A Quick Look of My Research Experience

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Date: Mar, 2022

01

CASE ONE

Thin film growth

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University of Science and Technology of China

A DDA model of thin film growth based on Kinetic Monte Carlo

基于动力学蒙特卡洛方法的一种薄膜生长DDA模型

01/ What did I do

中国科学技术大学
University of Science and Technology of China

01 Reviewed Growth Mechanism of Vapor Deposition Thin Films

02 Concluded important models for simulating thin film growth and Kinetic Monte Carlo Methods

03 Designed a deposition-diffusion-aggregation model based on KMC method

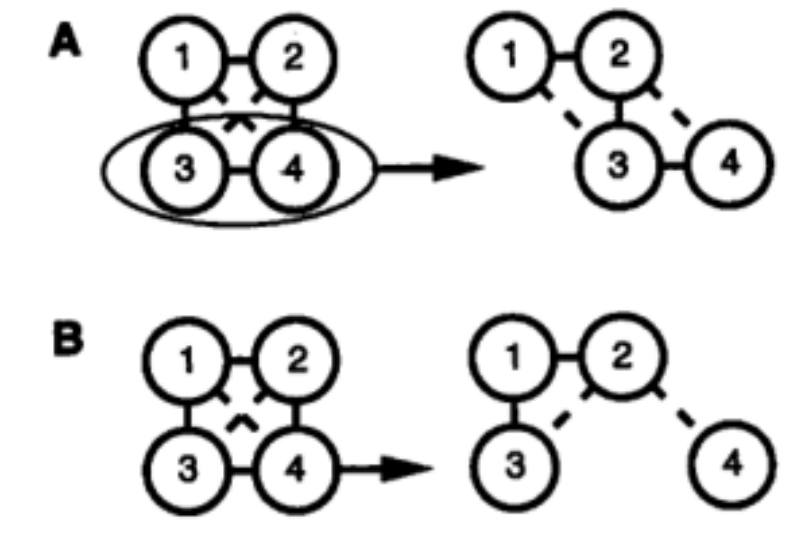
01 Reviwed growth Mechanism of Vapor Deposition Thin Films

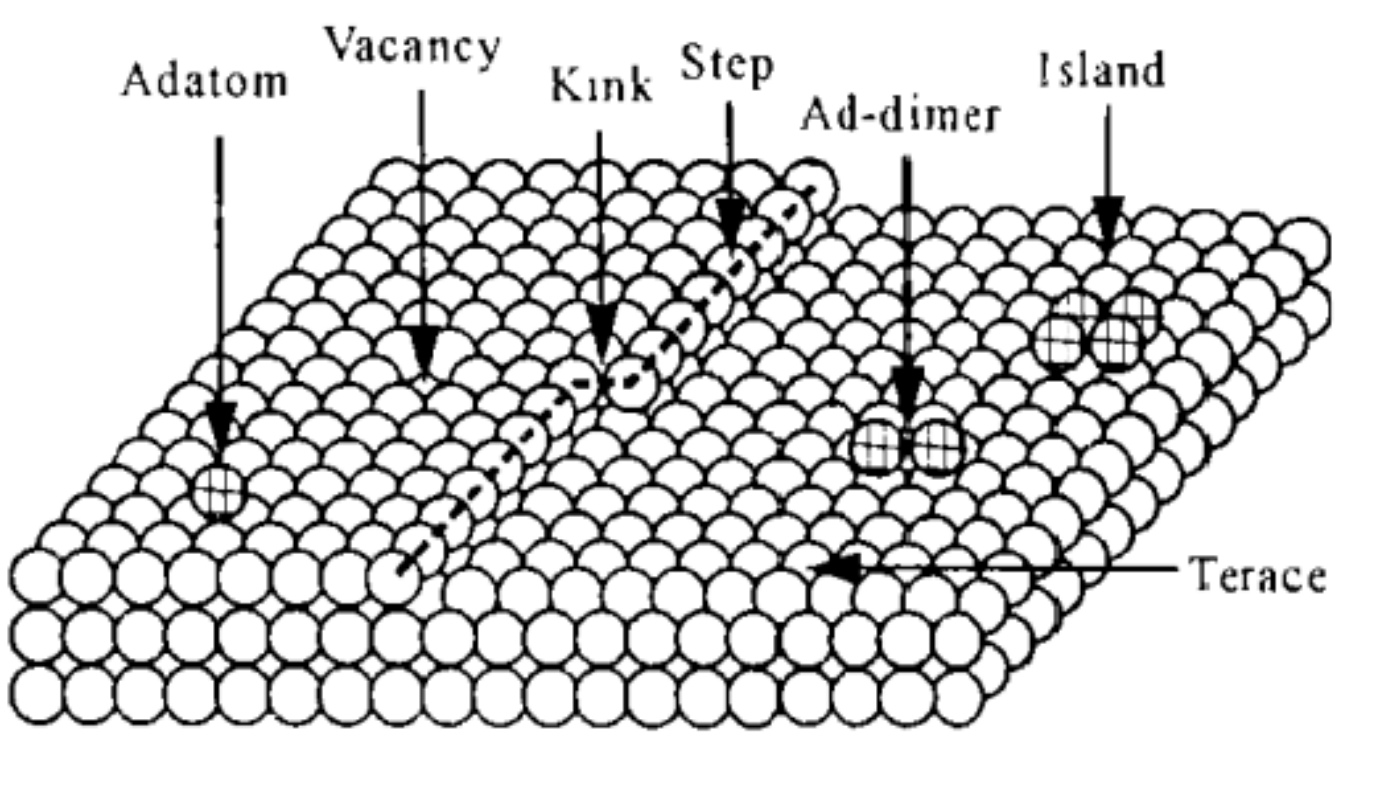
"Growth of thin films from atoms deposited from the gas phase is intrinsically a non-equilibrium phenomenon governed by a competition between kinetics and thermodynamics."——Zhang Zhenyu&Max.G.L, 1997

