Setting up the Wafer Orientation: Applications to Ion Implantation

Introduction

Properly setting the wafer orientation in Victory Process (VP) is critical for various processes such as ion implantation, etching, and deposition. For ion implantation in particular, the determination of the wafer orientation becomes crucial, given its profound impact on profile variations in channeling and non-channeling directions. Additionally, understanding the effects of crystal orientation in different materials, especially those with diamond and hexagonal structures, is essential due to the multitude of specifications in commercially available wafers. It is the aim of this article to demonstrate how to properly configure a wafer for a VP simulation, particularly for ion implantation. Emphasis will also be placed on the underlying crystal structure of the wafer because of its critical role in ion implantation.

Wafer Configuration

The INIT statement provides several options for configuring the orientation of the wafer. First, the option SUB.TYPE allows the user to choose between "diamond" and "hexagonal" structures. Depending on the selected structure, distinct orientation options become available for the wafer through the SUB.ORI setting. Specifically, if the "diamond" structure is selected, the available orientations are "100", "110", and "111". Conversely, when the "hexagonal" structure is selected, the available orientations are "0001", "000-1", "11-20", and "1-100". Each of these options corresponds to a different underlying crystal orientation of the wafer.

To distinguish the various configurations and facilitate the discussion, we define an orthogonal coordinate system xyz, as shown in Figure 1. This system will be used throughout this article. The xy-plane lies on the surface of the wafer, hence the z-axis is perpendicular to the surface of the wafer. Each configuration provided by SUB.TYPE and SUB.ORI corresponds to a different crystal orientation which will be described in relation to the xyz coordinate system.
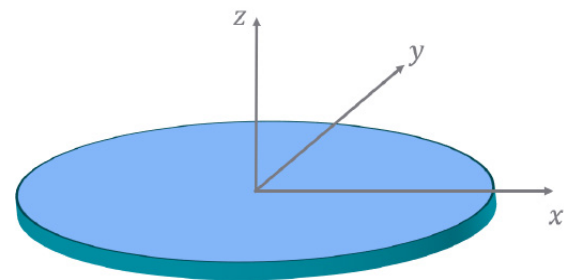

Figure 1. Representation of a wafer in the xyz coordinate system.

Table 1 summarizes the crystallographic direction corresponding to each axis x, y, and z for the different diamond wafer orientations available in VP. Notice that the name of each wafer orientation represents the crystallographic direction that is parallel to the z-axis of the coordinate system.

SUB.TYPE="diamond"			
SUB.ORI	z-axis	x-axis	y-axis
"100"	[100]	[010]	[001]
"110"	[110]	[-110]	[001]
"111"	[111]	[-110]	[-1-12]

Table 1. Wafer orientations and crystallographic directions for diamond structures (SUB.ROT=0).

Table 2 summarizes the crystallographic directions corresponding to each axis for the different hexagonal wafer orientations available in VP. A couple of differences compared to the diamond structures need to be clarified. First, in hexagonal structures, a crystallographic direction is represented by four indices [*hkil*]. The third index is redundant because of its relation to the first two indices, i.e.,

SUB.TYPE="diamond"			
SUB.ORI	z-axis	x-axis	y-axis
"0001"	[0001]	[1-100]	[11-20]
"000-1"	[000-1]	[1-100]	[11-20]
"1-100"	[1-100]	[000-1]	[11-20]
"11-20"	[11-20]	[1-100]	[0001]

Table 2. Wafer orientations and crystallographic directions for hexagonal structures (SUB.ROT=0). In SiC, "0001" corresponds to the Si-face, whereas "000-1" corresponds to the C-face.

i=-(h+k). Second, the (0001) direction in hexagonal crystals with two species, such as SiC, consists of separate layers of each element. Therefore, all the atoms in a plane perpendicular to the (0001) direction are the same species, i.e., either Si or C in SiC. To distinguish the two cases, we use "0001" and "000-1" for the Si-face and C-face, respectively.

