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Spontaneous Polarization Effects in Nanoscale Wurtzite Structures

Takayuki Yamanaka, Mitra Dutta, and Michael A. Stroscio
Nano Engineering Research Group, University of Illinois at Chicago, Chicago, IL, 60607.
email: tyaman1@uic.edu

INTRODUCTION

For nanoscale wurtzite structures such as quantum dots and nm-thick layers, the surfaces may terminate locally in different atoms; for example, GaN structures may terminate with Ga-surfaces or N-surfaces. In this paper, the spontaneous polarization is calculated and shown to be depend on these surface terminations.

DISCUSSION

Fig. 1 shows the unit cell of wurtzite crystals. The left hand side of Fig. 1 shows the geometry for ideal wurtzite structures. The lattice constant along a-axis of GaN is 3.189Å, consequently, the ideal height of the unit cell is 5.208Å. However, the actual height of the unit cell is 5.185Å. This is caused by the polarization in the crystal. In the wurtzite unit cell, the number of atom is identical for each layer. This means that the sheet charge density of each layer is same and the only the sign is different. If the horizontal area is large, the horizontal polarization can be approximated as zero. In the following, the vertical polarization is evaluated from the sheet charge density. Now, the large white circle in Fig. 1 is assumed to be a nitride, on the other hand, the gray circle is assumed to be a gallium. Thus, the sheet charge density is as shown in the left hand side of Fig. 2. The bottom area of the GaN unit cell is $(3.189\text{Å})^2 \sin 60^o = 8.807\text{Å}^2$. As a result, the sheet charge density σ is,

$$\sigma = (1.6 \times 10^{-19}\ \text{C})/(8.8 \times 10^{-20}\ \text{m}^2) = 1.8\ \text{C/m}^2$$

The contribution for polarization is half of the sheet density to consider both sides of the layer. The polarization P can be evaluated by averaging the total dipole moment of the unit cell with regard to the volume. The right hand side of Fig. 2 describes the dipole moment of each layer. Assuming a given area S, the polarization is expressed by

$$P = \sigma (c_1 - c_2)/2(c_1 + c_2)$$

At the same time, the height of the unit cell is $2(c_1 + c_2) = 0.5185$ nanometer as mentioned above. The spontaneous polarization of bulk wurtzite GaN is taken to be -0.029 C/m. From above equations and the spontaneous polarization, the thickness of layers in the equilibrium state is obtained as $c_1 = 0.1256$ nm and as $c_2 = 0.1338$ nm. Here, the polarization change from the spontaneous polarization is evaluated for four cases shown in Fig. 3. These two cases, 1 and 2, are possible arrangements to change the polarization. It is noted that there are two more cases, 3 and 4, that are simply turned upside down compared with cases 1 and 2, so, the polarization of the cases 3 and 4 will become the same value and the opposite direction of cases 1 and 2. Fig. 4 shows the polarization according to the number n, which is the number of the alternated units shown in Fig. 3. The two dotted lines in Fig. 4 represents 0.029 C/m^2 and –0.029 C/m^2, respectively. These spontaneous polarization effects are considered for different nanostructures.

CONCLUSION

Spontaneous polarizations have been calculated for nanostructures and the sensitivity of the results on the surface termination have been determined.

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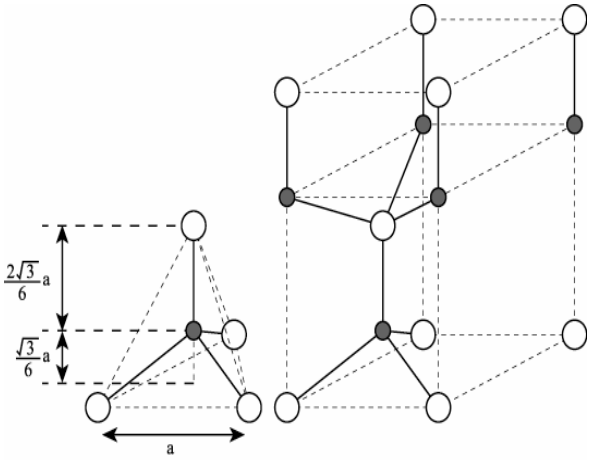

Figure 1. Wurtzite unit cell.

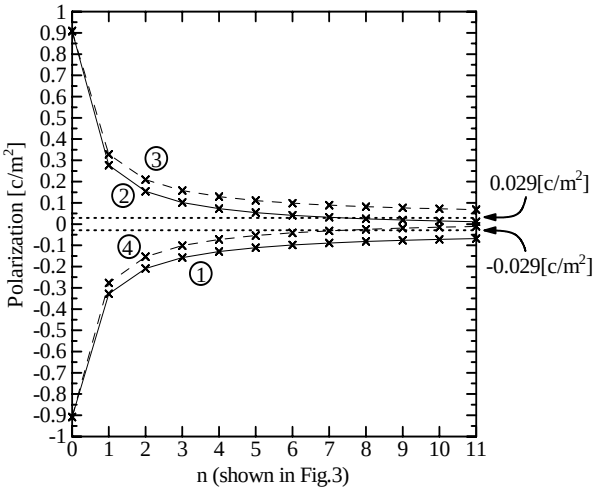

Fig. 4. Polarization change according to the number of layers.

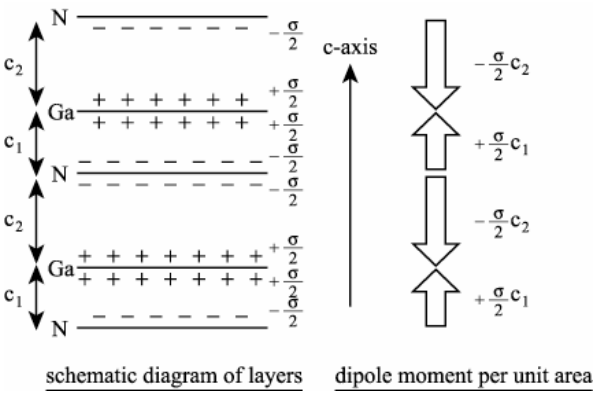

Figure 2. Sheet charge density and its dipole moment.

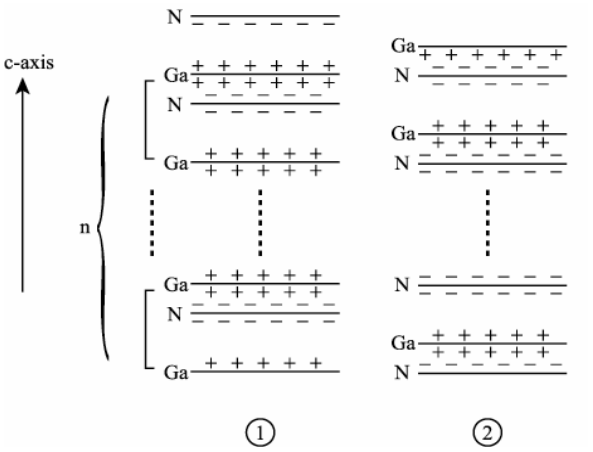

Figure 3. Arrangements to change the polarization.