So far, the microscopic mechanisms describing thin film growth are usually based on the so-called Terrace-Step-Kink (TSK) model.

Atomistic Processes in the Early Stages of Thin-Film Growth

Zhenyu Zhang and Max G. Lagally

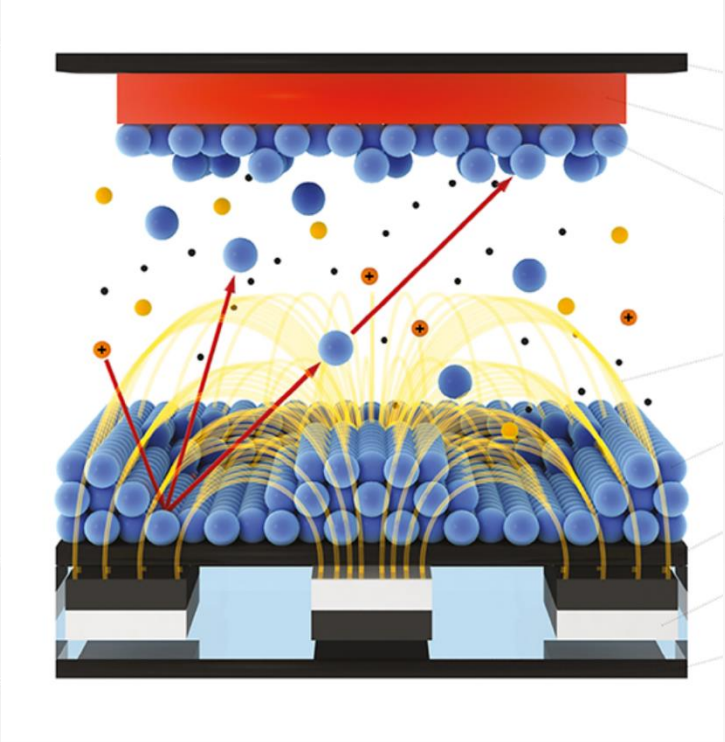


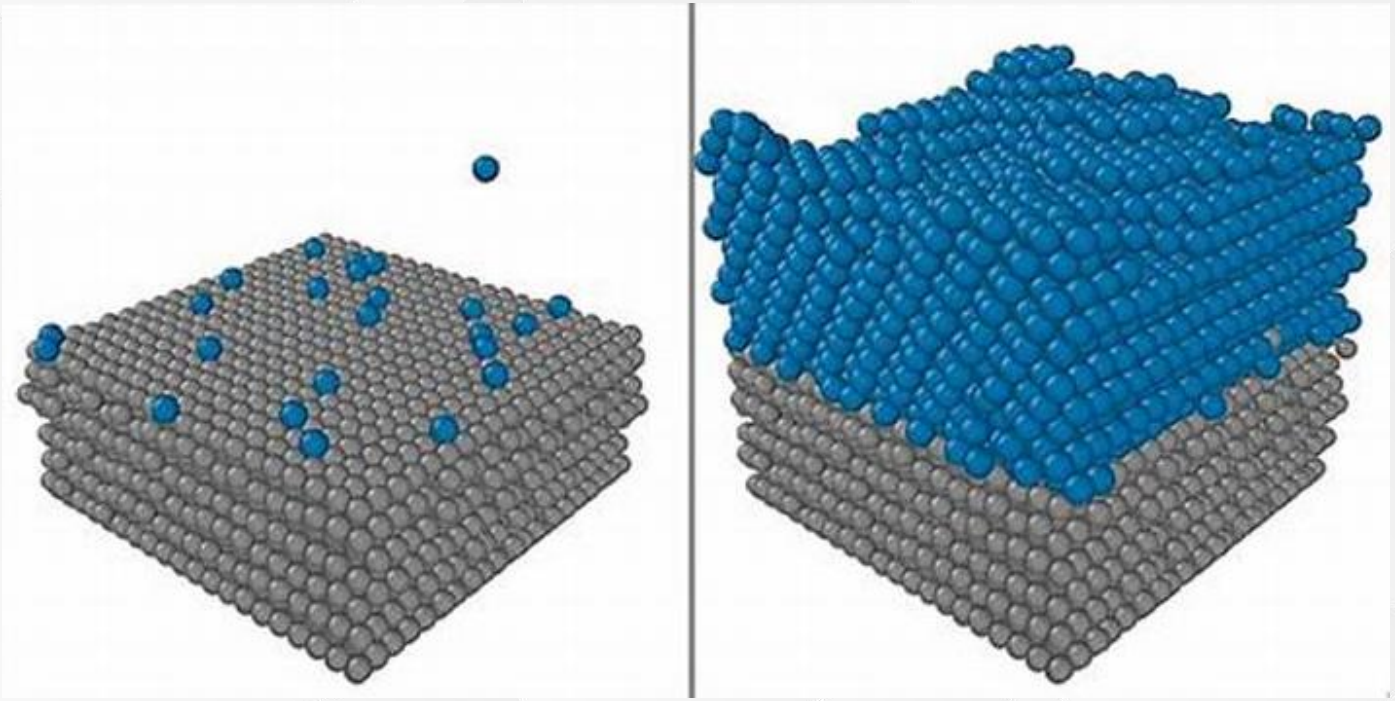


Since the actual formation process of the thin film is very complex, these processes are necessary to be summarized in the theoretical study and simplified to three main dynamic processes of atoms moving on the substrate surface: deposition process, diffusion process and desorption process:

(1) Deposition