Once the preferred orientation is selected, further operations can be conducted. The next operation is determined by the option SUB.ROT and is responsible for rotating the wafer clockwise about the z-axis by an angle S_R (in degrees). Figure 2 illustrates the operation conducted by SUB.ROT, where the arrow on the surface of the wafer is drawn to demonstrate the rotation. The orientations listed in Table 1 and Table 2 refer to SUB.ROT=0.
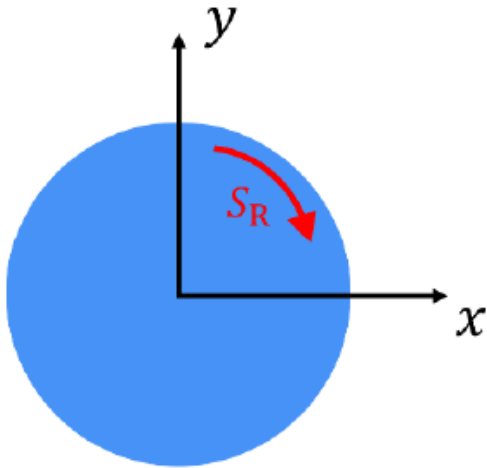

Figure 2. Rotation of the wafer by an angle S_R using the option SUB.ROT.

As shown in Figure 2, the xyz coordinate system is not affected by the SUB.ROT rotation. However, it is important to notice that the x and y axes are parallel to different crystallographic directions than the ones listed in Table 1 and Table 2 if the wafer is rotated. The z direction is not affected because the z-axis is the axis of rotation. As an example, consider the case of SUB.TYPE="diamond", SUB.ORI="100", and SUB.ROT=45. In this case, the x- and y-axis would be parallel to the [011] and [0-11] direction, respectively. Refer to Appendix A for more information and clarifications.

Finally, a feature that is often found in commercially available wafers, is the off-cut angle, also known as the miscut angle. Since this feature is common in SiC wafers, this material will be used as an example. The SiC boule is typically grown in the [0001] direction. Wafer manufacturers slice the boule at an angle ϑ to facilitate future homoepitaxial growth of the same polytype. Without it, the stacking information of the polytype would be lost, preventing future growth of the same polytype. The procedure of slicing off a wafer at an angle ϑ from the boule is shown schematically in Figure 3. Notice that the [0001] direction of the crystal is not perpendicular to the surface of the wafer after the slice. Instead, it is tilted at an angle ϑ.
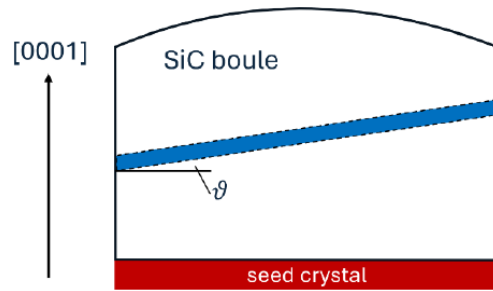

Figure 3. Growth of a SiC boule and a wafer (blue) sliced off at an angle ϑ.

In order to account for the miscut, two angles need to be configured in the INIT statement, i.e., SUB.MISCUT.THETA (ϑ) and SUB.MISCUT.PHI (ϕ). Both angles ϑ and ϕ are necessary for configuring the miscut of the wafer. Namely, the angle ϑ alone, which corresponds to the off-cut angle, is not enough to specify the miscut of the wafer. Figure 4 illustrates the slicing procedure and demonstrates the need for both angles to be defined.
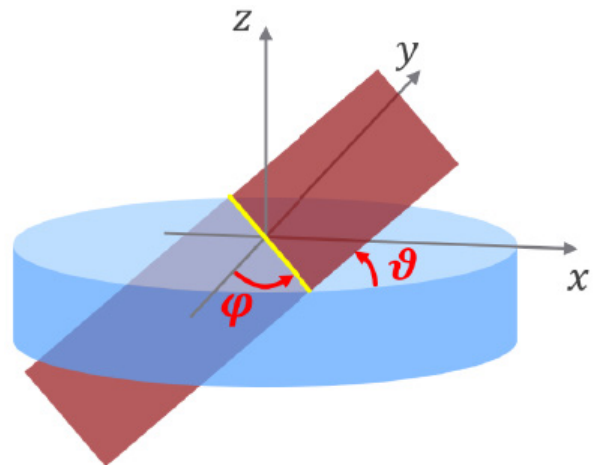

