Correlation Functions in Annealed Film Surface Grown by Molecular Beam Epitaxy Model

ฟังก์ชันสหสัมพันธ์ในผิวฟิล์มที่ผ่านการอบอ่อนซึ่งปลูกโดยแบบจำลองการปลูกชนิดโมเลกุลาร์บีมเอพิแทกซี

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ABSTRACT

Presently many researches focus on minimizing roughness of a film surface grown by Molecular Beam Epitaxy (MBE) technique. An annealing process is a technique which reduces the roughness of a film surface because it provides thermal energy for atoms on a substrate so that they can continue to diffuse after the deposition process has ended. In this work, we use correlation functions to characterize roughness of the film surface annealed at different temperatures. The simulation results show that the values of correlation functions decrease when the annealing temperature increases. This means that the roughness of the film surface significantly decreases as the annealing temperature increases. Furthermore, the results show that the annealed film still exhibits multiaffine behavior in the same way as the un-annealed film.

บทคัดย่อ

ปัจจุบัน งานวิจัยส่วนใหญ่ให้ความสนใจกับการลดความขรุขระของผิวฟิล์มที่ปลูกโดยเทคนิคโมเลกุลาร์บีมเอพิแทกซี กระบวนการอบอ่อนเป็นเทคนิคหนึ่งที่ลดความขรุขระของผิวฟิล์ม เนื่องจากให้พลังงานความร้อนกับอะตอมบนซับสเตรต ทำให้อะตอมสามารถแพร่ต่อไปได้หลังจากที่กระบวนการตกสะสมสิ้นสุดลง ในงานนี้เราใช้ฟังก์ชันสหสัมพันธ์แสดงลักษณะเฉพาะความขรุขระของผิวฟิล์มที่ถูกอบอ่อนด้วยอุณหภูมิที่แตกต่างกัน ผลของการจำลองปรากฏว่าค่าฟังก์ชันสหสัมพันธ์ลดลงเมื่ออุณหภูมิการอบอ่อนเพิ่มขึ้น ซึ่งหมายความว่าความขรุขระของผิวฟิล์มลดลงอย่างมีนัยสำคัญเมื่ออุณหภูมิของการอบอ่อนเพิ่มขึ้น นอกจากนี้พบว่า ฟิล์มที่ถูกอบอ่อนยังคงแสดงพฤติกรรมหลายสัมพรรคในทำนองเดียวกันกับฟิล์มที่ไม่ถูกอบอ่อน

Key Words: MBE model, Annealing, Correlation function

คำสำคัญ: แบบจำลองการปลูกชนิดโมเลกุลาร์บีมเอพิแทกซี การอบอ่อน ฟังก์ชันสหสัมพันธ์

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Introduction

Molecular Beam Epitaxy (MBE) is a technique to produce a high quality epitaxial film where atomic arrangement of the film is the same as the crystallographic structure of the substrate. In general, MBE growth is performed in an ultra-high vacuum environment in order to decrease contamination, and to increase a mean free path of an atom (Arthur, 2002). Atoms from the beam are deposited on a substrate maintained at a fix temperature. A deposited atom can diffuse or desorb if it has enough energy. The relevant processes in MBE growth, deposition, diffusion, and desorption process, are shown in Figure 1.

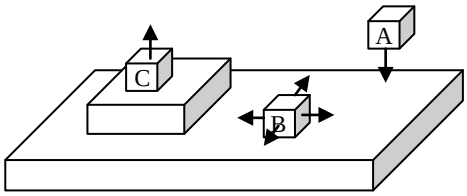

Figure 1 Schematic depiction of MBE growth processes: deposition of atom A, diffusion of atom B, and desorption of atom C.

At present many experimental researches have concentrated on finding ways to minimize roughness of a film surface. Annealing process is one of the most common techniques used. The annealing process is a heat treatment after deposition has ended. This increases the diffusion probability of an atom on the surface because it provides thermal energy to the substrate. An atom on surface acquires enough energy to break bonds formed during its deposition and therefore can diffuse to other positions.

Objectives of the study

In this work, our motivation is to study the role of annealing on a film surface grown by MBE. The law governing the diffusion rate in our simulations follows the Arrhenius law. We analyze properties of the film surface using the time evolution of film surface morphology and correlation functions.

Methodology

In our simulations, the MBE growth model is performed on two dimensional flat substrates. The model is restricted to obey periodic boundary conditions. To simplify the film growth under MBE condition, desorption process is neglected because the probability of desorption is much lower than deposition and diffusion. In this work, the deposition rate is fixed at 1 ML/s which means $L \times L$ atoms are deposited on a substrate of the size of $L \times L$ lattice sites during 1 second. When an atom is randomly deposited on the substrate, it uses up L^{-2} s which is called the deposition time. Diffusion will occur, if the deposition time is larger than the diffusion time. The diffusion time, t_R is calculated according to the Arrhenius Law (Barabasi and Stanley, 1995; Das Sarma and Tamborenea, 1991; Ghaisas and Das Sarma, 1992)

