СЕКЦИЯ 2
РАДИАЦИОННЫЕ ЭФФЕКТЫ В ТВЕРДОМ ТЕЛЕ

SECTION 2
RADIATION EFFECTS IN SOLIDS

ATOMIC-SCALE INVESTIGATION OF HYDROGEN PLATELET DEFECTS IN PROTON-BOMBARDED n-TYPE GaAs USING PROBE-Cs-CORRECTED STEM AND 4D-STEM

Ezra Jacobus Olivier, Johannes Henoch Neethling, Samesh Naidoo
Centre for HRTEM, Physics Department, Nelson Mandela University, Gqeberha, South Africa, jolivier@mandela.ac.za

Probe-Cs-corrected high-angle annular dark-field (HAADF) scanning transmission electron microscopy (STEM) and 4D-STEM ptychography were used to investigate planar defects on {111} planes in high-dose proton-bombarded n-type GaAs. The defects, present at the projected range of implanted 300 keV protons to a total dose of 10^{17} H^+ cm^{-2}, consist of single or double self-interstitial GaAs {111} dislocation loops, but also a newly observed platelet-like planar {111} disruption without a self-interstitial layer. These lower-density zones are proposed to be hydrogen platelet structures, consisting of molecular H_2 agglomerations trapped at tetrahedral interstitial sites. This work explores the use of experimental 4D-STEM phase retrieval techniques to visualise possible H_2 configurations in this new defect.

Keywords: GaAs; proton implantation; hydrogen platelets; STEM; 4D-STEM; ptychography.

Introduction

Gallium arsenide (GaAs), a III-V semiconductor, is widely utilised in high-frequency and optoelectronic devices due to its high electron mobility and direct bandgap. Control over its electrical properties is crucial for device functionality, with hydrogen ion implantation being a versatile method for modifying carrier concentration through dopant and defect passivation [1, 2].

At higher proton doses, defects are observed on {111} planes, forming extended platelet-like structures, in GaAs [3, 4]. Previous STEM studies of proton-bombarded GaAs revealed loop-like defects on {111} planes, consisting of self-interstitial arrangements of GaAs, associated with the presence of hydrogen [5].

Interestingly, single-layer disruptions in the interplanar stacking distance of GaAs {111} planes (Fig. 1), without the presence of self-interstitial layers, have also recently been observed. These observations suggest the possible formation of isolated hydrogen platelet configurations.

Limitations in conventional (S)TEM resolution and contrast have complicated the direct identification of hydrogen within these defects. Recent advances in probe-Cs-corrected STEM and 4D-STEM ptychography now allow for improved structural and chemical characterisation at the atomic scale, making direct identification of hydrogen possible [6, 7].

Experimental

Commercial n-type Si-doped GaAs (carrier concentration ~10^{18} cm^{-3}) was implanted with 300 keV protons at 7° off the [001] axis to minimise channelling, to a total dose of 10^{17} H^+ cm^{-2}. Post-implantation annealing was carried out in a tube furnace under flowing argon. Cross-sectional specimens for STEM analysis were prepared using a Helios Nanolab 650 focused ion beam scanning electron microscope (FIB-SEM). HAADF STEM imaging was performed using a double-Cs-corrected JEOL

ARM 200F operating at 200 kV. 4D-STEM datasets were acquired under optimised microscope conditions for light-element contrast enhancement, guided by image simulations implemented in the ABTEM Python library [8]. The model incorporated hydrogen platelets along {111} planes, enabling the evaluation of phase contrast sensitivity to hydrogen. Experimental 4D-STEM datasets were processed using the Py4DSTEM Python library.

Results

In addition to planar defects consisting of self-interstitial {111} planes, disruptions in the interplanar spacing of the GaAs {111} planes were frequently observed in the absence of self-interstitial layers (Fig. 1). These findings align with established models, where atomic hydrogen diffuses within the GaAs lattice until it is immobilised through recombination into H_2 molecules at defects [9].

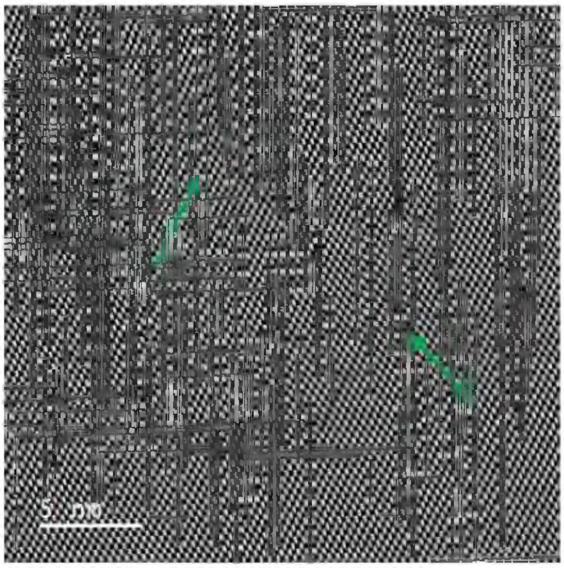

Fig. 1. HAADF STEM images show disruptions in the interplanar stacking distance of GaAs {111} planes

4D-STEM ptychography or annular bright field (ABF) imaging could provide enhanced sensitivity to light-element contrast. Image simulations validated these possibilities, demonstrating the feasibility of detecting hydrogen agglomerations at the atomic scale using this approach (contrast observed at defect core in Fig. 2).

