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Reactivity of the H–Si (111) surface

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Abstract

The H–Si (111) surface has been well characterized [Hricovini et al., Phys. Rev. Lett. 70 (1993) 1992], so the reactivity of this surface was studied. H–Si (111) surfaces exposed to Cl_2, Br_2, and 1-alkenes were studied with photoemission spectroscopy. These particular compounds were chosen because of their importance in semiconductor processing and surface functionalization. The observation of the growth of a Si 2p component at high binding energy, characteristic of halogen reactivity, confirmed that bromine and chlorine gases both reacted with the H–Si (111) surface. Reactions with 1-alkenes were confirmed by measuring both the Si 2p and the C 1s core level spectra. The C 2s-based molecular orbitals in the valence band revealed the identity of the alkyl monolayer on the Si (111) surface. Therefore, we found that the H–Si (111) surface, under certain conditions, was reactive.

1. Introduction

A standard method for preparing silicon surfaces used HF etching to remove native oxide layers and to protect the surface from chemical attack. However, HF etching left the surface atomically rough. Due to the surface roughness, mono, di and trihydride species were present [1,2]. Recently, a method for preparing ideal H-terminated Si (111) surfaces by chemically etching in aqueous NH_4F solutions was developed [1,2]. Infra-red spectroscopy has shown that this surface was terminated entirely by the monohydride and was flat on an atomic scale [1,2]. A high-resolution photoemission study of this surface showed that the Si 2p core level was very narrow, with a total linewidth of 0.160 eV, and that narrow features related to Si–H existed in the valence band [3]. These features in the core level and valence band spectra were much narrower than those for H–Si (111) prepared by H exposure in vacuum [4]. The discovery of this ideal H-terminated surface has opened up many possible avenues of study.

The most important area of study was in the area of chemical reactions of the H-terminated Si (111) surface. Chemical reactions with O_2, Cl_2, Br_2, and 1-alkenes were investigated. Higashi

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