Comparative TEM and HRXRD analyses of strain relaxation in step-graded GaInAs buffer-layers for high-efficiency solar cells

J. Schöne\textsuperscript{a,b}, E. Spiecker\textsuperscript{a}, W. Jäger\textsuperscript{a}, F. Dimroth\textsuperscript{b}, A.W. Bett\textsuperscript{b}

\textsuperscript{a}Faculty of Engineering, Christian-Albrechts-University, Kaiserstrasse 2, 24143 Kiel, Germany
\textsuperscript{b}Fraunhofer Institute for Solar Energy Systems ISE, Heidenhofstrasse 2, 79110 Freiburg, Germany

High resolution X-ray diffraction (HRXRD), especially the method of reciprocal space mapping (RSM), is a powerful tool for measuring strain and strain relaxation in graded buffer layers. On the other hand, transmission electron microscopy (TEM) allows to study individual misfit dislocations and dislocation networks which are the microscopic carriers of strain relaxation. While HRXRD is generally used as a quantitative tool for strain measurement, TEM analyses often remain qualitative in that they do not provide a statistical dislocation analysis. The main reason for this is that standard preparation techniques of cross-section samples do not prove to be suitable to bring out such a high number of dislocations required for a statistical analysis (e.g. figure 1A, left).

By applying the so-called bevel polish preparation method (sample grinding under a small angle of 4°) the buffer interfaces and layers of a GaInP/GaInAs/Ga\textsubscript{1-x}In\textsubscript{x}As/Ge epilayer structure, used for photovoltaic applications [1], are spread. Thus a significant number of 60° misfit dislocations is visible in the TEM micrographs (figure 1A, right), which allows an estimation of the total in-plane strain relaxation due to dislocations within all interfaces of the buffer layer system. Each misfit dislocation with $[\overline{1}10]$ line direction gives a contribution (corresponding to the magnitude of the misfit component of its Burgers vector) to the relaxation in $[\overline{1}0\ 1]$ direction. By evaluating a total number of ~ 150 misfit dislocations in the various interfaces the overall in-plane relaxation for the sample was estimated to 0.5%. This value is significantly lower than the nominal 1.1% mismatch between the Ge substrate and the Ga\textsubscript{0.35}In\textsubscript{0.65}P and Ga\textsubscript{0.83}In\textsubscript{0.17}As top layers indicating that only part of the in-plane strain has been released by dislocations.

By employing HRXRD the strain states of the top layers have been measured. As an example figure 1B shows a RSM of the asymmetric (224) reflection. From the difference $D_{220}$ an in-plane relaxation of 0.85% for the upper layers can be deduced. Assuming that the relaxation is solely caused by 60° misfit dislocations a considerably larger number of dislocations (factor 1.7) is expected in the buffer layer than actually observed. So far the origin of this apparent discrepancy could not be identified. One possibility is that undetected Lomer dislocations which result from the reaction of two 60° misfit dislocations contribute to the strain relaxation. Another possible explanation is that the number of dislocations studied by TEM is still too small to represent the complex dislocation network in the buffer structure. We are currently employing novel methods of bevel-polishing [3,4] which allow to produce TEM samples with even much smaller bevel angles (~
0.1°). The corresponding huge lateral spreading of the structure allows to study hundreds of dislocations in each individual interface.

In summary we have applied the bevel-polish preparation method to a step-graded GaInAs buffer of a high-efficiency solar cell structure. TEM samples prepared by this method allow to analyse the dislocation networks in each individual interface. By measuring dislocation densities the degree of in-plane strain relaxation can be estimated. In order to improve the statistics for a quantitative comparison with HRXRD novel bevel-polish sample preparation techniques have to be employed.

References

Fig. 1: A: TEM bright-field micrographs of a Ga$_{1-x}$In$_x$As/Ge buffer structure from a cross-section sample (left) and from a bevel polished sample (right). In the latter image each individual interface with a large number of dislocations are clearly visible. B: Asymmetric (224) reciprocal space map of the complete solar cell structure. The in-plane strain relaxation can be measured directly from the difference between the in-plane peak positions of the Ge substrate and the upper layers.