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Study of the early stages of Cr/6H-SiC(0 0 0 1) interface formation

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Abstract

The early stages of the Cr/6H-SiC(0 0 0 1) interface formation at room temperature were investigated using XPS, LEED and work function (WF) measurements. Upon stepwise Cr evaporation in UHV up to a thickness of 5–10 monolayers (ML) at RT, the binding energy of the XPS Cr $2p_{3/2}$ core level peak shifted from 576.1 eV, at submonolayer coverage, to 574.7 eV (corresponding to metallic Cr) for the final Cr deposit, while the binding energies of the substrate XPS core level peaks remained stable. The WF exhibited a steep decrease of about 0.5 eV from the initial SiC substrate value, upon submonolayer coverage, but then increased gradually to saturation at a value of about 4.8 eV (polycrystalline Cr film with some chemisorbed oxygen). The growth of the ultrathin film was via 3D-cluster formation. The height of the Schottky barrier for the Cr/6H-SiC(0 0 0 1) contact was found by XPS to be 0.5 ± 0.1 eV. The results, generally, indicate the absence of any extended interfacial silicide-like interaction at RT.

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Keywords: Silicon carbide; Chromium; Ohmic metal contacts

1. Introduction

Metal/SiC interfaces are important for high temperature and high power microelectronic devices [1–4] because of the high breakdown field and the wide band gap of SiC. Metal/SiC contact formation at room temperature has been studied for a large number of metals in recent years [5–18]. Cr/SiC is an interesting system for applications in SiC-based integrated-circuit technology; given that the Cr/Si contact was widely investigated in the past for Si semiconductor industry applications [19–26] and that SiC is a very promising material for the same applications area. Although there have been a number of reports on the interfacial reactions between thick Cr films and SiC at high temperatures [27–33], there is none investigating the initial steps of the Cr/SiC interface formation at RT.

In this work, the very early stages of the Cr/6H-SiC(0 0 0 1) interface formation at room temperature were studied by X-ray photoelectron and Auger electron spectroscopy (XPS/XAES), low energy electron diffraction (LEED) and work function (WF) measurements. The height of the interfacial Schottky barrier was obtained from the XPS data.

2. Experimental

All measurements were performed in a conventional ultra high vacuum chamber (base pressure 9×10^{-10} mbar) equipped with a Leybold LHS-12 hemispherical electron energy analyser and a twin-anode X-ray gun for XPS. Photoelectrons were excited using the Al Kα line at 1486.6 eV. A Kelvin probe with a gold-plated vibrating reference electrode (piezoelectrically driven) was used to monitor WF changes. Single crystal 6H-SiC wafers, Si-face, from Cree Research Inc. [34] were used as substrates. The wafers were n-type, nitrogen-doped (3×10^{17} to 3×10^{18} cm^{-3} net doping density) and oriented 3–4° off-axis with respect to the ideal (0 0 0 1) plane towards the [11–20] direction. Before the samples were mounted onto the ultra high vacuum system, they were subjected to standard chemical cleaning to remove the native oxide. In UHV, the specimens were heated up to 1000 K. The substrates exhibited a good 1×1 hexagonal LEED pattern. A small XPS O 1s peak was observed in the XPS spectrum of the as prepared surface of the samples indicating oxygen coverage of about 1/2 ML.

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Chromium was evaporated in UHV from a home-built evaporation source. After a stepwise deposition of chromium at room temperature, the Schottky barrier height was determined from the XPS data. After each deposition step, XPS/XAES and WF measurements were taken. The chromium coverage, in equivalent monolayers, was estimated by calibrating the source doses from the exponential decay of the Si 2p core level peak intensity, assuming a 2D growth at the early deposition stages, thus underestimating the coverage by about 20%. One monolayer (ML) corresponds to an average film thickness of 0.26 nm, or a Cr surface atom density of 2×10^{15} atoms cm^{-2}.

3. Results and discussion

Upon the early stages of Cr deposition at RT, the 1×1 LEED pattern of the initial surface weakened continuously with increasing background intensity and no new spots were observed. Thus at RT no Cr induced superstructures are formed.

Fig. 1 shows the variation of the Cr $2p_{3/2}$/Si 2p peak intensity ratio with Cr coverage for two different samples from the same Si-face 6H-SiC wafer. The solid line corresponds to a layer-by-layer or Frank–van-der Moerve (FM) model and was calculated using attenuation lengths of 1.6 and 1.3 nm for the Si 2p and Cr $2p_{3/2}$ peak energies respectively in Cr [35]. Chromium growth seems to follow a 3D-model after the first monolayer, as the experimental points begin to fall clearly beneath the calculated solid line.

