

# Non-polar Substrates for III-V-based Solar Cells: Directing dimers of Si(100) and Ge(100) Surfaces in an MOVPE Process Ambient

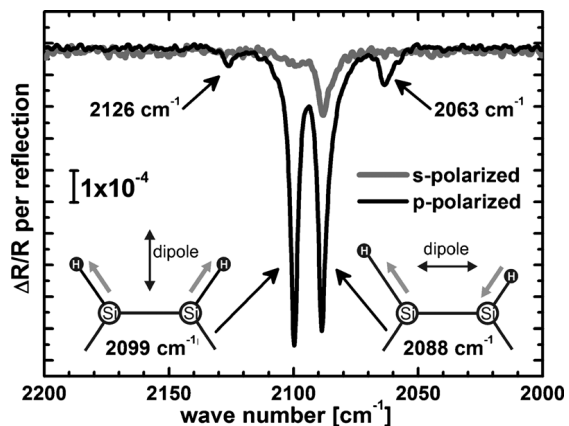
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Nowadays, triple junction solar cells based on Ge(100) show efficiencies significantly over 40%. Despite this outstanding results, the microscopic III-V/Ge(100) nucleation and its interface formation has not been fully understood so far. On the other hand, one of the most promising ways to further reduce the cost of multijunction solar cells is to manufacture them on cheap substrates such as Si(100). An important requirement to achieve low defect densities in the III-V epilayers is a suitable surface preparation of the group IV(100) substrate prior to heteroepitaxy [1]. Only little is known about the Ge and Si(100) surfaces prepared in metal-organic vapor phase epitaxy (MOVPE) ambient regarding its atomic surface structure since access to surface sensitive tools is limited due to the presence of a process gas. We applied in situ reflectance anisotropy spectroscopy (RAS) and benchmarking to ultra-high vacuum (UHV) based surface science to study Ge and Si(100) surfaces during preparation. Our experimental strategy allowed for the analysis of the atomic surface structure of these MOVPE prepared surfaces as well as observation of interactions between H<sub>2</sub> process gas and the substrates in situ.

Absorption lines in Fourier-transform infrared (FTIR) spectra after cooling the samples in H<sub>2</sub> ambient were identified as stretch modes of coupled H-Si-Si-H monohydrides [2] (Fig. 1), in agreement with Si-dimers observed by scanning tunneling microscopy (Fig. 2 inset), or H-Ge-Ge-H, respectively. Tip-induced H-desorption by STM proved the complete saturation of all dangling bonds after VPE-preparation. The polarization dependence of the anti-symmetric stretch mode distinguished different dimer orientations and verified a clear preference for one of the (2x1)/(1x2) surface reconstruction domains. The vicinal Si(100) surfaces exhibit a strong majority surface reconstruction domain as demonstrated by a (2x1) diffraction pattern (Fig. 2, left inset), where most terraces are separated by D<sub>B</sub> type double layer steps as shown by STM (right inset). In situ RAS showed the absence of Si-H bonds at elevated annealing temperature and enabled us to conduct a detailed study of the hydrogen termination process during cooling: Even above 1000 K, the Si(100) surface is mostly terminated by H-Si-Si-H dimers, while stability of Si-H bonds in the process gas ambient requires temperatures well below 750 K. Adjustment of hydrogen coverage employing alternative process gases provides experimental access to hydrogen adsorption and

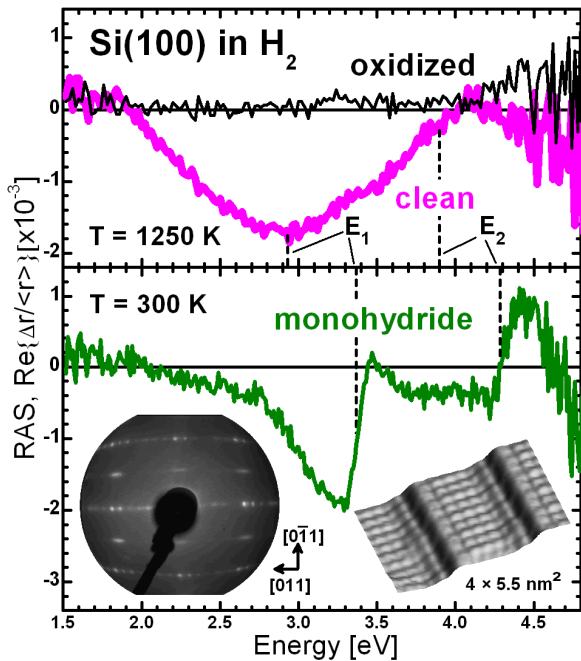
desorption characteristics, valid for annealing procedures in a VPE ambient

Vicinal Ge(100) surfaces feature characteristic RA spectra after preparation in H<sub>2</sub>, whereas the RA spectrum of Ge(100) after cooling in N<sub>2</sub> agrees in line shape with the spectrum of UHV prepared clean Ge(100). According to FTIR measurements, cooling in H<sub>2</sub> leads to a monohydride termination of the Ge(100) surface. Thus, observed differences of our Ge(100) RA spectra after cooling in H<sub>2</sub> and N<sub>2</sub> to UHV results are related to the formation of Germanium hydrogen bonds in case of H<sub>2</sub> as process gas.

