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Influence of (7 × 7)–"1 × 1" phase transition on step-free area formation in molecular beam epitaxial growth of Si on Si (111)

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ABSTRACT

The step-flow growth condition of Si on Si (111) near the (7 × 7)–"1 × 1" surface phase transition temperature T_C is analysed within the framework of Burton–Cabrera–Frank theory. In particular, coexistence of both surface phases well below T_C and their specific influence on the step-flow growth behaviour is considered. We presume that under dynamical condition of growth, the surface initially covered by only the (7 × 7) phase separates into domains surrounded by "1 × 1" areas. On such a surface, the overall supersaturation should be reduced drastically compared to a surface with only (7 × 7), resulting in much larger critical terrace width for nucleation.

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1. Introduction

The Si (111) surface exhibits a surface phase transition from (7 × 7) to disordered "1 × 1" surface structure at a temperature $T_C \approx 1100$ K. Recently, we investigated the development of surface morphology in Si molecular beam epitaxy (MBE) on mesa-structured Si (111) surfaces near T_C [1]. For a small increase in T, significant changes in surface morphology were found, accompanied by a strong increase in step-free area dimension (Fig.1), what has not been reported so far.

Therefore, a deeper understanding of the unusual observation is needed. In our earlier studies, the coexistence of "1 × 1" and (7 × 7) surfaces under certain growth conditions and their specific influence on the growth behaviour was already discussed in such a context [1]. Here, we present a more quantitative interpretation to support this prediction using a simple step-flow growth model and data known from the literature. The results show that indeed under dynamical condition of growth the coexistence of both surface phases well below 1100 K could explain our experimental findings.

2. Results and discussion

At $T < T_C$, the 7 × 7 surface phase exhibits a smaller surface energy than the "1 × 1" surface. However, long range order elastic and electrostatic interactions of surface structure domains allow the coexistence of (7 × 7) and "1 × 1" domains over an extended T-range around T_C [2]. Thereby, the size of the domains is dependent on T and the rate of T changes. Moreover, area fraction of the two surface phase domains was found to be also strongly dependent on the terrace width. Triangular domains with up to 1 μm side length were observed on terraces > 4 μm [3]. The size of domains for a given T is determined by the difference in surface free energy $\Delta\gamma$ between the 7 × 7 and "1 × 1" surface phase, where the T-dependence of $\Delta\gamma$ is determined by the entropy difference ΔS between both phases and can be expressed near T_c by: $\Delta\gamma = (T - T_C)\Delta S$, with $\Delta S = 0.013 k_b$ (k_b - Boltzmann constant) [3].

Further studies show, that surface supersaturation has also a strong impact on the formation and extension of surface phases. Hannon et al. found that near T_C the size of individual (7 × 7) domains within a "1 × 1" surface matrix decreases under the presence of an external Si flux [4]. The external Si flux results in a supersaturation of adatom concentration n with respect to the equilibrium mobile adatom density (n_{eq}) at the surface, giving rise to an adatom chemical potential $\Delta\mu = k_b T \times \ln(n/n_{eq})$. They pointed out that the energy cost of (7 × 7) domain formation relative to the uniform "1 × 1" phase with higher n_{eq} has to be modified by the energy associated with the transfer of excess adatom density to the surrounding "1 × 1" area on the terrace. This energy is expressed by: $\Delta\mu \times (n_{\text{"1 × 1"}} - n_{7\times7}) = \Delta\mu \times \Delta n$, [4] where $n_{\text{"1 × 1"}}$ and $n_{7\times7}$ are the n_{eq} values of the "1 × 1" and (7 × 7) phase, respectively. From STM investigations $n_{\text{"1 × 1"}} \approx 0.2$ monolayer's (ML) and $n_{7\times7} \approx 0.08$ ML were obtained, [5] which results in an excess mobile adatom density of $\Delta n \approx 0.12$ ML (1 ML = 7.83×10^{14} atoms/cm^2). This effect changes the surface free energy $\Delta\gamma$ by $\Delta\mu \times \Delta n$, which makes the "1 × 1" phase more favourable than the (7 × 7) phase (Fig. 2). Consequently, phase transition is shifted by $\Delta T = T_C' - T_C$ to lower T. Assuming no change of γ around T_C, ΔT can be roughly estimated by $\Delta T = -(\Delta n \times \Delta\mu)/\Delta S$ [4].