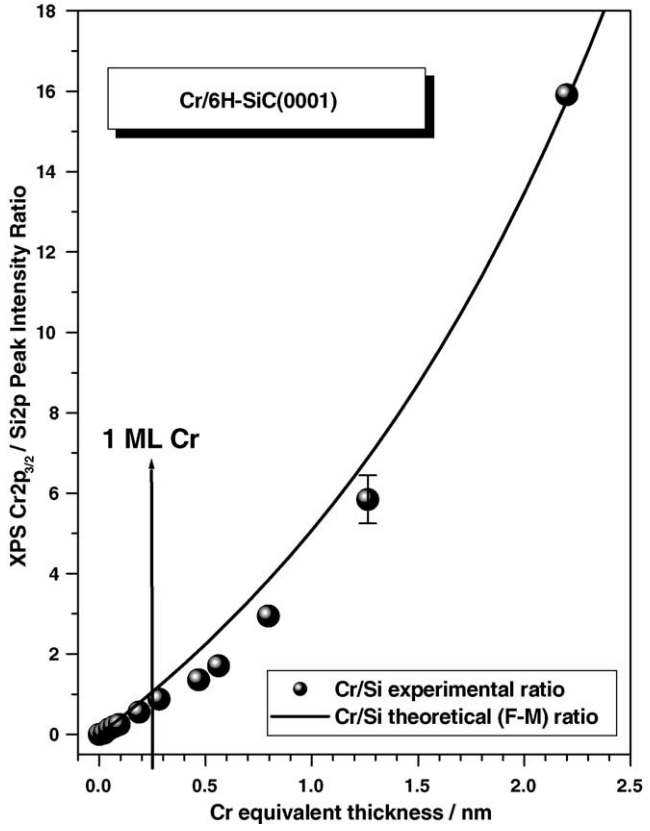

Fig. 1. XPS Intensity ratio of the Cr $2p_{3/2}$ and Si 2p peaks as a function of Cr equivalent thickness, compared with the theoretically calculated layer-by-layer (FM) growth mode curve.

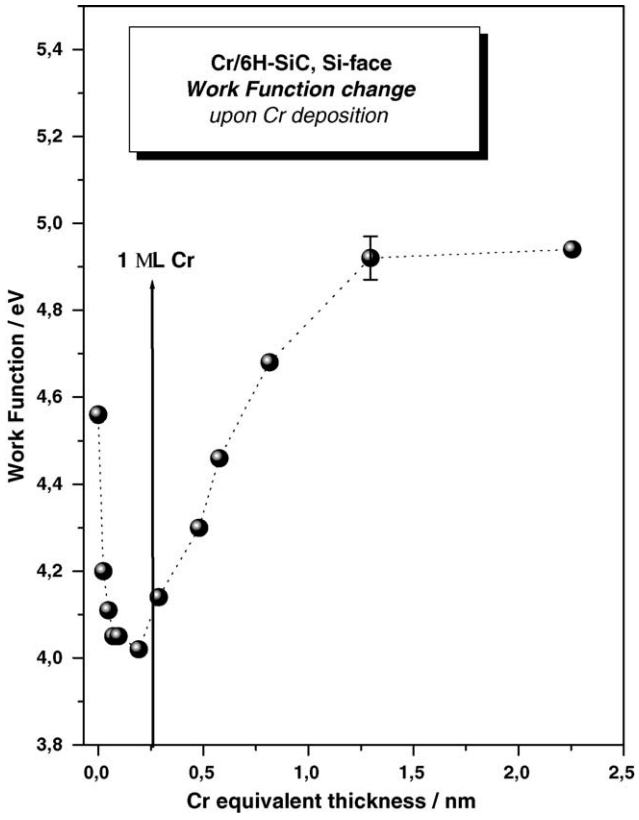

Fig. 2. Change of the WF upon chromium deposition.

The change of the WF upon Cr deposition is shown in Fig. 2. In principle, it can be seen in Fig. 2 that the initial value of the WF is slightly higher than that corresponding to the clean 6H-SiC(0 0 0 1) surface (4.5 ± 0.1 eV) [10,13,18]. This is due to the residual adsorbed oxygen (~1/2 ML) onto the surface during the sample preparation. For submonolayer Cr coverage, the WF decreases from its initial value (~4.55 eV) and reaches a minimum of 4.0 eV at about 0.4 ML Cr. Then, the WF increases gradually to saturation at ~4.9 eV. The initial steep decrease of the WF is partly attributed to Cr-substrate dipoles caused by a small charge transfer upon adsorption of Cr, probably on surface defect sites like steps, as in the case of the Cu/6H-SiC system [18]. In the latter case, the minimum of the WF was obtained for a Cu coverage of ~0.15 ML. Chromium is much more reactive than Cu, so the initial interaction with the substrate extends beyond the steps and probably involves also the adsorbed oxygen. The fact that the WF reaches saturation at a Cr coverage of about 8 ML is consistent with the aforementioned 3D character of chromium film growth. Furthermore, the final WF values are higher by ~0.3 eV than the value from the literature [22,36,37] for polycrystalline Cr films. This is probably due to further oxygen adsorption onto the Cr film surface during the deposition procedure.

Fig. 3 focuses on the binding energy change of the Cr 2p core level doublet at various stages of Cr deposition, as determined from the respective XP spectra. For a coverage of 0.1 ML, the Cr 2p doublet is broad and the BE for Cr $2p_{3/2}$ at ~576.2 eV could be related both to the small particle size of the deposit or to some degree of oxidation. The BE for Cr $2p_{3/2}$ decreased