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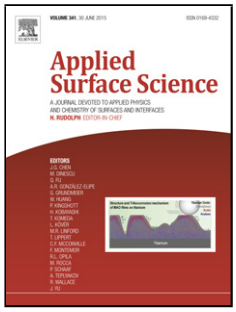

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Authors: F.B. Wiggers, Y. Yamada-Takamura, A.Y. Kovalgin, M.P. de Jong

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Selenidation of epitaxial silicene on ZrB_2

F. B. Wiggers[1,*], Y. Yamada-Takamura[2], A. Y. Kovalgin[1], and M. P. de Jong[1]
[1]*MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands*
[2]*School of Materials Science, Japan Advanced Institute of Science and Technology, Nomi, Ishikawa 923-1292, Japan*
*Correspondence to: F.B.Wiggers@utwente.nl

Highlights

- Deposition of Se on epitaxial silicene results in the formation of $SiSe_x$ species.
- Subsequent annealing leads to the desorption of Se and Si, leaving bare ZrB_2 surface area.
- A novel $ZrB_2(0001)$-$(\sqrt{7}\times3)$R40.9° reconstruction is observed, attributed to a Se-termination.

Abstract
The deposition of elemental Se on epitaxial silicene on ZrB_2 thin films was investigated with synchrotron-based core-level photoelectron spectroscopy and low-energy electron diffraction. The deposition of Se at room temperature caused the appearance of Si 2*p* peaks with chemical shifts of n×0.51±0.04 eV (n = 1-4), suggesting the formation of $SiSe_2$. This shows that capping the silicene monolayer, without affecting its structural and electronic properties, is not possible with Se. The annealing treatments that followed caused the desorption of Se and Si, resulting in the etching of the Si atoms formerly part of the silicene layer, and the formation of bare $ZrB_2(0001)$ surface area. In addition, a $ZrB_2(0001)$-$(\sqrt{7}\times3)$R40.9° surface reconstruction was observed, attributed to a Se-termination of the surface of the transition metal diboride thin film.
Keywords: silicene; ; ; ; , selenium, transition metal diboride, low-energy electron diffraction, photoelectron spectroscopy

Introduction
Silicene is a two-dimensional (2D) material with an atomically buckled, honeycomb lattice of Si atoms.[1] This material is predicted to exhibit charge carriers that behave as massless Dirac fermions,[1] and the quantum spin Hall effect.[2] Due to the relatively weak π-bonds of silicene, the surface is more chemically reactive than that of e.g. graphene. This currently restricts the characterization and processing of epitaxial silicene to vacuum systems that are also capable of *in situ* synthesis, or requires sample transport after synthesis to another system without breaking the vacuum. A capping layer of Se is commonly used for Se-based 2D materials, such as WSe_2 and $MoSe_2$, and can be desorbed again by annealing at 200 °C.[3] This motivated us to investigate Se as a capping layer for epitaxial silicene on ZrB_2 thin films.
In the current work, Se was deposited on epitaxial silicene on $ZrB_2(0001)$ thin films on Si(111) substrates at room temperature, and subsequently annealed up to 600 °C. The chemical composition and ordering of the surface was measured after both deposition and several annealing steps using synchrotron-based high-resolution photoelectron spectroscopy (HR-PES) and low-energy electron diffraction (LEED), respectively.

Experimental
Single-crystalline ZrB_2 epitaxial thin films were grown on Si(111) substrates by ultra-high vacuum chemical vapor epitaxy which is described elsewhere.[4] All subsequent sample preparation steps and measurements were performed at the MatLine beamline of the ASTRID2 synchrotron at the University of Aarhus, Denmark. The endstation consists of a loadlock (base pressure 7×10^{-8} mbar), and an analysis chamber (base pressure 4×10^{-10} mbar) equipped with a Scienta SES200 hemispherical analyzer for HR-PES measurements. Annealing is carried out in the analysis chamber by means of direct e-beam heating on the backside of the sample through a hole in the sample plate, while the