Figure 4. Miscut of a wafer at an angle ϑ. The intersection of the slicing plane and the xy-plane (yellow) forms an angle ϕ with the y-axis.

Mathematically speaking, the slicing of the wafer occurs at a plane that intersects the xy-plane at an angle ϑ. We call this plane the slicing plane, shown as maroon in Figure 4. However, there are infinite possible slicing planes that intersect the xy-plane at a given angle ϑ. To uniquely specify a single plane, the angle φ is also needed. The intersection of two planes is always a straight line. Angle φ defines the angle between the intersection line, yellow in Figure 4, of the two planes and the y-axis. Therefore, ϑ and φ uniquely define the slicing plane by specifying the angle between the slicing plane and the xy-plane and the angle between the intersection line and the y-axis, respectively. As a last step, the wafer is rotated in space about the intersection line so that the surface of the sliced wafer becomes parallel to the xy-plane, i.e., the normal to the slicing plane, is aligned with the z-axis.

To summarize, the set of parameters {`SUB.TYPE`, `SUB.ORI`, S_R, ϑ, φ} in the `INIT` statement correspond to a configuration vector which uniquely defines the underlying crystal configuration of the wafer. As described, each *configuration vector* corresponds to a set of operations that involve the rotation of the wafer and the underlying crystal structure in space. Therefore, the order of each operation is important. First, the wafer with a specific orientation is defined through `SUB.TYPE` and `SUB.ORI`. Second, a simple rotation is performed through `SUB.ROT`. Finally, the miscut is applied through the angles ϑ and φ.

As a practical example, we configure a commercially available SiC wafer [1] in VP. According to the manufacturer's specifications, the primary flat of the wafer indicates the [11-20] direction and the wafer is cut at an angle of 4° towards the [11-20] direction. Let us also assume that this is a Si-face wafer. Therefore, we start by setting `SUB.TYPE`="hexagonal" and `SUB.ORI`="0001". Setting a rotation is not necessary, therefore `SUB.ROT`=0. As listed in Table 2, that would align the y-axis with the [11-20] direction of the crystal. Hence, the wafer's primary flat will be parallel to the y-axis. The next step is to configure the miscut angle. Since the manufacturer specifies a miscut angle of 4° towards the [11-20] direction, we need to set `SUB.MISCUT.THETA`=4 and `SUB.MISCUT.PHI`=90. The choice of ϑ=4° is obvious. For the choice of φ=90° we need to consider that the slicing plane needs to be towards the [11-20] direction per the manufacturer's specification. Therefore, the intersection line should be perpendicular to the y-axis. Alternatively, we could have achieved the same result by setting `SUB.ROT`=90, `SUB.MISCUT.THETA`=4, and `SUB.MISCUT.PHI`=0. In this case, the [11-20] direction would be parallel to the x-axis and therefore no φ angle would be necessary. The only difference in this configuration is that the wafer flat would be parallel to the x-axis. Notice that the choice of SUB.ROT is mostly a matter of preference. However, this choice affects the configuration of the miscut afterwards.

Implantation

The settings discussed so far have a global character since they are configured in the INIT statement. The IMPLANT statement provides a couple more settings required for positioning the beam appropriately with respect to the wafer and the crystal structure. Specifically, these settings are the TILT (T) and ROTATION (R) angles of the beam.