Hannon et al. estimated $\Delta T = -3$ K for a Si flux of 4.4×10^{12} atoms/cm^2 s, which corresponds to $\Delta\mu = 2 \times 10^{-4}$ on a

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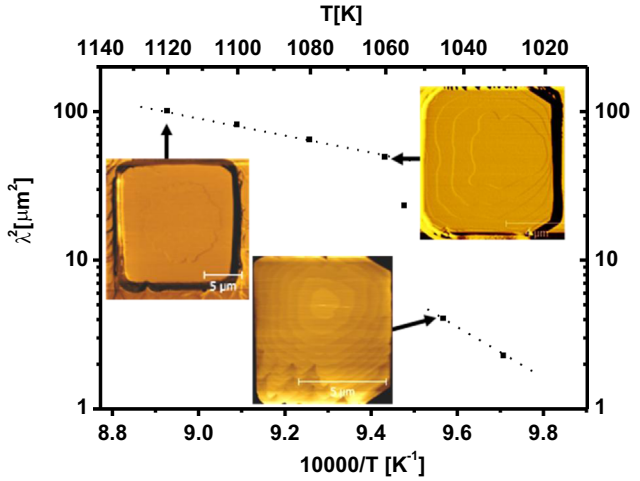

Fig. 1. Summarised data of step-free areas (λ^2) (λ – step-free terrace width) as a function of temperature (T) (Arrhenius graph), with corresponding AFM images of the mesa surfaces.

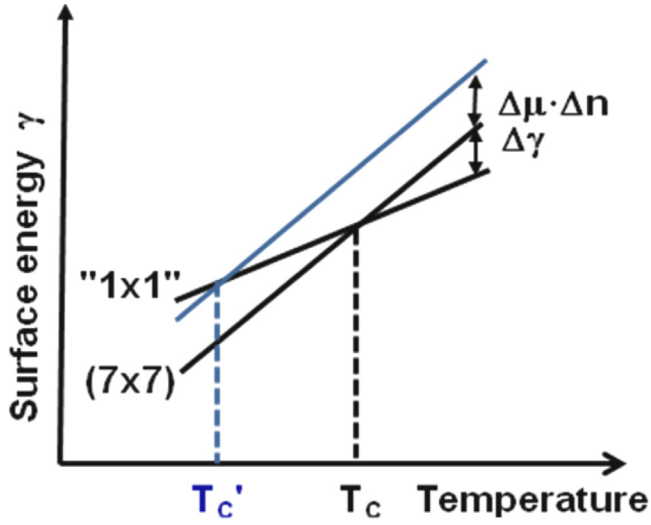

Fig. 2. Schematic illustration of the change in surface energy of the "1×1" and 7×7 phase at T around T_C and the shift in T_C due to the energy associated with the transfer of excess adatom density ($\Delta\mu\times\Delta n$).

2 μm wide terrace [4]. They also suggested already that typical growth rates used in semiconductor epitaxy lead to a more significant change in T_C. In our experiments, we use a Si flux of about 4×10^{13} atoms/cm^2 s, which results in a change in T_C by at least 30 K considering the same terrace width. Moreover, $\Delta\mu$ becomes larger on wider terraces, which consequently could result in a further increase in "1×1" domains or shrinking of (7×7) domains, respectively. Since we observed the (7×7)–"1×1"phase transition at 1100 K under static conditions, a significant amount of "1×1" domains could be present already at $T\leq1070$ K under the dynamical conditions of growth in our experiments. This is the T-range, where we observed a drastic change in surface morphology and a strong increase in step-free areas.