The process in which the atoms of the thin film material reach the substrate surface in a certain way and then be adsorbed by the substrate is related to the adsorption and state of the atoms on the substrate surface and the potential energy distribution of the substrate surface.



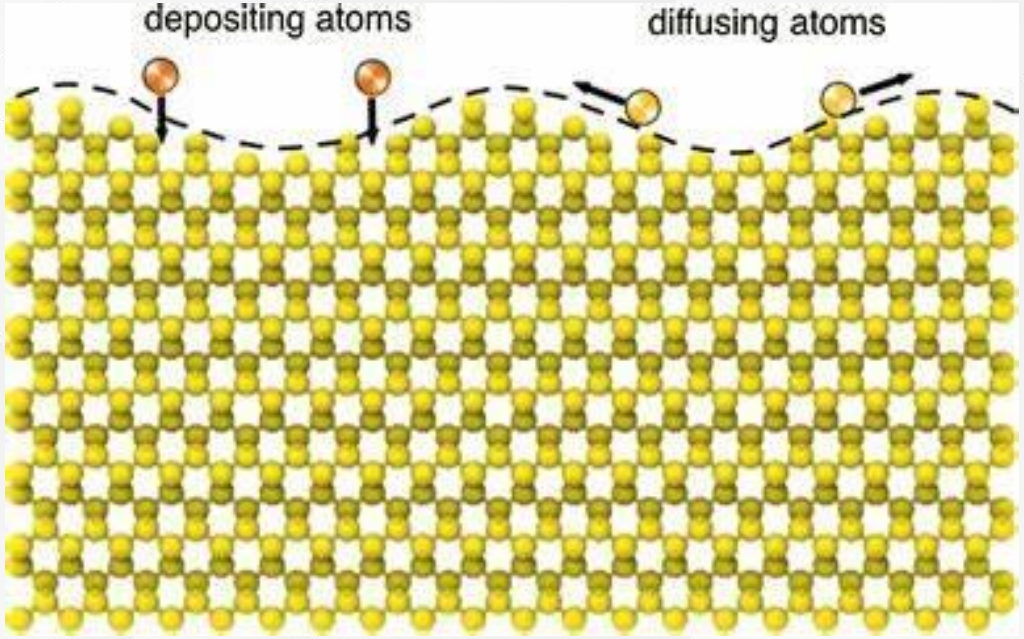


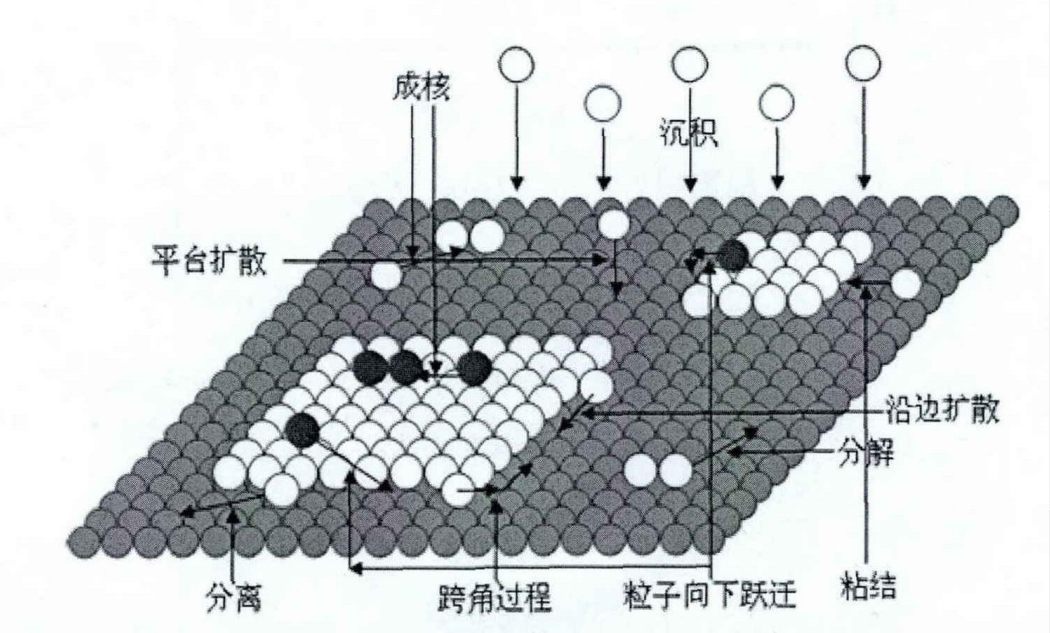
(2) Desorption

There are two ways for adatoms to be released from the system, one is that the atoms directly collide with the substrate surface elastically during the incident process to break away from the substrate, and the other is that the incident atoms are adsorbed on the substrate and obtain a certain amount of energy when they diffuse. energy, thereby freeing it from the growth surface and desorbing it from the growth surface.