$$t_R = \frac{h}{2k_B T} \exp\left[\frac{E_0 + nE_b}{k_B T}\right]. \qquad (1)$$

It depends on the number of bonds n and the substrate temperature T. The activation energy of a free atom with no bond E_0 and the bonding energy per bond E_b are chosen to be $E_0 = 1$ eV and $E_b = 0.3$ eV respectively. The number of bonds is $n =$ 1, 2,..., 5 (Barabasi and Stanley, 1995; Elsholz, Meixner and Schöll, 2003). In growth simulations, we randomly choose a deposited atom with the smallest diffusion time on the surface to diffuse to one of its nearest neighbor sites. A new atom is deposited when the summation of the diffusion time is larger than

the deposition time. For annealing process simulations, the deposition ends after a predetermined growth time t_G and the atoms diffuse until the provided annealing time t_A is reached.

In this work, we analyze the film surface's roughness via the time evolution of film surface morphology and the correlation functions. The correlation function, G, which is the height-height correlation function, is defined (Das Sarma, Ghaisas and Kim, 1994) as

$$G(r,t) \equiv \sqrt{\frac{1}{L^2}\sum_{\vec{x}}[h(\vec{x}+\vec{r},t)-h(\vec{x},t)]^2}, \qquad (2)$$

where $h(\vec{x},t)$ is the height at position $\vec{x}$ at time t and $\vec{r}$ is a position vector that points from the site $\vec{x}$ to other lattice sites on the substrate. At a fixed time, it is a function of the distance r. In general, the interested distance is $r \le L/2$ for thin film growth with periodic boundary condition. At small distances, the heights between any two sites are not independent and the correlation function G scales with the distance r as

$$G \sim r^{\alpha'}, \quad \text{when} \quad r << \xi. \qquad (3)$$

The exponent α' is called the *local roughness* exponent, and ξ is the *correlation length*. At large distances, the heights between any two sites are completely independent and the correlation function G becomes constant. The value of the saturated G depends on the growth time t as

$$G_{sat} \sim t^{\beta'}, \quad \text{when} \quad r \ge \xi. \qquad (4)$$

The exponent β' is called the *growth* exponent. In a growth model with multiaffine scaling, the correlation functions have q-dependent exponents and the generalized height-height correlation function is defined as (Krug, 1994)

$$G_q(r,t) \equiv \left[\frac{1}{L^2}\sum_{\vec{x}}\left|h(\vec{x}+\vec{r},t)-h(\vec{x},t)\right|^q\right]^{1/q}. \qquad (5)$$

Note also that G of Eq. (2) can be found by substituting $q=2$ into Eq. (5).

Results

In this work, we model the MBE growth on the substrate size 256×256 sites. In order to study effects of annealing process on the roughness of the film surface, the growth substrate temperature T_G and the growth time t_G are fixed at $T_G = 750$ K and $t_G = 10^3$ s, while the annealing temperature T_A is varied within the range from 750 to 900 K. The morphology of the film grown by MBE growth model is shown in Figure 2. The film surface is very rough.

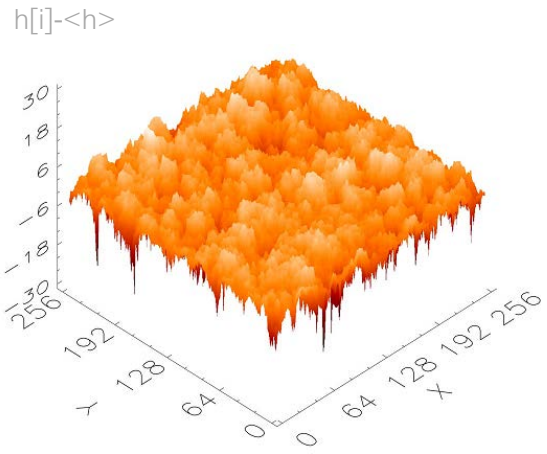

Figure 2 The film surface morphology for MBE growth model with $T_G = 750$ K at the time $t_G = 10^3$ s.

The film is then annealed for annealing time $t_A = 10^4$ s at various T_A. The results are shown in Figure 3. The figure shows that the film surface morphology is smoother when the annealing temperature is increased.

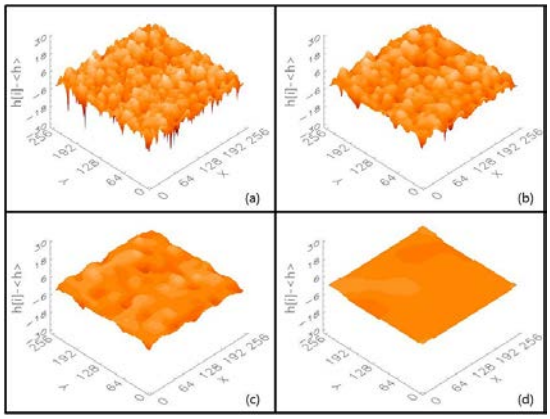

Figure 3 Morphologies of the film grown as in Figure 2 then annealed at (a) $T_A = 750$ K (b) $T_A = 800$ K (c) $T_A = 850$ K (d) $T_A = 900$ K for time $t_A = 10^4$ s.

