Stabilization of Au Monatomic-High Islands on the (2×2)-Nad Reconstructed Surface of Wurtzite AlN(0001)

Benoit Eydoux\textsuperscript{1,2}, Bulent Baris\textsuperscript{1}, Hassan Khoussa\textsuperscript{1,3}, Olivier Guillermet\textsuperscript{1,2}, Sébastien Gauthier\textsuperscript{1}, Xavier Bouju\textsuperscript{1} and David Martrou\textsuperscript{1}

(1) Centre d'élaboration de matériaux et d'études structurales, CEMES-CNRS, UPR 8011, Nanosciences Group, 29 rue Jeanne Marvig, F-31055 Toulouse, France
(2) Université Toulouse III, UPS, 118 route de Narbonne, F-31062 Toulouse, France
(3) Laboratoire LSMC, Université d’Oran 1 Ahmed Ben Bella, 31100 Oran, Algeria

RHEED spectra and low temperature NC-AFM images demonstrate that Au grows on the AlN(0001) (2×2)-Nad reconstructed surface as large (>100 nm) monolayer islands that form moiré patterns \cite{1}. These experimental data allow us to build atomic models that are used as input for first-principles DFT calculations. These calculations show that the hexagonal Au adlayer interacts locally with the substrate via the acceptor and donor sites existing on the (2×2)-Nad reconstructed surface \cite{2}. These interactions lead to local distortions of the hexagonal layer. Au adsorption is accompanied (i) by a global vertical charge transfer from the AlN substrate, that fulfills the electrostatic stability criterion for a polar surface, (ii) by lateral charge transfers mediated by the reaction of Au with the acceptor and the donor sites of the polar substrate.

The stabilization of the monolayer is the consequence of these two mechanisms that lead to energy gains of electrostatic and chemical origin. This study rationalizes the physico-chemical effects associated with the adsorption of metallic islands on a polar substrate with a nonstoichiometric reconstructed surface and opens routes for the fabrication of metallic pads particularly interesting in the context of molecular electronics. These 2D metallic pads can also be the seeds for the growth of thick 2D gold electrodes. Such electrodes with a controlled metal-semiconductor interface could improve the reliability of the nitride active devices.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{(left) NC AFM image of Au nano-islands on AlN(0001) ; (middle) Atomic resolution NC AFM image obtained at low temperature (5K) showing the moiré pattern formed by the Au monolayer; (right) Superposition of the model calculated by DFT (yellow : Au atom, violet : Al atom, grey : N atom) on the experimental NC-AFM image.}
\end{figure}

References

Corresponding author email: dmartrou@cemes.fr