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Thermal stability and crystallization of magnetron sputtered Si_2C

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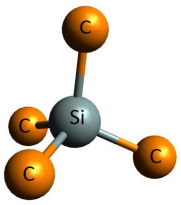
Introduction

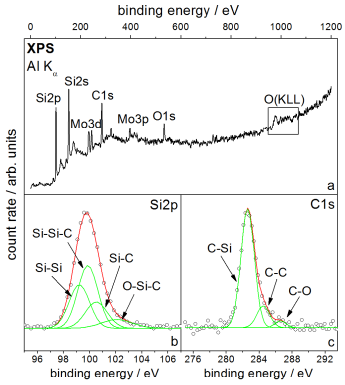
During the last decades amorphous silicon carbide (SiC) has attracted much attention in several fields of scientific research. This wide band gap semiconducting material is associated with several applications ranging from high power, micro- and optoelectronic devices, operations in harsh environmental conditions like high temperature, to utilization in photovoltaic applications such as solar cells. The thermal stability of silicon carbide and its crystallization is of particular interest. In this regard the thermal stability of thin films of amorphous Si_2C deposited by magnetron sputtering on silicon substrates was studied by means of electron spectroscopic (XPS, AES) and microscopic (AFM, SEM, TEM) techniques.



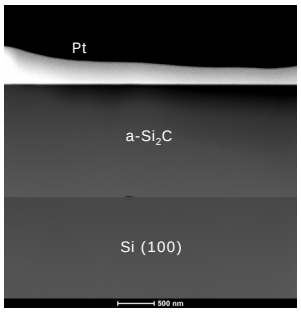
Experimental

Thin amorphous films of silicon carbide (Si_2C) were deposited on single crystalline single silicon (111) wafers (CIS, Germany) by a r. f. cosputtering technique. X-Ray Photoelectron Spectroscopy (XPS) was carried out in an ultra high vacuum apparatus with a base pressure of 5×10^{-11} hPa using the Al K_α line (photon energy 1486.6 eV) . Annealing of the films was performed in-situ inside the Ultra High Vacuum (UHV) using a sample heater based on electron impact heating of the backside of the sample and in an external furnace respectively. The topography of the as-deposited Si_2C and the annealed Si_2C-surfaces is determined by Atomic Force Microscopy (AFM). All measurements are performed in Tapping Mode. Auger Electron Spectroscopy (AES) and Scanning Electron Microscopy (SEM) were carried out in a Scanning Auger Electron Microscope (Omicron NanoSAM). All SEM images were taken with a primary electron energy of 5 keV. AES is performed at an electron energy of 5 keV. Transmission Electron Microscopy (TEM) analyzes were carried out with a FEI Titan 80-300 at the Karlsruhe Nano Micro Facility (Karlsruhe, Germany).

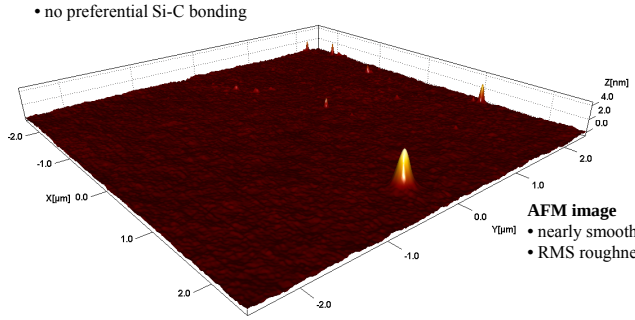
As-deposited Si_2C



XPS survey and detail spectra
- only silicon and carbon are detectable (Mo from sample holder)
- variety of Si and C bonding states, typical for the amorphous phase [1]
- no preferential Si-C bonding



