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Intrinsic Stress and Misfit Relaxation Ge/Si(001)

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1. Introduction

Ge films on Si substrates are promising candidates for the fabrication of Si-based optoelectronic devices (e.g. strained-layer superlattices or uniform quantum-dot arrays). On Si(001) film growth proceeds by SK (Stranski-Krastanov) mode, i.e. 3D islands nucleate on top of a several ML (monolayer) thick wetting layer. Whereas at temperatures below 800 K the initial 3D islands preferentially are small square pyramids of uniform size distribution ('hut'-clusters') [1, 2], at higher temperatures larger ('macroscopic') islands with more complex facet structures are formed [3]. In view of the large misfit of about 4.1 %, which corresponds to compressive misfit stress of −6.0 GPa, it is interesting that the 3D islands of Ge are dislocation-free up to lateral dimensions as large as 100 nm [3]. According to current theory [4] and confirmed recently by x-ray diffraction [5] the 3D islands partially relax the misfit strain by lattice expansion in upper layers.

Here we present in situ intrinsic stress measurements of the SK system Ge/Si(001) up to the film thicknesses at which the 3D islands percolate. Confirmed by the structural results of AFM (atomic force microscopy) and LEED (low energy electron diffraction) direct information on onset and thickness range as well as the strain relief of the three growth stages of SK mode [(i) pseudomorphic layer-by-layer stage, (ii) nucleation and growth and (iii) coalescence of 3D islands] is obtained.

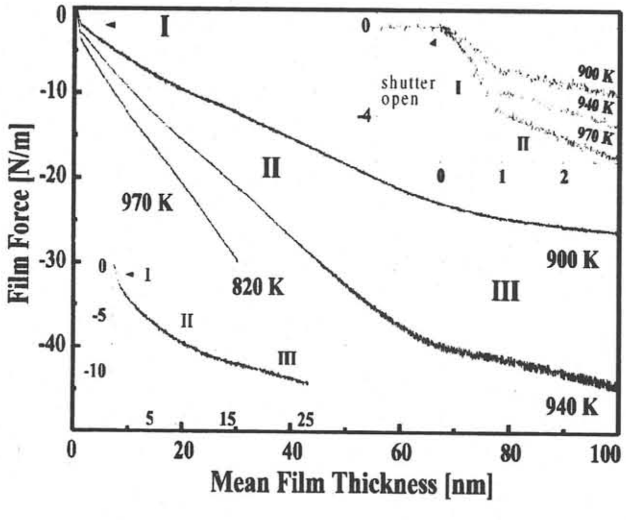

FIG. 1: Representative examples of the film forces (see text) of Ge/Si(001) vs. average mean film thickness. Bends in the force curves separate different stages of SK growth: I wetting layer, II nucleation and growth, III coalescence of 3D islands. In the upper right insert the signal recorded before the Ge deposition is plotted on the same time scale.

2. Experimental

The experiments were performed in a UHV chamber with base pressure better than 1×10^{-10} mbar. It is equipped with a cantilever beam device for measuring the intrinsic film stress continuously during film deposition and a four-grid LEED optics for in situ control of the epitaxial film quality [6]. Ge was evaporated out of boron nitride crucibles at deposition rates of 0.008 ± 0.002 nm/s and pressures better than 2×10^{-9} mbar. The Si(001) substrates were carefully outgassed at 1000 K for several hours and heated to 1150 K for 30 minutes in order to remove the oxide; sharp LEED patterns of Si(001)(1x2) were routiney obtained. The absolute substrate temperature which was controlled by a reference thermocouple is accurate within ±30 K, but the relative error is considerably smaller (±5 K). The AFM investigations of the Ge films were performed in air in the contact mode.

3. Results

Fig. 1 summarizes the intrinsic stress results of Ge/Si(001) at deposition temperatures of 700 − 1050 K. The film forces plotted in Fig. 1 as a function of the average Ge thickness t_{Ge}, represent the integral force F_{tot} acting in films of unit width. The slope of the force curves F_{tot} *vs.* t_{Ge} correspondingly yields the instantaneous film stress ($\partial F_{tot}/\partial t_{Ge}$). Each of the force curves of Fig. 1 clearly reveals three different regimes, which are characterized by declining slopes, i.e. incremental stress values, which can be directly related to the three growth stages of SK mode:

Stress-Regime I coincides with the pseudomorphic layer-by-layer stage. The film stress is dominated by the misfit and assumes values between −2.8 and −5.8 GPa, which are of the same order of magnitude as the bulk misfit stress of −6.0 GPa. The deviations at lower temperatures, which definitely are beyond experimental error (≈10%), indicate partial strain relief already in the wetting layer.