(3) Diffusion

Atoms deposited on the substrate surface are not stationary after being adsorbed by the substrate surface due to adsorption, but can also diffuse in all directions on the substrate plane and between layers.





According to the surface morphology of the film, the growth process of the film can be divided into the following three modes:

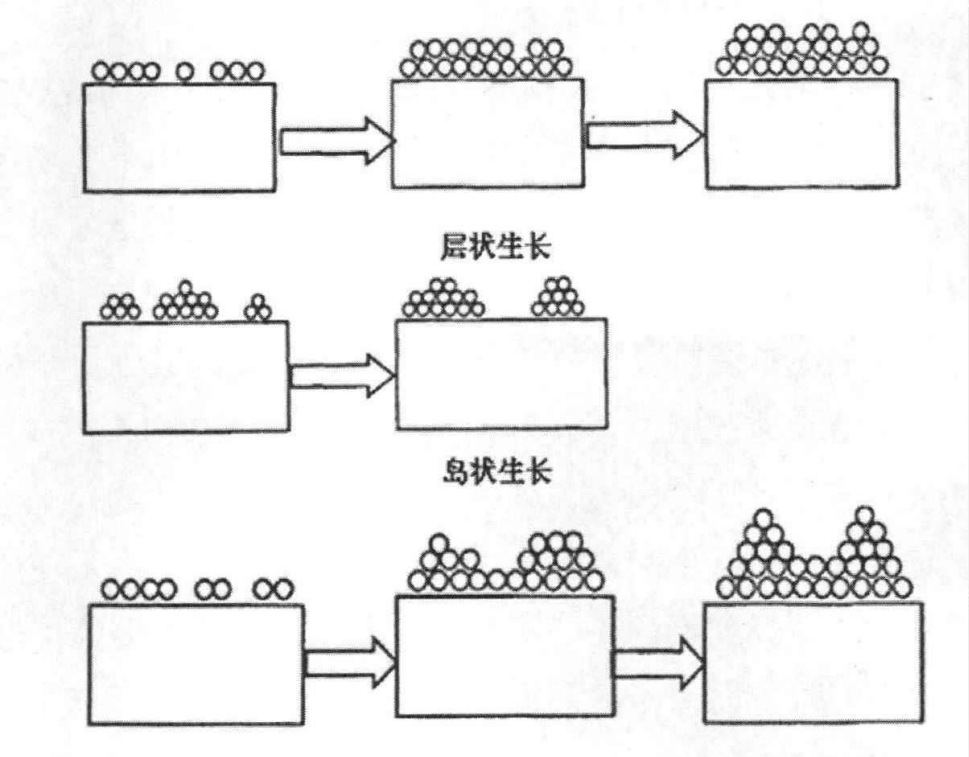
Frank-van der Merwe

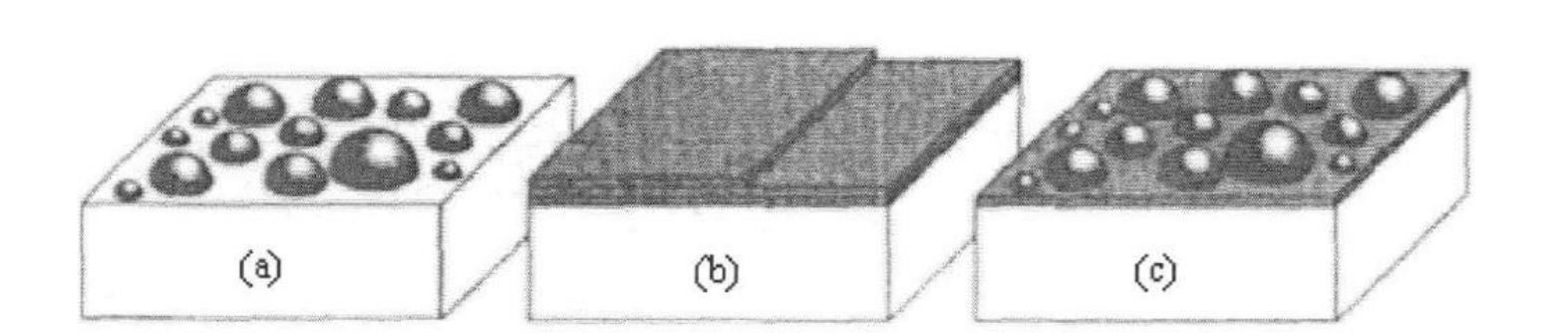
When the wettability between the deposition material and the substrate is good, the bonding ability between the deposition atoms and the substrate atoms is relatively strong, and the bonding between the deposition atoms and the deposition atoms is relatively weak. So the deposited atoms tend to bond with the substrate atoms.

