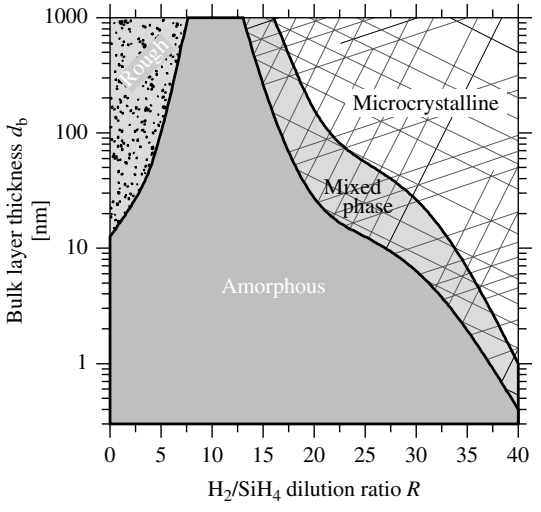

Figure 12.13 Phase diagram for the structure of plasma-deposited silicon thin films for varying dilution ratios R of silane in hydrogen and film thickness d_b; thin films were deposited onto a single-crystal Si substrate. For lower dilutions ($R < 10$) the films remain amorphous, but undergo a roughening transition in thicker films. For high dilutions, films start out as amorphous, develop and silicon crystallites, and ultimately become entirely microcrystalline. Based upon the phase diagram proposed by Ferlauto *et al*. [115] on the basis of *in situ* spectroscopic ellipsometry measurements

growing thin film first adopts an amorphous structure. As the film thickens, crystallites form in the amorphous matrix (creating a "mixed phase"). Ultimately, the film becomes entirely microcrystalline. The details of the phase diagram do depend upon the details of deposition, in particular upon power and substrate conditions, but the structure of the phase diagram is thought to be universal.

These effects of hydrogen dilution during growth are likely owing to the following effects. (1) Atomic hydrogen "etches" a growing film, removing strained weaker bonds that are in energetically unfavorable locations; (2) a high flux of atomic hydrogen promotes the surface diffusivity of adatoms so that they can move around to more energetically stable positions and form stronger bonds; (3) atomic hydrogen diffuses into the network, restructuring it and promoting a more stable structure. For the same reasons, sufficiently large hydrogen dilution induces the formation of microcrystalline Si. The enhancement of short-range and long-range order through hydrogen dilution has been observed in many deposition techniques, including PECVD (DC, RF, VHF, and MW) and HW CVD; of course, the transitions from amorphous to microcrystalline structures occur at different dilution levels for different deposition techniques. There is evidence that the more stable amorphous silicon is deposited under the conditions that are close to the microcrystalline formation [116].

The hydrogen dilution level for the transition from amorphous to microcrystalline silicon thin films depends on other deposition conditions as well. At higher substrate temperatures (above 300°C), the transition from amorphous to microcrystalline state occurs at a higher H dilution; this effect is likely to be due to the low sticking coefficient