Structural study of the commensurate-incommensurate low-temperature phase transition of Pb on Si(111)

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It is well known that adsorbates and impurities can induce significant reorganization of the atoms on semiconductor surfaces. Such reconstructed surfaces have been extensively investigated at room temperature (RT) in the past. Recently it has been found that a number of systems exhibit low temperature (LT) phases with unusual properties. We present the results of our investigations on the phase transition from the hexagonal incommensurate (HIC) phase of lead on silicon(111) at RT to the $\left(\frac{3}{2}, \frac{1}{1}\right)$ commensurate phase at LT.

The sample was prepared in an ultra high vacuum (UHV) system and RHEED and LEED techniques were used to monitor the Pb deposition and to confirm that the sample was purely HIC. After preparation the sample was transferred into a UHV-LT chamber which was mounted at the surface diffractometer at the BW2 beamline. In-plane and out-of-plane data sets were measured at a wavelength of $\lambda = 1.24$ Å with the angle of incidence $0.17^\circ$. The temperature was below 30 K. Due to the threefold symmetry of the substrate three surface domains with not overlapping fractional order reflections occur. The intensities of the symmetry equivalent reflections revealed that the three domains had equal populations so the reflections could be mapped on one domain. For solving the surface structure a starting model for the refinement was developed from the known surface reconstruction of the HIC phase. It consists of a lead overlayer with six atoms per unit cell. Refining only the positions of the lead atoms a $\chi^2 = 3.4$ was found which shows that the model contains all essential features. The measured and calculated inplane intensities are shown in Fig. 1a, the CTRs and fractional order rods in Fig. 1b and c (dotted lines). The fit could be improved by including the positions of one double-layer of silicon atoms and anisotropic Debye Waller (DW) factors for the lead atoms in the refinement. To avoid an unrealistic high out-of-plane DW factor for atom 1 (9.9 Å$^2$) a split position in the $z$-direction was assumed for this atom. The CTRs and fractional order rods calculated using the final model are shown as solid lines in Fig. 1b and c ($\chi^2 = 2.5$), the model is shown in Fig. 2.

The Pb overlayer consists of a sequence of three different rows of lead atoms in the direction of b. One row (atoms 1/1a and 2) lies on the mirror line (parallel to b, $[\overline{2}11]$ in Si bulk coordinates, indicated by the dash-dotted line in Fig. 2a). The atomic positions of these two atoms are essentially similar to those in the SIC model. The zig-zag row formed by atoms 3 and 4 is mapped onto the third row (atoms 5 and 6) by the mirror line. Compared to the SIC model these atoms are shifted close to T1 on-top positions above the uppermost silicon atoms.

Judging from next-neighbor distances the bonds between the lead atoms can be classified in covalent like bonds (below 3.15 Å), and metallic like bonds (between 3.30 and 3.55 Å). This is illustrated in Fig. 2a by gray and black lines between the lead atoms, indicating covalent- and metallic-like interatomic distances, respectively. From Fig. 2b it can be seen that atom number 1, which is located on a hollow site, is the only one without a covalent bond to a silicon atom. This is probably the reason for the disorder in $z$-direction. Judging from these atomic distances all of the five silicon dangling bonds within one $\left(\frac{3}{2}, \frac{1}{1}\right)$ unit cell are saturated. The partially covalent bonds between lead...
adatoms and the silicon substrate atoms seem to stabilize the system and in contrast to the situation at RT produce a commensurate surface reconstruction at LT. We speculate that the formation of such “covalent bonds” might be the driving force behind the formation of the \((\frac{3}{1}, \frac{2}{1})\) phase. This work was supported by the TMR-Contract ERBFMGECT950059 of the European Community.

Figure 1: (left): Measured and calculated intensities. (a) In-plane data set \((h, k, 0.015)\). The areas of the filled and empty semi-circles correspond to measured and calculated intensities. (b) Fractional order and (c) integer order rod scans. The solid lines show the fit with the final model, for the dotted line only the Pb positions are refined. The \((0.6, 0.6)\) rod is scaled with a factor of 0.5.

Figure 2: (right): The final Pb model in (a) top and (b) side view. Lead and silicon atoms are shown as gray and white circles. The unit cell is indicated by the dashed line, the mirror line by the dash-dotted line and that part of (a) which is shown in (b) in a side view by the thin dotted line.

References