Volmer- Weber

Stranka- Krastanov

Wettability becomes poor after growing to a few monolayers, which usually occurs when stress occurs in the film after 2D growth





The main factors affecting film growth include:

The elemental properties of the deposited material, the type of interaction between atoms, the type and structure of the growth substrate, the choice of substrate temperature, the deposition rate, direction and energy, assisted deposition, etc.

Various parameters have been proposed to describe the growth morphology of thin films, mainly including:

（1） Critical Island Size

The atomic number of the island when it has just reached stability

（2） Island density

Number of atomic islands per unit surface

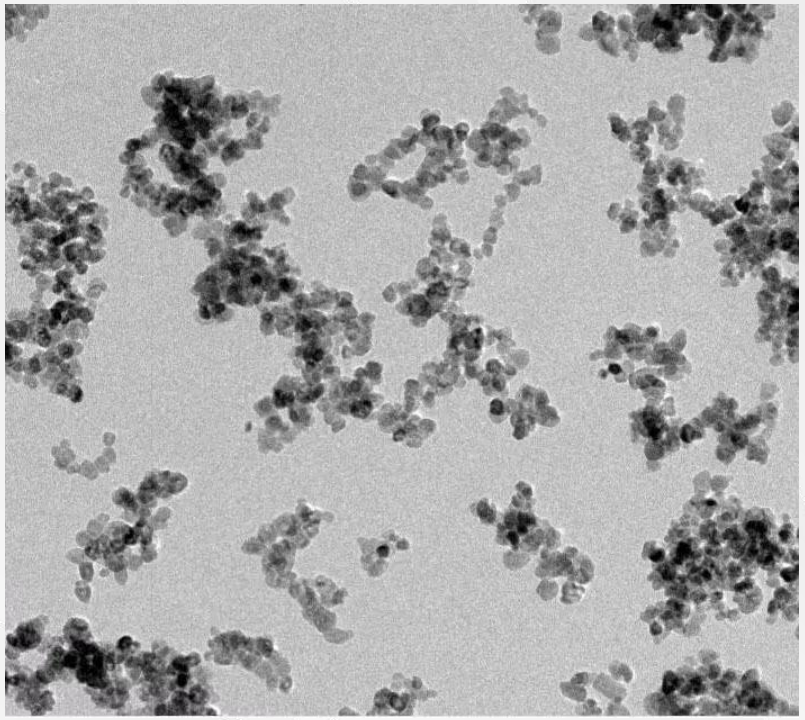
（3） Island size distribution

Distribution of atomic islands of different sizes on the substrate surface. Studies have shown that the size distribution of islands has a scaling behavior in the region of irreversible growth aggregation.

（4） Fractal dimension of islands

Treat islands of different sizes as different levels of the fractal, and calculate the Hausdorff dimension

The classical nucleation theory gives an expression for the scaling relationship between island density and critical island size i



$$N \approx \left(\frac{D}{F}\right)^{-\frac{i}{i+2}} \exp\left[\frac{E_i}{(i+2)k_B T}\right]$$

(Here, D is the diffusion coefficient of atoms on the substrate surface, Ei is the bond energy, F is the deposition flux)

For the 3D growth morphology of thin films, there are also:

(5) Coverage/Relative Density

$$m_d = 1 - \frac{N_1}{N_2}$$

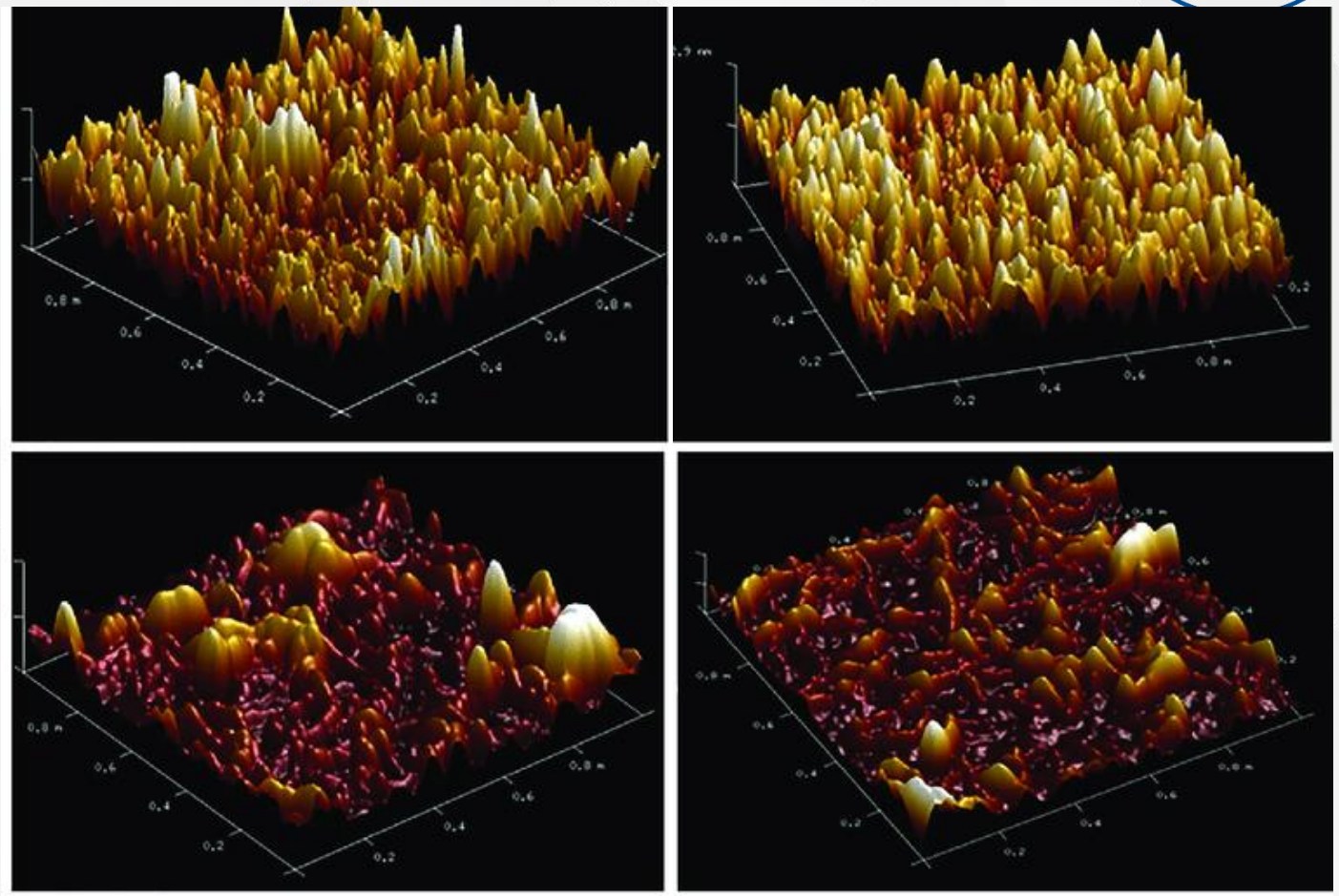
Among them, N_1 represents the number of atoms required to form a complete lattice, and N_2 is the number of unoccupied crystals in the film during the film formation process, that is, the number of vacancies. Therefore, the larger the m_d, the more complete the lattice structure of the film.