Figure 5 demonstrates the effects of TILT and ROTATION on the orientation of the beam. The beam tilts by an angle T from the z-axis on a plane that is typically referred to as implantation plane. For R=0° (no rotation), the implantation plane is parallel to the xz-plane of the coordinate system.
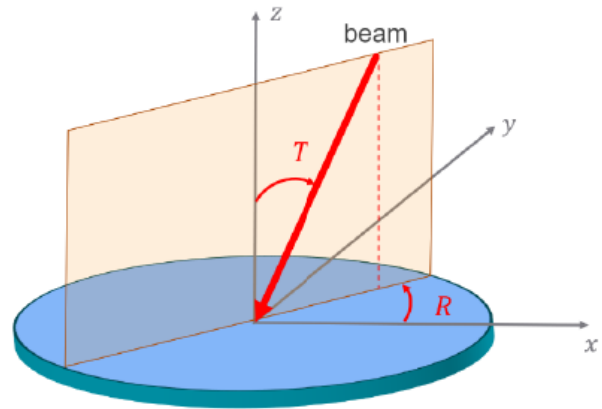

Figure 5. Tilt and rotation in ion implantation.

Notice that although tilt and rotation refer to the orientation of the beam assuming a fixed wafer in space, an equivalent perspective would be to consider a beam which is fixed and a wafer that rotates according to the IMPLANT settings instead. According to the latter view, ROTATION is equivalent to SUB.ROT of the INIT statement and TILT is equivalent to a miscut angle. Therefore, an appropriate combination of tilt and rotation can counteract any inherent miscut of the wafer.

To fully configure an implantation step, we need to specify the configuration vector {SUB.TYPE, SUB.ORI, S_R, ϑ, ϕ, T, R}. The first five parameters of this vector are specified in the INIT statement, whereas the last two are specified in the IMPLANT statement. As an example, we use the wafer we configured in the previous section, which had a configuration vector of {"hexagonal", "0001", 0, 4, 90, T, R}. Depending on the choice of T and R, we can achieve different implantation settings. For instance, to counteract the effects of miscut and access the [0001] channel, we need to set TILT=4 and ROTATION=90.

References

[1] Wolfspeed Silicon Carbide and Nitride Materials Catalog.

[2] K. Momma and F. Izumi, "VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data," J. Appl. Crystallogr., 44, 1272–1276 (2011).

Appendix A: Crystal Orientations

The top views of various orientations with their corresponding crystal directions in Si and SiC-4H are illustrated in this section using VESTA [2]. First, the orientations corresponding to diamond structure as listed in Table 1 are shown. The top view of the orientation corresponding to the configuration vector {"diamond", "100", 0} is shown in Figure 6.
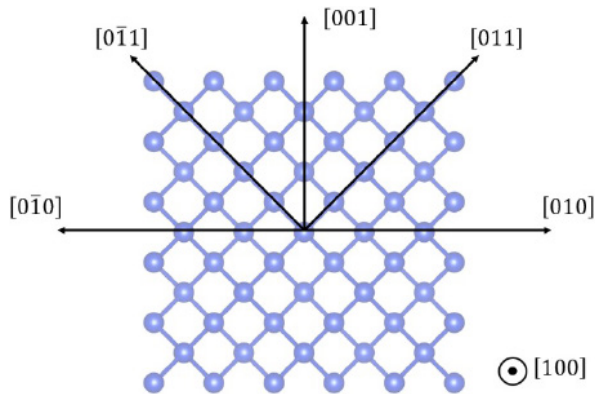

Figure 6. Top view of the crystal orientation corresponding to the configuration vector {"diamond", "100", 0}.

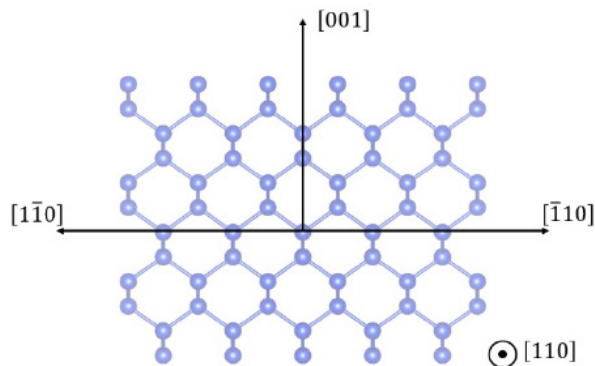The orientation corresponding to the configuration vector {"diamond", "110", 0} is shown in Figure 7.

