The three-dimensional shape of antiphase domains in GaP on Si(001)

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The integration of III-V semiconductors on Si(001) has been a long standing research aim to lower the cost of optoelectronic devices and simultaneously improve their performance. As the lattice mismatch between Si and GaP is smaller than 4%, this particular III-V semiconductor is used preferentially. However, due to charged, three-dimensional defects called antiphase domains (APDs) in GaP arising at the interface, its integration has proven to be quite challenging. While the search for growth conditions to avoid pronounced formation of these defects has been successful, the exact shape of the remaining ones is not yet fully understood.
In this work, APDs in GaP on Si(001) are investigated by means of transmission electron microscopy (TEM) and cross-sectional scanning tunneling microscopy (XSTM), two methods that offer unique insight into the appearance of APDs' cross sections due to their high surface sensitivity and resolution. The progression of the cross sections of the antiphase boundaries (short: antiphase boundaries) that separate the crystal's mainphase from the antiphase could be analyzed all the way down to the atomic level, allowing for an identification of the individual crystal planes along which the antiphase boundaries form. The accurate analysis of their progression by means of XSTM is illustrated by Fig. 1. After a thorough investigation of the antiphase boundaries' appearances on plane-view TEM and on the (110) and the (1-10) cleavage planes by means of XSTM, it has been possible to develop a true-to-scale, three-dimensional model of antiphase domains.
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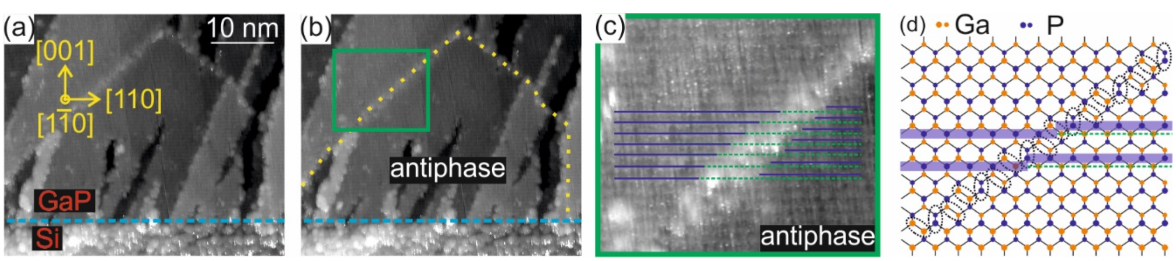

Figure 1: (a) XSTM image of GaP/Si(001) obtained at a sample bias of U = - 3.2 V and a tunneling current of I = 20 pA; the dashed light blue line approximates the position of the interface; (b) same image, with the dotted yellow line denoting the approximate progression of the antiphase boundary, a zoom into the area inside the green box is shown in (c). Here, chains of P atoms are marked by solid dark blue lines. A shift of one quarter of their separation in growth direction when crossing over from the mainphase to the antiphase can be observed which is emphasized by the dashed green lines and explained by the ball and stick model given in (d).

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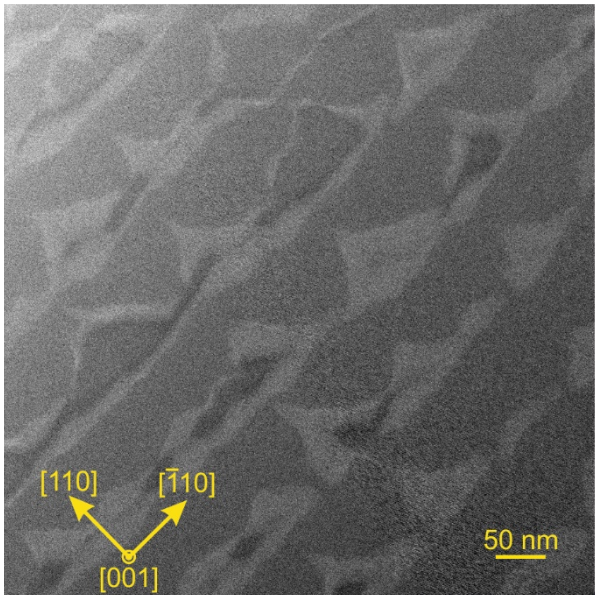

Fig. 1: Scanning transmission electron microscopy image from a plane view sample at low magnification showing the approximate alignment of the antiphase domains with the silicon surface steps.