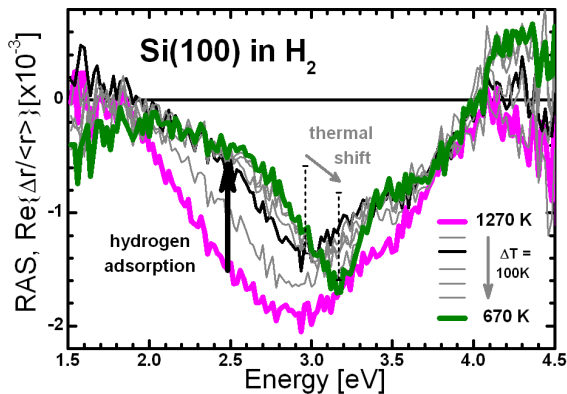


**Fig. 1** FTIR spectra measured in an ATR configuration at H<sub>2</sub> annealed Si(100).

We distinguish characteristic configurations of vicinal Si(100) by in situ RAS (Fig. 2): covered by protective oxides (black line), cleaned by thermal annealing (magenta line), and the formation of monohydrides during cooling (green line) [3], in agreement with RA spectra from UHV based studies of vicinal Si(100) [4]. In situ RAS investigation of vicinal Si(100) while cooling from 1270 to 670 K under H<sub>2</sub> flow (Fig. 3) show the transformation from clean vicinal Si(100) (thick magenta line) to a monohydride termination of the surface (thick green line) [3]. Hydrogen adsorption is accompanied by a decay of signal intensity around 2.5 eV (large arrow) and the formation of a characteristic shoulder around 3.4 eV. The results shown in Fig. 3 clearly suggest a monohydride termination of vicinal Si(100) in the hydrogen-based MOVPE process ambient for annealing temperatures up to more than 1000 K.



**Fig. 2** In situ RAS of vicinal Si(100) and benchmarking to surface science in UHV.

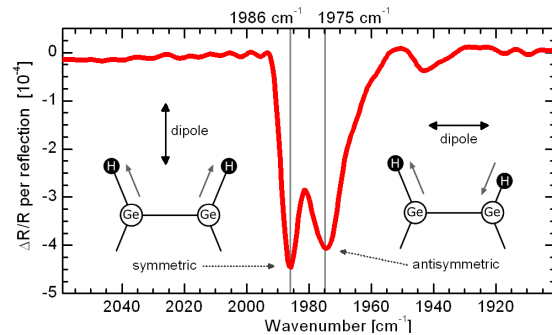


**Fig. 3** In situ RAS of vicinal Si(100) while cooling from 1270 to 670K.

Since UHV investigations showed significant desorption from monohydride terminated Si(100) at 800 K and even below, our in situ observations most probably represent the dynamic balance of hydrogen adsorption and desorption events, which heavily depend on the respective process conditions.

Regarding Ge(100) substrate preparation in MOVPE ambient, we confirmed oxide and carbon removal by hydrogen annealing with XPS and characterized the (2x1)/(1x2) surface reconstruction with LEED. In analogy to vicinal Si(100), LEED and STM showed the formation of a strong majority surface reconstruction domain and a

mainly D<sub>B</sub> stepped surface with dimers oriented parallel to the step edges.



**Fig. 4** FTIR spectra measured in an ATR configuration at H<sub>2</sub> annealed Ge(100).

Similar as shown for Si(100) in Fig. 1, ATR mode FTIR spectroscopy revealed coupled H-Ge-Ge-H stretch modes indicating a monohydride termination of our Ge(100) surfaces after cooling in H<sub>2</sub> ambient (Fig. 4). Confirmation of characteristic in situ RA spectra which distinguish between both surface configurations of Ge(100) allowed dedicated in situ investigations of the hydrogen adsorption and desorption characteristics [5] of the Ge(100) surface and Ge dimer orientation in dependence of temperature, pressure, termination, and process gas in the MOVPE reactor.

In summary, we studied the atomic surface properties of Si(100) and Ge(100) substrates in the hydrogen ambient of a MOVPE reactor, step structures, and dimer orientations. Cooling in H<sub>2</sub> leads to formation of a monohydride terminated surface in both cases. In situ RAS allowed us to observe the hydrogen adsorption and desorption in dependence of different process parameters such as temperature, pressure and process gas. Our results demonstrate in situ access to the interaction of Si(100) and Ge(100) surfaces with hydrogen ambient, which we consider crucial for the development of unique atomic surface structures by MOVPE based processes.

## REFERENCES

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