

Surface Passivation Mechanism of Atomic Layer Deposited Al₂O₃ Films on c-Si Studied by Optical Second-Harmonic Generation

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increased Au deposition. Time-of-flight (TOF) spectroscopy was used to collect charge-resolved spectra of scattered 2 keV ${}^7\text{Li}^+$ and ${}^{39}\text{K}^+$ ions. Spectra collected following small Au depositions display only a sharp single scattering peak, while multiple and plural scattering features are present following larger depositions. The change in spectral shape is indicative of the formation of multilayer nanoclusters. The experimental findings are interpreted with the aid of Monte-Carlo ion scattering simulations. The neutral fraction of scattered K^+ , which provides an indication of the filled quantum states, starts at $\sim 50\%$ for small Au coverages and decreases with further deposition, indicating changes in the quantum state occupancy with cluster size. The lack of any angular dependence to the neutralization implies that the clusters behave as atomic-like structures. Further experiments will investigate how the clusters evolve when deposited onto the substrate by heating to desorb the ASW layer.

11:20am SS1-FrM10 Initial Nucleation and Growth of Oxide Scale on Haynes® 214® Alloy, V. Shuthanandan, S.V.N.T. Kuchibhatla, A.S. Lea, Z. Zhu, M.H. Engelhard, S. Thevuthasan, Pacific Northwest National Laboratory, P. Singh, University of Connecticut, V. Deodshumukh, Haynes International, Inc., H. Ghezelayagh, Fuel Cell Energy, Inc.

A combination of ion beam and electron spectroscopy techniques have been used to precisely understand the initial oxidation of a multicomponent alloy system, Haynes®214®. Surface sensitive nature of these techniques has been rightly exploited to precisely identify different phases formed at different times of oxidation. Haynes® 214® is a high temperature, Ni-Cr-Al-Fe based alloy, widely used in a plethora of applications ranging from “clean firing” of ceramics to the gas turbine industry. Various reports exist in the literature, which describe the long term stability of this alloy under oxidizing environments at temperatures above 900°C. *Despite the number of applications and significant interest in this alloy, a clear mechanism of the early stage oxidation has not been documented.* An effort is underway to estimate the initial nucleation and growth of oxide scale on this alloy in various environments (such as dry and humid air). A combination of ion and electron based techniques such as Rutherford backscattering spectrometry (RBS), nuclear reaction analysis (NRA), particle induced x-ray emission (PIXE), secondary ion mass spectrometry (SIMS) and Auger electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS) were used to measure the initial nucleation of the oxide scale on this alloy. NRA was used to track the oxygen depth profile while PIXE and RBS were used to track the changes in matrix components of the alloy for the formation of oxide scale for as-low-as 1 min of oxidation. Chemical analysis of this early stage of oxidation formation was studied by AES and XPS. Chemical surface mapping obtained from Auger analysis indicated that the initial oxide formed is chromia which is completely dominated by alumina after 7 min of oxidation treatment at 900°C in air. Various merits of this work will be discussed along with possible future scope for using ion beam techniques for processes such as oxidation of metals, a most widely studied problem.

Surface Science

Room: N - Session SS2-FrM

Semiconductor Surfaces and Interfaces II: Si

Moderator: C.L. Hinkle, University of Texas at Dallas

8:20am SS2-FrM1 Observation of Realtime Oxidation of Si(111) Surfaces using Second Harmonic Generation, K. Gundogdu, B. Gokce, E.J. Adles, D.E. Aspnes, North Carolina State University

Realtime material diagnostics during material growth is commonly used in industrial applications. Linear optical methods specifically spectroscopic ellipsometry (SE) probe thin film thickness with a nanometer precision by measuring the change in dielectric susceptibility during material growth. However SE is a spatially averaging technique and therefore can not probe the chemical change at the bond level. In this work we show that second harmonic generation experiments can be used to directly visualize changes in interface and surface bonds in realtime, providing a powerful bond structure characterization tool. We employed SHG experiments to probe the oxidation of hydrogen terminated Si(111) surfaces. We are able to extract the oxidation rates for different bonds on Si(111) surfaces that are nominally flat and with vicinal cut. We found that the initial hydrogen termination process effects the oxidation rate in the bond level. We compare the results of SHG measurements with that of spectroscopic ellipsometry.

