Low-temperature epitaxial growth of SiGe thin film on silicon substrate by Reactive Thermal CVD

As shown in Fig. s1, Si_2H_6 , GeF_4 and He are used as source gases, in which, GeF_4 is selected as the Ge source material and Si_2H_6 is used as the reductant gas. He is the carrier gas. The redox reaction between Si_2H_6 and GeF_4 will happen when they arrive at the silicon substrate, and Ge layer incorporated with some Si atoms will be deposited on the substrate. This deposition exhibits selective growth characteristics. The rate of the redox reaction is mainly controlled by the gas flow ratio between Si_2H_6 and GeF_4 , the gas pressure and the substrate temperature. Here, the redox reaction can only take place when the substrate temperature reaches a certain value (the optimum value locates in between $300 \sim 375^{\circ}$ C). If the substrate temperature is lower than this threshold, no film can be grown. On the other hand, if the substrate is much higher than this threshold (e.g. 400°C), pyrolysis of Si_2H_6 will happen. In this case, the selective growth will be suppressed and many silicon atoms will incorporate into the film, resulting in a poor crystalline quality.



Fig. s1 (a)the skech map of Reactive Thermal CVD and (b) the redox reaction between Si_2H_6 and GeF_4

During the redox reaction, Si_2H_6 is oxidized into SiH_nF_m or SiF_4 , and GeF_4 is reduced into GeF_2 . In this reaction system, GeF4 shows three important characters: firstly, it reacts with Si2H6, and contributes to the deposition of Ge, as shown in Fig. s2. Secondly, it can react with silicon atoms which incorporates into the film surface, as a result, Si is substituted by Ge and the component of Si in the epilayer decreases. Thirdly, GeF₄ can react with Ge atoms and generated GeF₂, which can easily move away from the growth surface. During this process, the weak bonds between atoms are broken and atoms re-structure on the surface, which can suppress the three-dimensional growth and promote the structural relaxation of the film network. The latter two surface chemical reactions can assist the improvement of film quality.



Fig. s2 the schematic drawing for the epitaxial growth mechanism of RTCVD