Figure 7. Top view of the crystal orientation corresponding to the configuration vector {"diamond", "110", 0}.

The orientation corresponding to the configuration vector {"diamond", "111", 0} is shown in Figure 8.
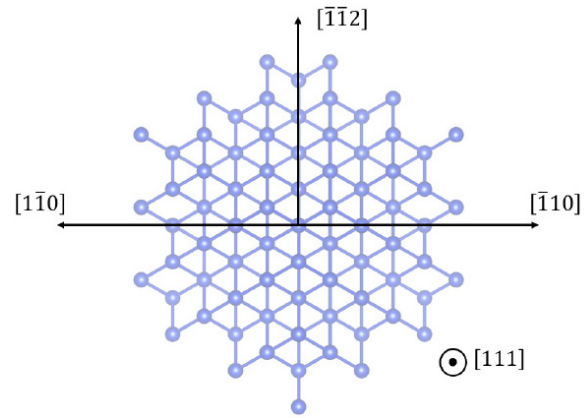

Figure 8. Top view of the crystal orientation corresponding to the configuration vector {"diamond", "111", 0}.

Notice that in all cases, a different channel of the diamond structure is accessed in ion implantation assuming no tilt of the beam.

Next, the orientations of SiC-4H are shown for the settings listed in Table 2. First, the orientation corresponding to the configuration vector {"hexagonal", "0001", 0} is shown in Figure 9. Additionally, the shape of the wafer is drawn around the crystal structure to indicate the most commonly available wafer, i.e., the primary flat is parallel to the [11-20] direction.
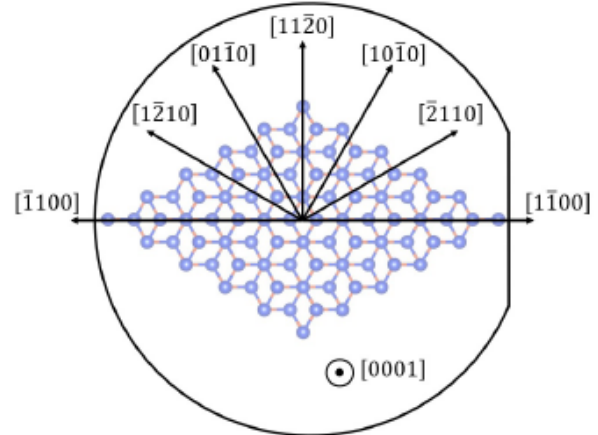

Figure 9. Top view of the crystal orientation corresponding to the configuration vector {"hexagonal ", "0001", 0}. The wafer shape is drawn for reference.

The orientation corresponding to the configuration vector {"hexagonal", "000-1", 0} is effectively the same as in Figure 9 with the only difference being that the surface consists of carbon atoms. The orientation corresponding to the configuration vector {"hexagonal", "1-100", 0} is shown in Figure 10.
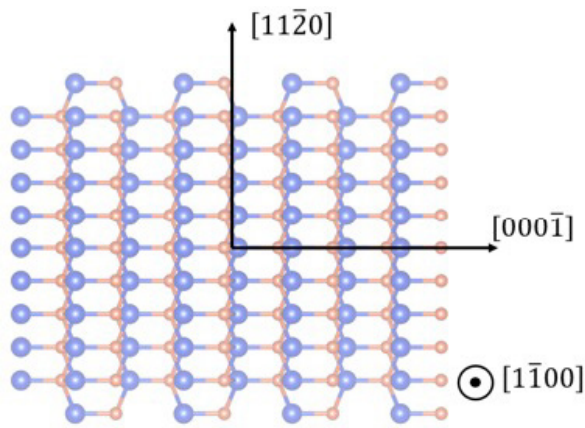
Figure 10. Top view of the crystal orientation corresponding to the configuration vector {"hexagonal ", "1-100", 0}.

