Solving the Phase Problem of Diffraction: X-Ray Standing Waves Imaging on Bismuthene / SiC(0001)

Niclas Tilgner [1], Susanne Wolff [1], Serguei Soubatch [2], Tien-Lin Lee [3], Fabian Göhler [1], F. Stefan Tautz [2,4], Thomas Seyller [1], Philip Schädlich [1], and Christian Kumpf [2,4]

[1] Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany
[2] Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, Jülich, Germany, and Jülich-Aachen Research Alliance (JARA), Fundamentals of Future Information Technology
[3] Diamond Light Source Ltd., Didcot, Oxfordshire, United Kingdom
[4] Experimentalphysik IV A, RWTH Aachen University, Aachen, Germany

Over the decades, a variety of diffraction-based techniques for determining the structure of materials at an atomic level has been developed and employed. These techniques have contributed significantly to our understanding of the properties and functionalities of physical systems and devices in many fields, particularly in surface and interface science. However, a fundamental limitation of such methods is the so-called 'phase problem', as diffraction techniques can only measure intensities (i.e., the squared magnitudes of the complex scattering factors), while their phases remain inaccessible in an experiment. If both amplitudes and phases of the structure factors were available, it would be straightforward to use an inverse Fourier transform to reconstruct the three-dimensional atomic density distribution. One way to overcome this limitation is to exploit the direct relationship between the phase of the structure factor and the phase of the X-ray standing wave (XSW) generated by a Bragg reflection from a crystalline substrate. This technique, known as XSW imaging, was first proposed 40 years ago [1], but its application has remained limited due to the demanding experimental requirements involved.

In this study, we demonstrate the potential of XSW imaging to reveal atomic-scale processes and structural transformations on surfaces. As a case study, we investigated bismuthene, a quantum spin Hall insulator prepared by intercalating Bi between a graphene layer and a silicon carbide substrate [2,3]. The electronic, spintronic, and topological properties of the bismuthene layer are discussed in the contribution by N. Tilgner. Here, we focus on the structural properties, in particular on the mechanism driving the reversible phase transition between the bismuthene phase and its topologically trivial precursor phase (the so called ***β*** phase). Using several Bragg reflections, we identified the position of the Bi atoms in both phases and, as a reference, those of the Si and C bulk species in the unit cell of the 4H-SiC crystal. The key finding is that the adsorption site of the Bi atoms changed during the phase transition [2]. This is accompanied by a reorganization of chemical bonds at the interface, resulting in the formation of the distinctive electronic band structure characteristic of two-dimensional bismuthene.

References:

[1] M.J. Bedzyk and G. Materlik, Phys. Rev. B **32**, 6456 (1985).
[2] N. Tilgner et al., 2D Materials **12**, 045020 (2025)
[3] N. Tilgner et al., Nature Commun. **16**, 6171 (2025)

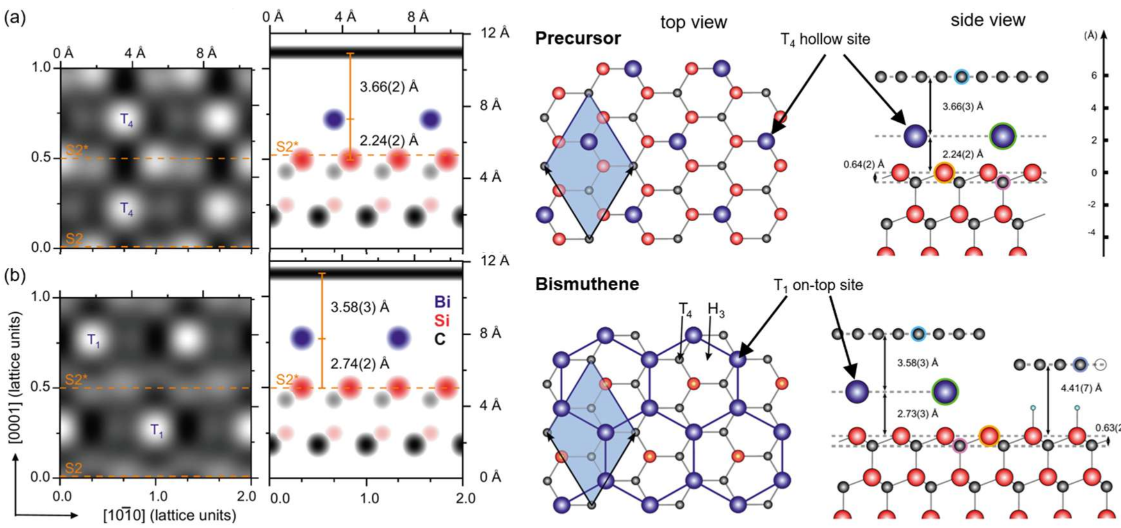

Fig. 1: Atomic densities, as obtained from XSW imaging, and atomic models (top- and side view) for (a) the topologically inactive precursor phase (***β*** phase) and (b) the bismuthene phase.