(6) Surface roughness

$$\mathrm{W(r,t)} = [\langle \mathrm{h^2(r,t)} \rangle - \langle \mathrm{h(r,t)} \rangle^2]^{1/2}$$

In which

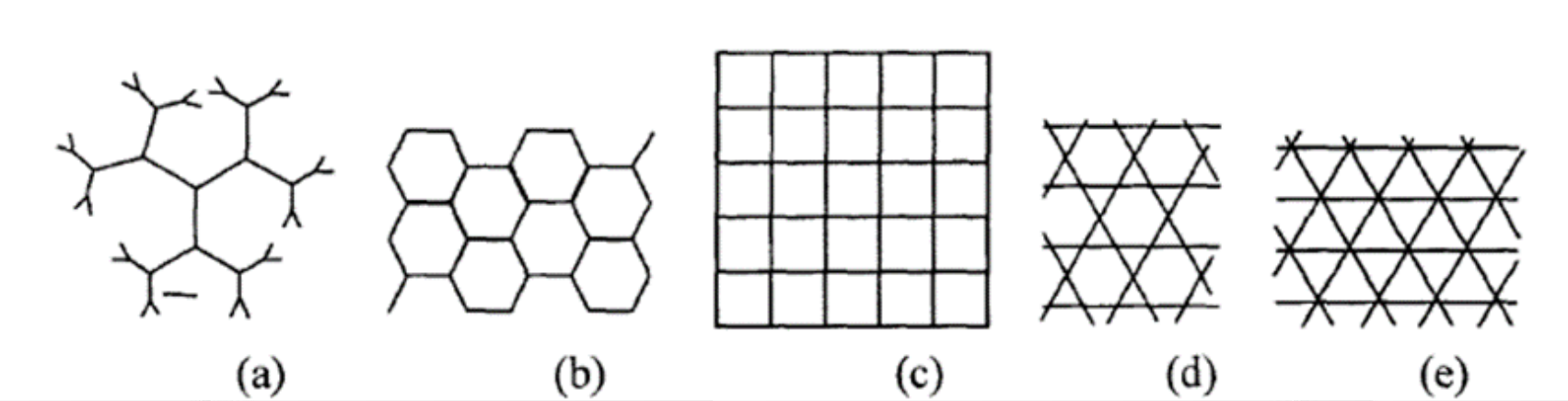
$$\langle \mathrm{h^n(r,t)} \rangle = \overline{\mathrm{L^{-2}} \sum_{\mathrm{r}} \mathrm{h^n(r,t)}}$$



02 Concluded important models for simulating thin film growth and Kinetic Monte Carlo Methods

There are two forms of space processing in the growth model: continuous space, that is, the particles under consideration can be in any position in the space; the other more common is discrete space, which discretizes the space, and the particles can only occupy the discrete space. on the center of the regular space grid node or grid point. There are many types of lattice points used in discrete spaces, including different crystal planes of various crystal systems. An important parameter of the lattice type is the coordination number of each node. For thin film growth, this discretization can reduce the computational complexity and is a reasonable approximation.

If boundary effects need to be reduced, the boundary problem of the growth surface can be handled with periodic boundary conditions. This makes it possible to perform computations on infinitely large models in a finite space.



