142bc Adsorption and Dissociation Kinetics of Dichlorosilane on Silicon Surface

Deepthi Gopireddy and Christos G. Takoudis

Dichlorosilane is a widely used precursor for silicon epitaxial growth since it produces higher quality silicon epitaxial layers than silane. For silicon atomic layer epitaxy (ALE), we propose to deposit single epitaxial silicon layers by alternating injections of dichlorosilane (SiH_2Cl_2) and silane (SiH_4) in a reaction chamber at temperatures less than 700 K. This technique will allow for control of atomic layer growth at much lower temperatures (conventional reaction temperature > 1100 K). The surface chemistry of SiH_2Cl_2 adsorption kinetics and the surface coverage play a pivotal role in determining the chemistry of silicon ALE. In this talk we explore the adsorption and the decomposition of SiH_2Cl_2 on silicon surfaces in a hot-walled chemical vapor deposition (CVD) chamber.

The adsorption of SiH_2Cl_2 on silicon (100) surfaces is studied using Auger electron spectroscopy (AES) and X-ray photoelectron spectroscopy (XPS). These surface sensitive analytical techniques are used to identify the chemical bonding states of surface species. Prior to exposing the silicon to SiH_2Cl_2, it is essential to obtain a hydrophobic silicon surface, which is predominantly terminated by Si-H bonds at about 1 monolayer density. Next, the samples were annealed for 6 min in $1X10^{-3}$ vacuum and 700 K temperature to desorb the hydrogen from the Si-H_2 and Si-H surface species to produce silicon dangling bonds at the surface. The AES and XPS spectra of silicon surface following saturation SiH_2Cl_2 exposures at different temperatures reveal the presence of primarily dichloride (Si-Cl_2) surface species. The stability of these surface species is examined as a function of the annealing time and temperature. The spectral changes indicate that the dichloride species are converted to monochloride species with increase in annealing temperature and time.

In an effort to support the experimental results, we modeled SiH_2Cl_2 adsorption and decomposition kinetics using first principle electronic structure computations and density functional theory. The transition states and reaction pathways are computed for possible reactions. A comparison of the reaction energies of different mechanisms reveals lowest energy of reaction for adsorbed dichloride species on the surface. Furthermore, the investigations show that on annealing the dichloride species are converted to monochloride species by Si-Cl bond breakage.

The experimental coupled with theoretical studies reveal the diclorosilane adsorption and desorption pathways on silicon surfaces. The amount of the dichloride molecules adsorbed on the surface plays a critical role in determining the growth of the silicon layer using ALE. This will help clarify the mechanism of silicon ALE when DCS and silane are used as precursors.