Stress-Regime II: When 3D islanding sets in, a sharp bend of the force curves to considerably smaller incremental stress values of 0.4 − 1.7 GPa is observed. AFM investigation of Ge films of regime II indeed reveals 3D islands with a narrow size distribution. Examples of 25 nm and 40 nm thick Ge films deposited at 875 K and 970 K, respectively are shown in Figs. 2a and b. Individual islands still are isolated from each other, which is confirmed by respective single scans (e.g. of Figs. 2a and b) revealing height levels parallel to the Ge wetting layer between neighboring islands. With increasing deposition temperature the density of islands decreases, whereas their dimensions increase; at 970 K the average island size is about 1 µm.

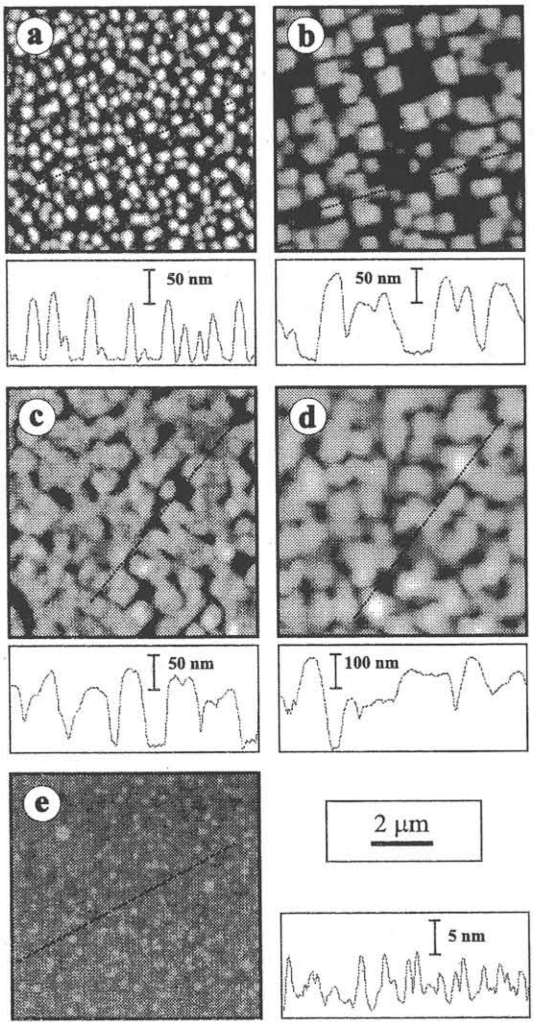

FIG. 2: AFM images of Ge/Si(001): a) 875 K, t_{Ge} = 25 nm, b) 970 K, 40 nm, c) 940 K, 55 nm, d) 940 K, 200 nm, e) 790 K, 25 nm. The height profiles are taken in [100] direction along the dashed lines marked in the topviews.

Furthermore the island shapes become more and more regular, at 970 K mainly square truncated pyramids with sides parallel to [100] and [010] have formed. Quantitative evaluation of the AFM images reveals predominately angles of ≈20° with respect to (001) indicating the preferred formation of {103} facets in agreement with LEED. In accordance with previous studies [4, 5] the 3D islanding is accompanied by a partial relief of the misfit strain. The decrease of the incremental stress of regime II at higher thicknesses indicates the incorporation of misfit dislocations by larger islands (see also [3, 7]). .

Stress-Regime III is characterized by a further reduction of the incremental stress to values of 0.10 – 0.17 GPa. The additional strain-relief is observed when the 3D islands of the SK films merge. AFM images of Ge films with thicknesses near the second bend of the force curves (e.g. Fig. 2c) reveal a morphology typical for island growth close to percolation. Coalescence of neighboring islands is also confirmed by arbitrary single scans that no longer include the height level of the continuous Ge layer (Fig. 2c). At this growth stage the strain is further relieved by misfit dislocations in agreement with recent TEM (transmission electron microscopy) studies [7]. Obviously the formation of misfit dislocations is facilitated by the coalescence of relaxed epitaxial islands as the boundary provides energetically favorable sites for the insertion or omission of extended atomic rows (i.e. dislocations). On further growth the thickness of the continuous layer increases (Fig. 2d). Notice that at 800 K regime III is reached at thickness values lower than 10 nm (Fig. 1b) leading to a rather flat continuous film at 25 nm (Fig. 2e).

4. Conclusions

Our experimental results on the strained SK system Ge/Si(001) nicely demonstrate that – as indicated already by previous studies – the relief of misfit-strain proceeds mainly in two steps, namely upon (i) formation and (ii) growth and coalescence of 3D islands. Ge films of regime III have relaxed more than 97 percent of the theoretical misfit stress. It is noteworthy that the strain-relief by the 'hut-clusters', which preferentially are formed below 800 K [1], is less efficient than by the macroscopic islands. Moreover our stress measurements reveal that the maximum strain-relief by 3D islanding at deposition temperatures of about 900 K. This finding, i.e. decreasing strain-relief at higher temperatures, is in contradiction to a plain energetic model, thus pointing to a kinetic pathway for the 3D islanding of Ge/Si(001) [8].

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