8:40am SS2-FrM2 Surface Passivation Mechanism of Atomic Layer Deposited Al_2O_3 Films on *c*-Si Studied by Optical Second-Harmonic Generation, N.M. Terlinden, J.J.H. Gielis, V. Verlaan, G. Dingemans, M.C.M. van de Sanden, W.M.M. Kessels, Eindhoven University of Technology, Netherlands

Recently, it was shown that Al_2O_3 thin films synthesized by (plasma-assisted) atomic layer deposition (ALD) provide excellent surface passivation of *n*, *p* and *p*⁺ type *c*-Si as highly relevant for *c*-Si photovoltaics. It was found that a large negative fixed charge density (up to 10^{13} cm^{-2}) in the Al_2O_3 film plays a key role in the passivation mechanism of Al_2O_3 [1, 2]. The surface passivation quality of Al_2O_3 strongly increases with film thickness before reaching saturation around 10 nm as determined by carrier lifetime spectroscopy. In this contribution a study into the thickness effect will be presented in order to distinguish between the influence of field-effect passivation, *i.e.* electrostatic shielding of charge carriers by the fixed negative charge, and chemical passivation, *i.e.* by a reduction of the interface defect density. To this goal the nonlinear optical technique of second-harmonic generation (SHG) has been utilized. SHG is highly surface and interface specific and allows for the contactless determination of internal electric fields ($\geq 10^5 \text{ V/cm}^{-1}$). Spectroscopic SHG, carried out with a femtosecond Ti:sapphire laser tunable in the 1.33-1.75 eV photon energy range, has revealed a thickness independent electric field for Al_2O_3 films with thicknesses ranging from 2 to 20 nm. This implies that the field-effect passivation is not affected by the film thickness and that the thickness dependence in passivation quality can be attributed to a changing level of chemical passivation. Moreover, this result confirms that the fixed negative charges are located at the Al_2O_3 interface as also indicated by conventional C-V measurements. In addition, SHG shows clear differences between measurements performed on Al_2O_3 films grown by thermal and plasma-assisted ALD. These are likely related to the properties of the interfacial SiO_x induced by either growth process. The presence of this oxide is suggested to be responsible for the chemical passivation quality. Furthermore, the differences indicate a smaller contribution of field-effect passivation for the Al_2O_3 grown with thermal ALD compared to the film from the plasma-assisted process. These results have led to a deeper understanding of the *c*-Si surface passivation by Al_2O_3 as will be discussed.

[1] B. Hoex *et al.* J. Appl. Phys. **104**, 044903 (2008)

[2] J.J.H. Gielis *et al.* J. Appl. Phys. **104**, 073701 (2008)

9:00am SS2-FrM3 Influence of Alkali-Metal Adsorption on Phase Transition of In/Si(111)-4 × 1 Surface, H. Shim, W. Lee, G. Lee, Inha University, Republic of Korea, S. Yu, J. Koo, Korea Research Institute of Standards and Science

One monolayer of In on a Si(111) surface forms 4×1 structure at room temperature (RT). This In/Si(111)-4×1 surface has a quasi- one dimensional (1D) metallic electronic structure and undergoes a symmetry-lowering phase transition into an insulating 8×2 phase at low temperature (LT) upon cooling the sample below approximately 130 K [1]. Adsorption of Na atoms on the surface was reported to convert the 4x1-RT phase into the 8x2-LT phase even at RT [2]. We investigated using low-energy electron diffraction (LEED) the influence of alkali-metals (Na, K, Li) adsorption on the structural phase transition of this quasi-1D In/Si(111) surface. Introducing the alkali metals with low coverage on the surface at room temperature was found to affect the 4×1-to-8×2 structural phase transition by lowering the transition temperature (*T_c*). The *T_c* decreased almost linearly and the transition becomes more rounded when the amount of deposited alkali-metals atoms was increased. The decrease of *T_c* with the increase of the amount of adsorbed Na atoms is suggested to be due to the doping of electrons from adsorbates to the substrate [3]. In the high-coverage regime, new superstructures appear in LEED with the adsorption of alkali metals. Comparison of the adsorbate-induced superstructures in low-coverage and high-coverage regimes will be made and discussed.

[1] H. W. Yeom, *et al.*, Phys. Rev. Lett. **82**, 4898 (1999)

[2] S. S. Lee, *et al.*, Phys. Rev. Lett. **88**, 196401 (2002)

[3] H. Shim, *et al.*, Appl. Rev. Lett. *in press* (2009)

9:20am SS2-FrM4 The First Attachment of Polybutadiene and Functionalized Polybutadiene to Hydrogen-Terminated Silicon, with Post-Derivatization of these Adsorbed Species, E. Nelsen, T. Wickard, Brigham Young University, H. Schlaad, Max Planck Institute of Colloids and Interfaces, Germany, R.C. Davis, M.R. Linford, Brigham Young University

We report the first attachment of polymers with pendant vinyl groups to hydrogen-terminated silicon(111) (Si(111)-H) under mild conditions; 1,2-addition polybutadiene (Mw 3200-3500) in solution was attached to Si(111)-H at room temperature with only visible light activation. We also report the partial functionalization, in solution, of 1,2-addition polybutadiene with various thiols using thiol-click chemistry and the