	6,1	6,2	6,3	6,4	6,5	6,6	
1,6	1,1	1,2	1,3	1,4	1,5	1,6	1,1
2,6	2,1	2,2	2,3	2,4	2,5	2,6	2,1
3,6	3,1	3,2	3,3	3,4	3,5	3,6	3,1
4,6	4,1	4,2	4,3	4,4	4,5	4,6	4,1
5,6	5,1	5,2	5,3	5,4	5,5	5,6	5,1
6,6	6,1	6,2	6,3	6,4	6,5	6,6	6,1
	1,1	1,2	1,3	1,4	1,5	1,6	

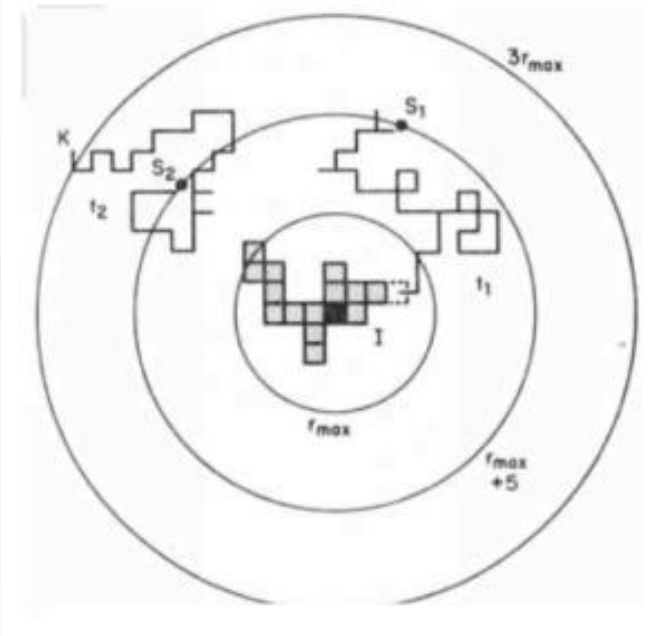
According to the dominant factor of nucleation, thin film growth models can be divided into

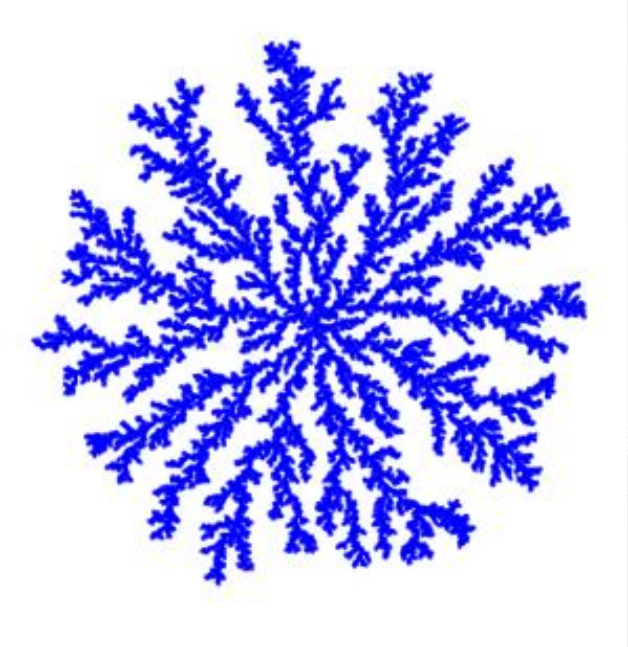
1. Diffusion-controlled nucleation growth model

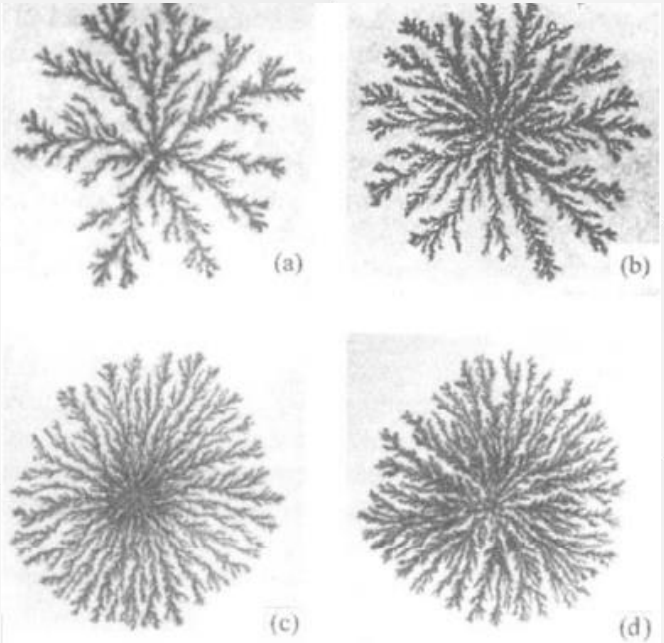
(1) Diffusion-Limited Aggregation (DLA) Model

This is the earliest model proposed by people. The main idea is: place a seed particle at the center of the lattice, and the particles generated in the distance diffuse randomly. When the diffused particle diffuses to the neighboring position of the seed particle, it stabilizes and becomes an aggregate. part. This process is repeated until aggregates with fractal structures are formed. The DLA model intuitively explains the fractal structure formed in the early growth stage of some metal films at lower temperatures, which is similar to the cluster morphology of electrochemical deposition.

