattered intensity of a (full triangles), b (full circles) and c (full squares) dislocation segments (along lines indicated in figure 2b) that is as a function of the relative position of the light beam along the [110] direction.
3.3 Burgers vector determination

As shown in figure 2b, the light scattered by dislocations depends on the polarization of incoming light. The outcome of the simulation performed with the method described in section 2 for the three possible Burgers vectors of the theoretical loop in (11-1) plane is shown in figures 4a-c. Figure 4d displays the observed scattered intensities. For the \(a\), \(b\), and \(c\) segments, the MSI positions correspond to different polarization angles: for segment \(b\) the MSI is close to \(\beta = 85^\circ\), for segment \(a\) it is at \(50^\circ\), while the intensity from segment \(c\) shows basically no polarization dependence. This behavior depends on the orientation of the Burgers vector of the dislocation and its slip plane. Thus, the Burgers vector orientation can be determined by comparing the experimental dependence of scattered light on polarization (figure 4d) of the beam with the simulations of figure 4a-c. Our measured data correspond well to the Burgers vector direction [101]. Accordingly, segment \(a\) being oriented along [011] and segment \(b\) along [-110] both correspond to 60° dislocations while segment \(c\) oriented along [101] is of screw character. The values used in calculation for elasto-optical coefficients are: \(p_{11} = -0.094\), \(p_{12} = 0.017\), and \(p_{44} = -0.051\) [13, 14].

![Figure 4](image)

**Figure 4.** Simulation outputs for the dislocation lines orientation in (11-1) plane ([-110] continuous line, dotted line [101] and continuous line with crosses [011]). (a) Burgers vector parallel to [011], (b) Burgers vector parallel to [101], and (c) parallel to [-110]. (d) Scattered intensity of dislocation segments \(a\), \(b\) and \(c\) (along lines indicated in figure 2b) as a function of \(\beta\).

4. Discrimination between non-decorated and decorated dislocation

Additional information about the morphology of the light scattering defects is provided by the analysis of the scattered intensity dependence on the polarization of the illuminating beam [8]. For small particles, where the Rayleigh approximation works, the scattering distribution of linear polarized light is similar to a dipole radiation pattern. Scattered intensity is proportional to \(\sin^2(\beta)\). It means that small defects are visible only when incoming light has a polarization component perpendicular to the observation direction. In practice, the objective lens collects scattered light within an angle of about 11°, which leads to non-zero defect intensity when polarization of the incoming light is parallel to the...
objective optical axis. Examples of scattered intensity dependence on polarization of the illuminating beam are shown in figure 5a for oxygen precipitates of different sizes.

The wafer in which non-decorated dislocations were developed was annealed at 950°C for 2 hours to obtain oxygen precipitation along the dislocations. Figure 5b shows the scattering behavior of the dislocation half loop analyzed in the previous section, after this anneal. The polarization dependence of scattered intensity has completely changed and is now very close to the one observed for small oxygen precipitates. This experimental result corroborates our hypothesis that the generation and fast movement of dislocations during the first anneal resulted in non-decorated loops. During the second anneal the dislocation did not move and became decorated by oxygen atoms or small precipitates.

![Figure 5](image)

Figure 5. (a) Scattered intensity dependence on polarization of the beam for oxygen precipitates of different sizes with $d \ll d_{eff}$, and (b) the same profiles as in figure 4d after annealing at 950°C for 2 hrs.

5. Conclusion

Non-decorated glide dislocations in Si have been used as model defects to develop a characterization method based on the tomography and polarization options of LST 300A. The glide plane of the dislocation is determined by tomography, while the polarization dependence of the scattered intensity allows the Burgers vector to be identified. A simulation code calculating the incoming light polarization dependence of scattering by a dislocation has been developed and is able to identify the Burgers vector by comparison with the experiment. LST enables to distinguish between non-decorated and oxygen-decorated dislocations in Si using the polarization dependence of the scattered light. The reported results confirm as well that non-decorated glide dislocations can be created in silicon crystals.

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