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Bulk and Surface Reactions of Atomic H with Crystalline Si(100)

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Si(100) surfaces were exposed to gas-phase thermal-energy hydrogen atoms, H(g). We find that thermal H(g) atoms etch, amorphize, or penetrate into the crystalline silicon substrate, depending on the employed T_s range during the H(g) exposure. We find that etching is enhanced as T_s is lowered in the 300 - 700 K range, while amorphous silicon hydride (*a*-Si:H) formation dominates at a T_s below 300 K. This result was well explained by the fact that formation of the etching precursor, SiH_x(a), and amorphization are both facilitated by a lower T_s, whereas the final step for etching, SiH_3(a) + H(g) → SiH_4(g), is suppressed at a lower T_s. We also find that direct absorption of H(g) by the crystalline bulk of Si(100) substrate occurs within a narrow T_s window of 420 - 530 K. The bulk-absorbed hydrogen evolved out molecularly from Si(100) at a T_s 80 - 120 K higher than that for surface monohydride phase (β_1) in temperature-programmed desorption. This bulk-phase H uptake increased with increasing H(g) exposure without saturation within our experimental limits. Direct absorption of H(g) into the bulk lattice occurs only when the surface is atomically roughened by surface etching. While pre-adsorbed hydrogen atoms on the surface, H(a), were readily abstracted and replaced by D(g), the H atoms previously absorbed in the crystalline bulk were also nearly all depleted, albeit at a much lower rate, by a subsequent D(g) exposure at a fixed exposure T_s. Implications of the evolution of isotopically scrambled HD(g) at the peak temperature in TPD from the substrate sequentially treated with H(g) and D(g), together with a gas phase-like H_2 Raman frequency of 4160 cm^{-1}, will be presented.