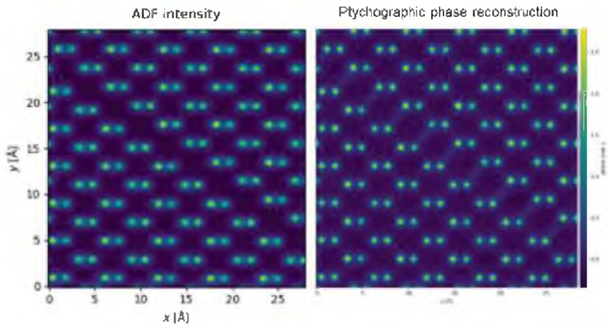

Fig. 2. Simulated annular dark field (ADF) and ptychographic phase reconstructed images of a hydrogen platelet model

Unfortunately, the successful acquisition of experimental 4D-STEM datasets from the proposed hydrogen platelet regions has been complicated due to the likely diffusion of hydrogen from the site of interest when interacting with the electron beam.

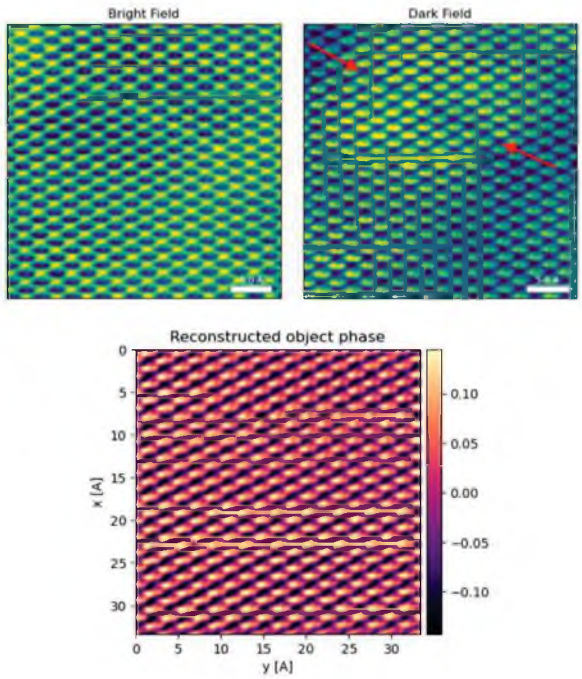

Fig. 3. Reconstructed STEM bright field, dark field and object phase images from an experimental 4D-STEM dataset containing a platelet defect

Discussion

The formation of earlier reported hydrogen-related self-interstitial platelet defects on {111} planes in proton-bombarded GaAs is consistent with earlier reports of hydrogen behaviour in semiconductors [1,3,4]. The adjacent regions of reduced density suggest hydrogen accumulates near interstitial defect planes, in line with theoretical predictions of H_2 stabilisation in tetrahedral sites [9]. It is possible that the observation of platelet configurations at disrupted {111} planes in the GaAs could be an arrangement of such tetrahedrally stabilised H_2 sites viewed in-plane.

Compared to conventional STEM imaging, 4D-STEM ptychography provides a means of visualising the weak scattering features associated with hydrogen, as demonstrated from simulated data obtained from a hydrogen platelet model.

The experimental utilisation of this technique, however, is challenging and will depend on the stability of the defect under the electron beam during data acquisition. Conventional focused probe 4D STEM acquisition of experimental datasets using pixel dwell times down to 40μs and probe currents less than 20 pA failed in capturing the defect structure in its native state.

Conclusions

This study demonstrates the formation of planar defects on {111} planes in proton-bombarded n-type GaAs, different to the previously reported self-interstitial defects. Disruptions in the stacking sequence of {111} planes, without the presence of a self-interstitial layer, are observed. The presence of isolated hydrogen platelet configurations is proposed.

The application of probe-Cs-corrected HAADF STEM and 4D-STEM ptychography, supported by image simulations, enabled atomic-scale study of these defects. These findings contribute to a deeper understanding of hydrogen behaviour in GaAs and demonstrate the utility of advanced electron microscopy techniques for investigating light-element defects.

Future work will explore alternative approaches, such as defocused probe or low-dose ptychography, along with data acquisition at cryogenic temperatures.

References

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