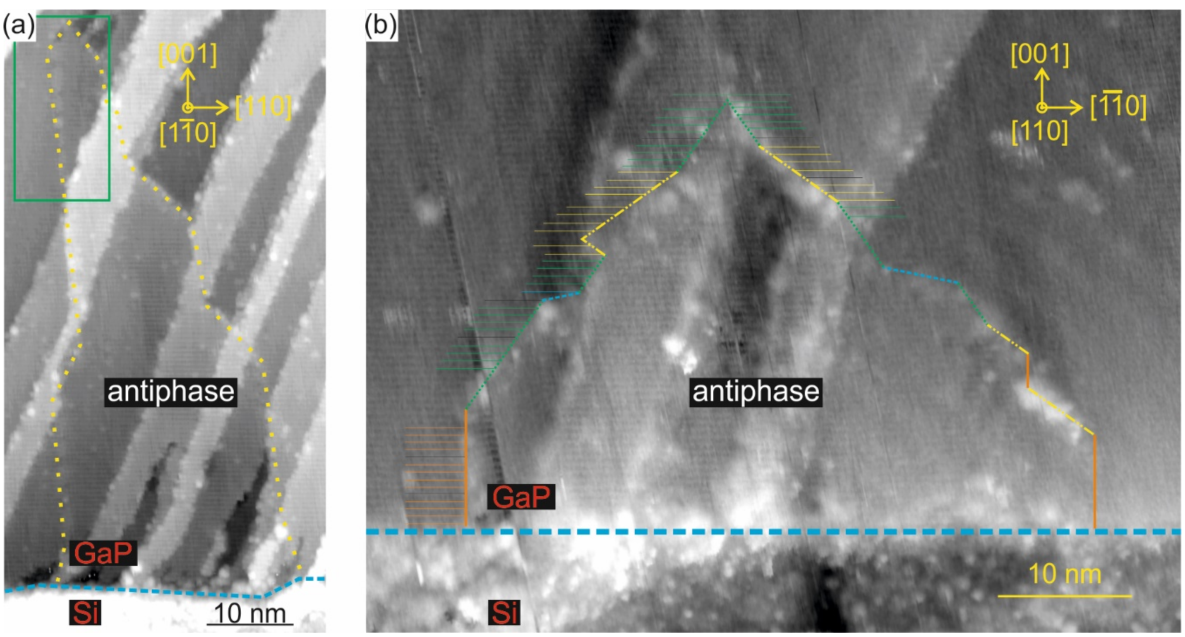

Fig. 2: (a) XSTM image of an antiphase domain on the (1-10) cleavage plane obtained at a sample bias of U = -3 V and a tunneling current of I = 20 pA. The progression of the antiphase boundary is denoted by a dotted yellow line; (b) XSTM image of an antiphase domain on the (110) cleavage plane obtained at a sample bias of U = -2.9 V and a tunneling current of I = 30 pA. The antiphase boundary is broken down into sections at angles corresponding to the planes that antiphase boundaries are commonly observed to progress along. Different line types as well as colors have been chosen for the different sections to guide the eye. The dashed light blue line marks the approximate position of the GaP/Si interface in both images.

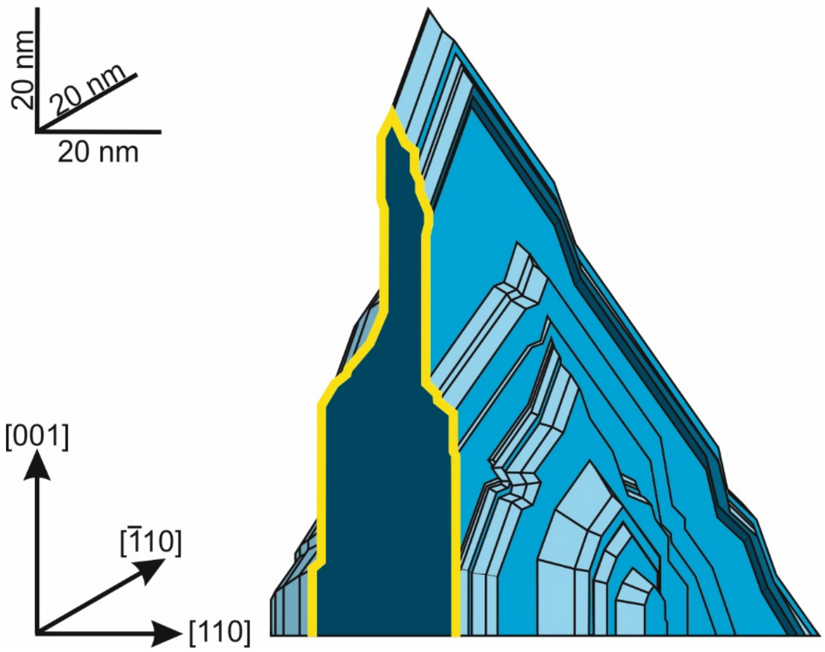

Fig. 3: True-to-scale, three-dimensional representation of an antiphase domain. Kinks along the [-110] direction as well as kinks along the [110] direction are included in the model. All dimensions have been chosen in accordance with measured values derived from XSTM data. Further kinks arise in a real antiphase domain which are not shown in order to avoid confusion. A look at the (1-10) cleavage plane reveals a realistic depiction of an antiphase domain cross section as it could be found in a GaP crystal, see fig. 2 (a). Its shape is emphasized by the thick yellow line.