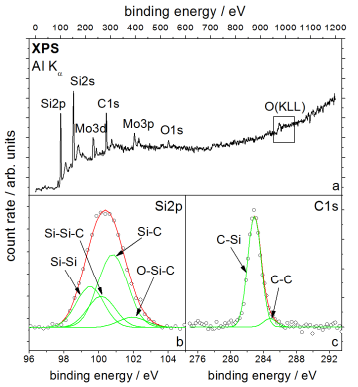
STEM cross section
- the amorphous Si_2C layer and its surface show a smooth structure
- only a small imperfection at the Si_2C/Si(100) transition can be found



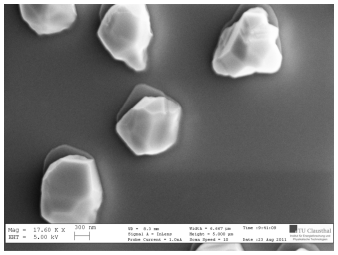
AFM image
- nearly smooth surface
- RMS roughness: 0.5 nm

In addition no crystalline phase could be found with GIXRD

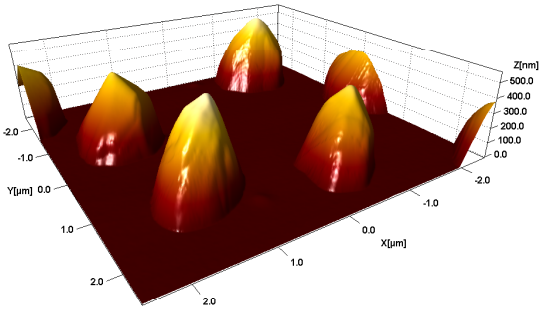
Annealed at 800 °C



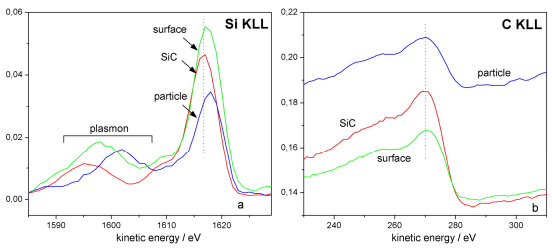
XPS survey and detail spectra
- increasing amount of Si-C bonds
- decreasing of Si-Si and Si-Si-C bonding states



SEM image
- small particles with a distinct faceting and a diameter of 1.1 – 1.5 µm can be found, confirming the findings of AFM

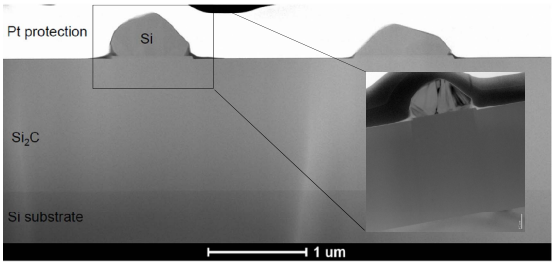


AFM image
- particles of 400 – 600 nm height and 1.4 µm in diameter have formed
- uniformly dispersed over the surface



AES spectra
- the spectra of the particles and the surface in between show differences in peak shape and kinetic energy which can assigned to Si-Si bonds and mixed bonding states, respectively

STEM cross section
- no imperfections in the amorphous layer after annealing
- BF-TEM (inset) show a pronounced faceting of the particles, typical for a crystalline structure



In addition GIXRD revealed the existence of crystallized Si while no SiC has been found

Summary

- magnetron sputtering of Si_2C on Si(100) lead to a homogeneous amorphous film containing a variety of bonding states with major contributions relating to Si-Si and non-stoichiometric Si-Si-C
- thermal annealing at 800 °C is associated with the decomposition of mixed Si-Si-C bonding states and reconstruction of additional Si-C bonds
- simultaneously crystallization of silicon takes place combined with the formation of silicon crystals at the surface, while no silicon carbide has been found

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Literature

[1] K. Mui, W. Smith, Phys. Rev. B **35** (1987), 8080-8088

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Atom- und Molekülphysik an Oberflächen