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Intensity analysis of polarized Raman spectra for off axis single crystal silicon

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ABSTRACT

In this work we demonstrate that polarized backscattered Raman spectroscopy can be used for identifying the crystallographic orientation of silicon cut off axis. The orientation of the crystal is defined by two angles one defined between the (0 0 1) crystal axis and the lab z-axis and the other as the angle of rotation of the crystallographic x-y plane about the crystal's z-axes. Theoretical Raman intensity profiles are generated by rotating wafers of different geometry about the lab z-axis in the backscattered configuration. This changes the polarization of the incident light with respect to the crystallographic axes. The impact of the off axis Si on the Raman intensity profile were investigated to identified specific signatures in the Raman spectra that are most effective in determining the degree of off axis cut for single crystal Si. The results show excellent agreement with experimental outcomes.

1. Introduction

Since 1928 when the first measurement was reported by C.V. Raman [1–4] and in particular after the introduction of laser spectroscopy in early 1960s, Raman spectroscopy has become invaluable for the characterization of vapor, liquid and solid phase materials. The Raman system is user friendly, requires minimal sample preparation and is therefore widely used in research and for quality monitoring in industry. From electronic materials to insulators, from organic materials to artificial structures, from single crystalline materials to amorphous and disordered structure, and from bulk to nano-structures, this contactless and nondestructive technique provides valuable information about optical, electronic, magnetic, and thermal properties of materials [5–9].

Single crystalline Si wafers are used extensively as substrates on which epitaxial thin films and nanostructured materials are grown to fabricate electronic devices. Variations in the crystallinity of the Si substrate and especially the angle at which the substrate is cut influence the growth of thin films and nanostructures. This and the electron mobility for different off-axis cuts of silicon affects implantation characteristics and device performance [10,11]. Raman spectroscopy is especially useful to study the properties of epitaxially grown materials [12–25]. These investigations commonly involve exploring changes in the Raman spectra of specific materials compared to what is expected for a single crystalline sample. Variations in the spectral signatures such as mode intensity, red-shifts and blue-shifts in peak positions, FWHM and asymmetry of the peak, are often studied. From these analyses information regarding impurities, doping, stress, strain, degree of crystallinity or micro-crystalline size in amorphous samples and nanostructural characteristics can be obtained. Polarization dependent characteristics of Raman scattering are dependent on single crystalline quality and crystallographic orientation of the substrate [26–29].

This report presents an in depth analysis of the Raman intensity profiles when an alternative approach is used to obtain polarized Raman spectra from single crystalline Si samples to that commonly used for this purpose. It demonstrates that comparing experimental intensity profiles of polarized Raman spectra to those determined by calculation allows the sample cut to be determined. The theoretical model presented here provides the details of Raman selection rules, using Raman tensors and calculating theoretical responses for various orientations of Si substrates. Fig. 1 represents the revised configuration where a horizontal polarization direction is maintained for the incident beam and the orientation of the analyzer could be set for horizontal (HH) or vertical polarization (HV). The sample is then rotated to control the angle between the crystal axis and incident beam polarization. This is in contrast to the more common approach to polarized Raman scattering where the sample is kept stationary and the desired scattering polarization direction is selected by adjusting the orientation of the optical analyzer, or in some cases altering the direction of the incident polarization by using a polarization rotator. The intent of the approach

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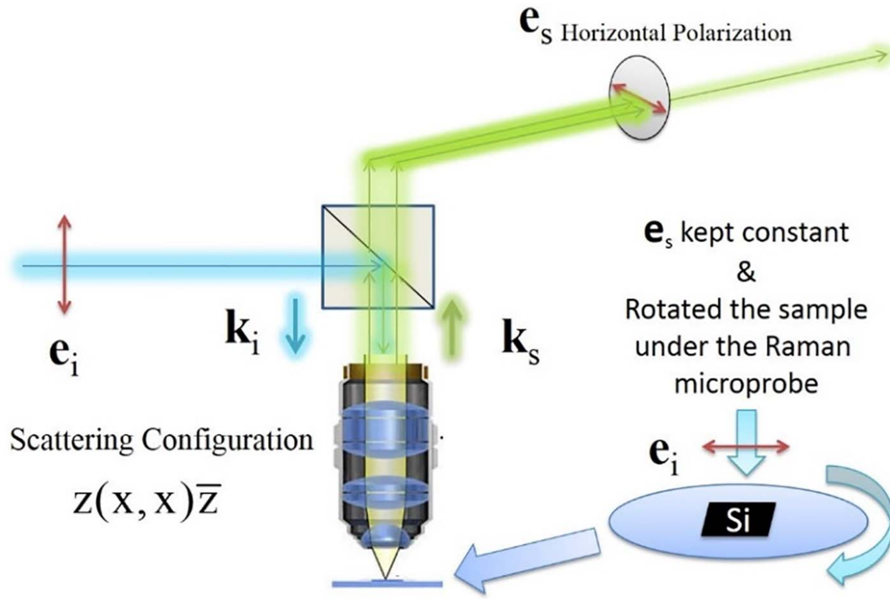

Fig. 1. Schematic diagram representing a revised approach for polarized Raman scattering measurement using fixed polarization directions while rotating the single crystalline sample.

presented here is to determine the specific theoretical profiles of Raman scattered signal from samples of the well-known diamond cubic crystalline Si cut off axis. Thus the focus is shifted away from the details of materials properties to examining of the crystalline orientation of samples in typical Si wafers widely used in devices.