Finally, the orientation corresponding to the configuration vector {"hexagonal", "11-20", 0} is shown in Figure 11.
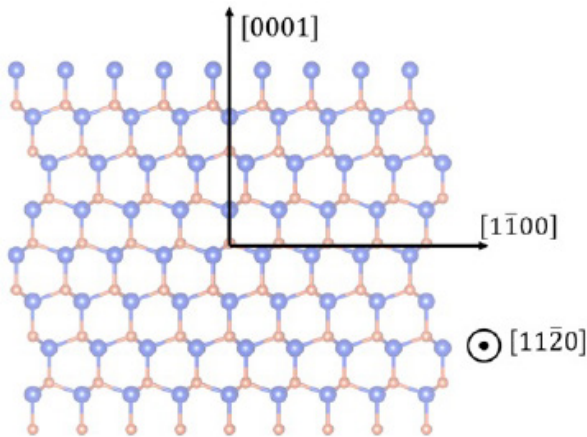

Figure 11. Top view of the crystal orientation corresponding to the configuration vector {"hexagonal ", "11-20", 0}.

Appendix B: Implantation examples

The following example demonstrates the implantation in the [0001] channeling direction of SiC-4H at a wafer with a miscut of 4° towards the [11-20] direction which is oriented parallel to the y-axis.

Example 1. Channeling implantation in the [0001] direction on a SiC-4H wafer with a miscut of 4° towards the [11-20] direction.

```
init material=sic-4h sub.type=hexagonal
sub.ori="0001" sub.rot=0
sub.miscut.theta=4 sub.miscut.phi=90

implant Phos energy=120 dose=1e12 BCA
n.ion=5e3 tilt=4 rotation=90
```

An equivalent way to access the [0001] channel is shown in Example 2. The difference in this case is that the x-axis is parallel to the [11-20] direction.

Example 2. Channeling implantation in the [0001] direction on a SiC-4H wafer with a miscut of 4° towards the [11-20] direction.

```
init material=sic-4h sub.type=hexagonal
sub.ori="0001" sub.rot=90
sub.miscut.theta=4 sub.miscut.phi=0

implant phos energy=120 dose=1e12 bca
n.ion=5e3 tilt=4 rotation=0
```

Another direction that exhibits strong channeling in SiC-4H is the [11-23] direction which occurs at 17° off the [0001] direction towards [11-20]. Example 3 demonstrates an implantation in this channel on a wafer with a miscut of 8° towards [11-20]. Notice that the tilt required to counteract this miscut is 25°.

Example 3. Channeling implantation in the [11-23] direction on a SiC-4H wafer with a miscut of 8° towards the [11-20] direction.

```
init material=sic-4h sub.type=hexagonal
sub.ori="0001" sub.rot=0
sub.miscut.theta=8 sub.miscut.phi=90

implant phos energy=120 dose=1e12 bca
n.ion=5e3 tilt=25 rotation=90
```

Example 4 demonstrates an implantation in the [110] channel of silicon. Notice that [110] can be accessed directly using SUB.ORI="110" without any tilt.

Example 4. Channeling implantation in the [110] channel of silicon in a [100] wafer.

```
init material=silicon sub.type=diamond
sub.ori="100" sub.rot=45

implant phos energy=120 dose=1e12 bca
n.ion=5e3 tilt=45 rotation=45
```

As a final example, Example 5 shows the implantation in the [211] channel of silicon.

Example 5. Channeling implantation in the [211] channel of silicon in a [100] wafer.

```
init material=silicon sub.type=diamond
sub.ori="100" sub.rot=45

implant phos energy=120 dose=1e12 bca
n.ion=5e3 tilt=35 rotation=0
```