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Local atomic structures of dissociatively adsorbed NO species on Si(100) below room temperature

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Great interest has been focused on silicon oxynitride due to the improved electrical reliability as well as the resistance to boron peneration compared with silicon oxide. Among various fabrication methods, many processes involve thermal or plasma-assisted reaction of NO. Thus many studies have been subject to the interactions and reactions between NO and the Si(100) surface.

Although there has been a lot of experimental[1] or theoretical[2] investigations on the NO decomposition processes on Si(100) surfaces, there are still debates on various issues concerning the reaction pathway and the intermediate reaction species.

We have employed high resolution photoemission spectroscopy using synchrotron radiation at PAL (8A1) to study the dissociatively adsorbed NO molecules on the Si(100)-2x1 surface at 150 K. N 1s, O 1s, as well as Si 2p core-level spectra were obtained for the series of NO exposures ranging from the very submonolayer regime to the initial saturation coverage. The metastable N species at 396.4 eV and 395.8 eV have been first observed and ascribed to the bonding configurations of $N=(Si-O_x)_2$ and $N=Si_2$ with dangling bonds, respectively. These components were found to disappear upon annealing above 350K suggesting that they are the metastable intermediate reaction species after dissociative NO adsorption. In the O 1s spectra, the major O species (related to $O=Si_2$) at 532.4eV was found to shift toward high binding energies by about 0.4 eV with increasing NO exposures as well as increasing substrate temperatures, which was explained by the changes in bonding configurations induced by oxygen agglomerations. From the above results, it was possible to explain the initial decomposition processes of NO on a single Si dimer, as was proposed in the previous theoretical studies.(2) However, our results suggest that there are more reaction channels than that proposed by theoretical calculations, or the changes of bonding configurations are also accompanied by the dissociation even at 150K.

[References]

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