2. Theory

Most semiconductor and electronic materials are opaque to the visible laser wavelengths generally used in Raman scattering. Therefore, the most common Raman scattering configuration used for electronic materials is backscattering geometry [30–32]. Under such scattering configuration the incident light wave vector ($\mathbf{k}_i$) is along z-axis and the scattered light wave vector ($\mathbf{k}_s$) is collected in 180° or anti-parallel to $\mathbf{k}_i$, along $-z$ (denoted $\bar{z}$). Thus for a backscattering geometry when the incident polarization vector ($\mathbf{e}_i$) is along x, and the scattered light polarization vector ($\mathbf{e}_s$) can be chosen to be along either x or y by placing an analyzer appropriately in the path of the scattered light. The scattering designation is shown as $z(xx)\bar{z}$ or $z(xy)\bar{z}$. These experimental geometries are referred to as the HH and HV cases.

We describe the principles used to present the theoretical model for the polarized Raman scattering intensities for a sequence of Si orientations starting with Si (0 0 1) in Sections 2 and 3. In Section 4 the experimental polarized Raman intensity measurements for Si as a function of the angle between the polarization and crystal direction is compared to the theoretical model. The results indicate that it would be possible to identify the angle at which the wafer is cut for different single crystalline Si samples. This becomes significant when off-axis cut Si has steps with nucleation points that benefit growth of epitaxial oxides such as $SrTiO_3$ [33].

2.1. Raman intensity model for Si (1 0 0) backscattering with fixed sample orientation

Si crystallizes in a diamond cubic structure and belongs to O_h class of the 32 crystal classes. It therefore has threefold degenerate F_{2g} Raman active optical phonons with two-Transverse Optic (TO) modes and one Longitudinal Optic (LO) mode. The unit polarization vectors of the incident and scattered laser beams are defined as, $\mathbf{e}_i$ and $\mathbf{e}_s$, respectively. The Raman tensor is presented as $\mathbf{R}_j$, with j representing x, y, or z components. Using the polarization vectors; $\mathbf{e}_i$ and $\mathbf{e}_s$, and Raman tensors; $\mathbf{R}_x$, $\mathbf{R}_y$, and $\mathbf{R}_z$, Raman intensity could be calculated using:

$$I \propto |\boldsymbol{e_i} \boldsymbol{R_j} \boldsymbol{e_s}|^2 \tag{1}$$

The polarization vectors, $\mathbf{e}_i$ and $\mathbf{e}_s$, are defined by the direction of the incident and scattered beams, while $\mathbf{R}_x$, $\mathbf{R}_y$, and $\mathbf{R}_z$, are representing the x, y, and z components of the Raman tensors that reflect the Si crystalline symmetry [5,31–33]. Note that $\mathbf{R_x}$ and $\mathbf{R_y}$ correspond to Transverse Optic (TO) modes, and $\mathbf{R_Z}$ corresponds to Longitudinal Optic (LO) mode. The Raman tensor components for Si are defined as [5]:

$$\boldsymbol{R_x} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & b \\ o & b & 0 \end{bmatrix}, \boldsymbol{R_y} = \begin{bmatrix} 0 & 0 & b \\ 0 & 0 & 0 \\ b & 0 & 0 \end{bmatrix}, \boldsymbol{R_z} = \begin{bmatrix} 0 & b & 0 \\ b & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{2}$$

The simplest case for the polarization configuration is when the incident and scattered polarization are aligned with the lab x- coordinate axis. The lab axes could be expressed as; x = ⟨1 0 0⟩, y = ⟨0 1 0⟩, and z = ⟨0 0 1⟩. Below we present the details of the polarized Raman selection rule calculations for this configuration and then we tabulate them for ease of comparison.

For the $z(x,x)\bar{z}$ configuration the Raman intensity calculation leads to a zero value, as shown below, indicating a Raman forbidden mode:

$$I \propto |\boldsymbol{e_i} \boldsymbol{R_x} \boldsymbol{e_s}|^2 = \left| [1 \;\; 0 \;\; 0] \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & b \\ 0 & b & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \right|^2 = \left| [1 \;\; 0 \;\; 0] \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \right|^2 = 0 \tag{3}$$

As reported in Table 1, the results of similar calculations leads to a zero intensity value for all TO mode configurations and for two parallel polarized LO mode configurations; $z(x,x)\bar{z}$, and $z(y,y)\bar{z}$,. However, Raman intensity calculations for the cross polarized LO phonon mode denoted as; $z(x,y)\bar{z}$, shows a non-zero value:

Table 1
Raman selection rules for backscattering from the (0 0 1) surface of single crystalline Si samples when laboratory axis and crystalline axis are aligned.

Polarization Configuration	Phonon modes (direction of atomic displacement)		
	LO (z-direction)	TO (x-direction)	TO (y-direction)
$z(x,x)\bar{z}$	0	0	0
$z(x,y)\bar{z}$	b^2	0	0
$z(y,y)\bar{z}$	0	0	0

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