The supersaturation is determined by the ratio of the actual density of mobile adatoms at the surface to n_{eq}. Following the work of Burton, Cabrera and Frank (BCF) [6], the adatom density n on a terrace is governed by the diffusion equation. The diffusion equation in the steady state regime valid for complete condensation, fast attachment–detachment kinetics as well as slow moving straight steps in x-direction scan can be written in a form

$$D\frac{d^2n(x)}{dx^2}+R=0 \tag{1}$$

with D is the diffusion coefficient, and R is the rate of atom flux towards the surface. The assumption of complete condensation is justified in view of the very low desorption rate (between 10^8 and 10^{10} atoms/cm^2 s^1 [7]) at T used in our experiments compared to the deposition rate (10^{13} atoms/cm^2 s^1). Furthermore, it has been shown that surface mass transport on Si (111) is governed by diffusion of adatoms on terraces rather than attachment/detachment of atoms at steps within the T-range of our investigation [8]. Therefore, it can be suggested that $n(x)$ at the step edges is equal to n_{eq}: $n(0)=n(\lambda)=n_{eq}$. Introducing the dimensionless terrace width $X=x/\lambda$, solution of Eq. (1) is

$$\frac{n(x)}{n_{eq}}=1+\frac{R\times\lambda^2}{2D\times n_{eq}}X-\frac{R\times\lambda^2}{2D\times n_{eq}}X^2 \tag{2}$$

where $D\times n_{eq}$ represents the so-called mass diffusion constant. The corresponding supersaturation $\Delta\mu$, i.e. the adatom chemical potential, is given by

$$\Delta\mu=k_bT\times\ln\left[\frac{n(x)}{n_{eq}}\right]=k_bT\times\ln\left[1+\frac{R\times\lambda^2}{2D\times n_{eq}}X-\frac{R\times\lambda^2}{2D\times n_{eq}}X^2\right] \tag{3}$$

Midway the steps ($\lambda/2$), $\Delta\mu$ reaches its maximum value with

$$\Delta\mu=k_bT\times\ln\left[\frac{n(\lambda/2)}{n_{eq}}\right]=k_bT\times\ln\left[1+\frac{R\times\lambda^2}{4D\times n_{eq}}-\frac{R\times\lambda^2}{8D\times n_{eq}}\right]=k_bT\times\ln\left[1+\frac{R\times\lambda^2}{8D\times n_{eq}}\right] \tag{4}$$

or with simplification for small $\Delta\mu$

$$\Delta\mu=k_bT\times\frac{R\times\lambda^2}{8D\times n_{eq}} \tag{5}$$

Values in the range from $D\times n_{eq}=10^7$–10^8 s^{-1}were reported for the "1×1" surface [9,10]. In our analysis, we use a value of $D\times n_{eq}=8\times10^7$ s^{-1}derived for $T=1140$ K [8]. Furthermore, $D\times n_{eq}$ can be suggested to be thermally activated [10]

$$D\times n_{eq}=const.e^{-[(E_D+E_a)/k_bT]} \tag{6}$$

where E_D is the surface diffusion barrier and E_a is the adatom creation energy [10]. At $T\geq1100$ K, $E_D+E_a=1.3$ eV on "1×1"; with $E_D=1.1$ eV and $E_D=0.2$ eV were reported [8,10]. If this is applied to the value of $D\times n_{eq}=8\times10^7$ s^{-1}at 1140 K, we get $D\times n_{eq}=6.3\times10^7$ s^{-1} at 1120 K.

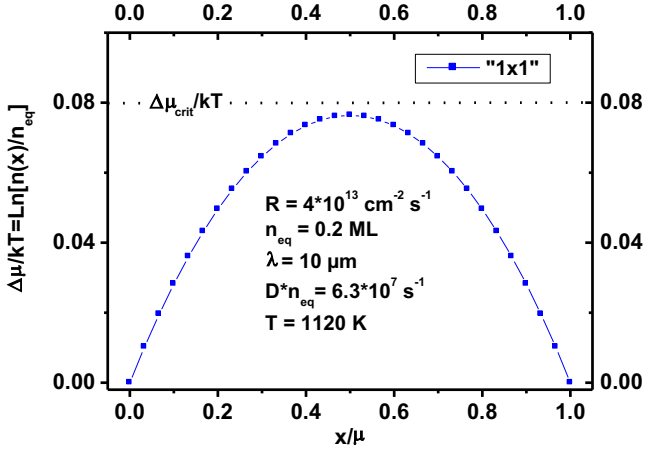

Fig. 3. Excess chemical potential profile across a 10 μm wide terrace calculated for a Si flux of 4×10^{13} cm^{-2} s^{-1} at 1120 K, where only the "1×1" surface phase was observed. Critical supersaturation for nucleation is also indicated by the dotted line.

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