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Hydrogen Absorption by Crystalline Semiconductors: Si(100), (110) and (111)

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Gas-phase hydrogen atoms create a variety of chemical and physical phenomena on Si surfaces: adsorption, abstraction of pre-adsorbed H, Si etching, Si amorphization, and penetration into the bulk lattice. Thermal desorption/evolution analyses exhibited three distinct peaks, including one from the crystalline bulk. It was previously found that thermal-energy gaseous H(g) atoms penetrate into the Si(100) crystalline bulk within a narrow substrate temperature window(centered at ～460K) and remain trapped in the bulk lattice before evolving out at a temperature as high as ～900K. Developing and sustaining atomic-scale surface roughness, by H-induced silicon etching, is a prerequisite for H absorption and determines the T_s windows. Issues on the H(g) absorption to be further clarified are: (1) the role of the detailed atomic surface structure, together with other experimental conditions, (2) the particular physical lattice sites occupied by, and (3) the chemical nature of, absorbed H(g) atoms. This work has investigated and compared the thermal H(g) atom absorptivity of Si(100), Si(111) and Si(110) samples in detail by using the temperature programmed desorption mass spectrometry (TPD-MS). Due to the differences in the atomic structures of, and in the facility of creating atom-scale etch pits on, Si(100), (100) and (110) surfaces, the H-absorption efficiency was found to be larger in the order of Si(100) > Si(111) > Si(110) with a relative ratio of 1 : 0.22 : 0.045. This intriguing result was interpreted in terms of the atomic-scale surface roughening and kinetic competition among H(g) adsorption, H(a)-by-H(g) abstraction, SiH_3(a)-by-H(g) etching, and H(g) penetraion into the crystalline silicon bulk.