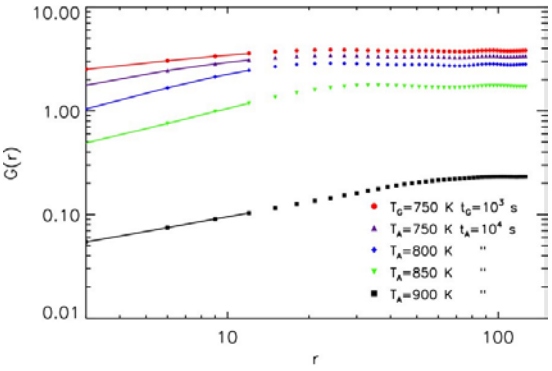

Figure 4 The correlation function G as a function of r for film grown at $T_G = 750$ K and the time $t_G = 10^3$ s then annealed for the time $t_A = 10^4$ s with different T_A.

The correlation functions are shown in Figure 4. The correlation functions become smaller after the film is annealed. This means that the film surface is smoother because the height difference between two sites decreases. The film with the highest annealing temperature is the smoothest surface.

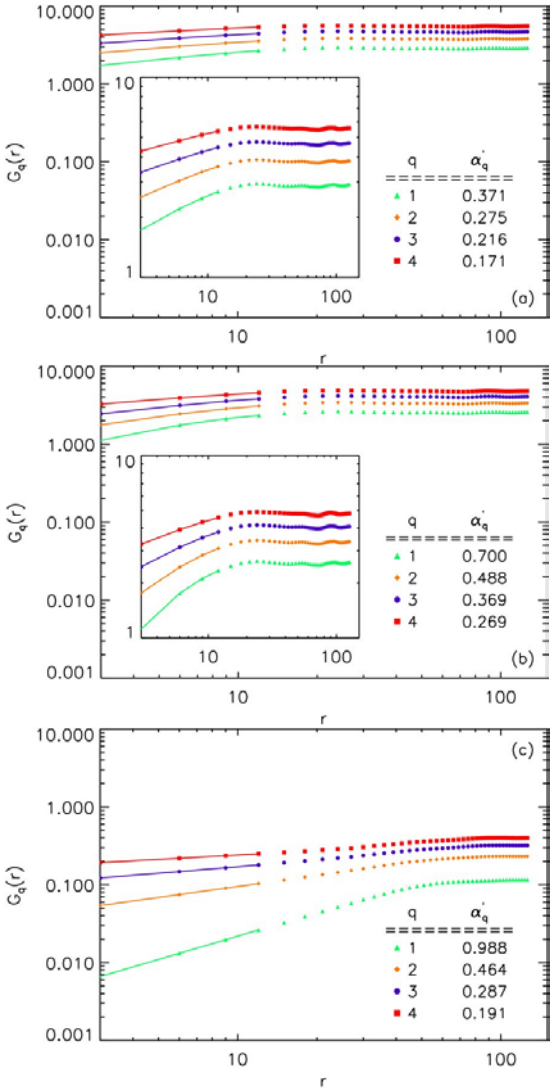

Figure 5 The height-height correlation function for four values of q from (a) the film grown with $T_G = 750$ K at the time $t_G = 10^3$ s and the film grown as in (a) then annealed for $t_A = 10^4$ s at (b) $T_A = 750$ K and (c) $T_A = 900$ K. The scales are fixed in all main plots while the insets show closed-up plots.

The multifractal aspect of the films is studied via the q-dependent correlation function. In Figure 5(a), the strong multifractality of the grown film can be seen. Figure 5(b) and 5(c) show the multifractality of film when the film is annealed.

Discussion and Conclusions

Figure 2 shows the film surface grown at $T_G = 750$ K on the system of 256×256 sites. It is very rough because the deposition time is smaller than the diffusion time. As a result, an atom cannot diffuse far away from the deposited site and the diffusion rarely happens due to a deposited atom being buried by newly deposited atoms. The annealing process reduces the roughness of the surface as can be seen in the film surface morphologies and the correlation function shown in Figure 3 and 4. This is because the deposition process is discontinued during the annealing process and only the diffusion process is allowed at an annealing temperature T_A. This causes the increase in the probability that an atom can diffuse to other positions. From equation (1), the diffusion time significantly decreases when T increases. Therefore, the film surface morphology of the system with the highest annealing temperature (Figure 3(d)) is the smoothest surface. This is in agreement with the correlation function at different annealing temperatures T_A. In Figure 4, during the growth process, the correlation function is very large (circles). After the growth process is completed and the annealing process starts, the correlation function become smaller and the correlation function with the highest annealing temperature (squares) is the smallest. In this work, we show that MBE film modeled with Arrhenius law has multifractal because the correlation functions have q-dependent roughness exponents as shown in Figure 5. Moreover, the film still shows the multifractal scaling after it is annealed.

Acknowledgements

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