The disadvantage is that it is too simple to explain other experimental laws.







(2) Extended DLA Model

The main idea is: the particles diffused to the edge of the aggregate will not stabilize immediately, but continue to move along the edge of the aggregate, and the stable position they seek is the position where the number of adjacent atoms is greater than or equal to 2. The particles diffused along the edges of the aggregates, which made the branches of the aggregates thicker and the number of branches decreased until a clump-like structure was formed.

(3) Deposition-diffusion-aggregation (DDA) model

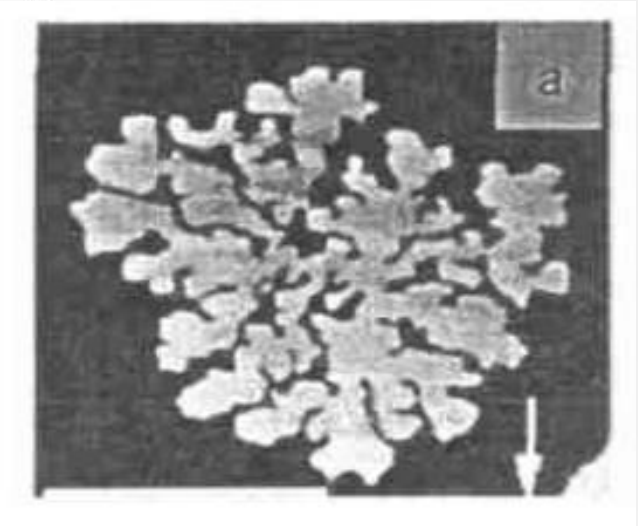
Atoms are randomly deposited onto the substrate and diffuse randomly across the surface of the substrate. Clusters are formed when diffusing atoms meet. Clusters can still continue to diffuse, and islands are formed when clusters meet diffusing atoms or other clusters. With the continuous deposition of atoms, the aggregates gradually grow into groups with fractal structure, and the fractal dimension of the groups increases with the increase of deposition coverage. The DDA model is more realistic than the DLA model for the thin film growth process.

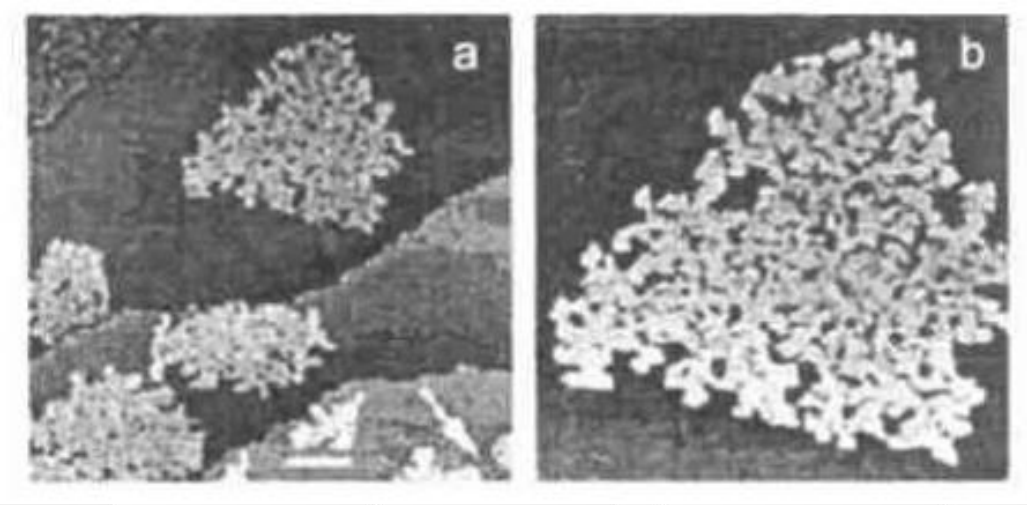
Other models include ballistic aggregation models, attractive potential interaction models, and so on.

2. Reaction-controlled nucleation growth model

As mentioned earlier, the introduction of a small amount of surfactant during the growth process in heteroepitaxial growth will make the growth mode transition from island growth to layer growth. In 1998, Tsong's group studied the shape and size distribution of 2D islands formed on the surface of sub-monolayer substrates in the early stages of growth under surfactant. Because the shape and size distribution of these 2D islands directly affects the quality of multilayer film preparation in heteroepitaxial growth. They were surprised to find that in the Ge/Pb/Si(111) epitaxial growth system, when the temperature was increased or the deposition rate was decreased, large fractal islands were formed on the substrate; compact island.

This conclusion is opposite to the case without surfactant and cannot be explained by the existing diffusion-limited aggregation (DLA) theory.





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Two-Dimensional Pattern Formation in Surfactant-Mediated Epitaxial Growth

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In the same year, a research team of four experts including Zhang Zhenyu and Wang Enge proposed a surface reaction limited aggregation (RLA) theory, which well explained the experimental phenomenon and became the main method for thin film epitaxial growth in the presence of surfactants. Model.

The surface reaction-limited aggregation (RLA) theory contains three basic assumptions. First, the deposited atoms need to overcome a large energy barrier to exchange positions with surfactant atoms before they can become stable nucleation centers. Second, later deposited atoms still need to overcome an energy barrier to exchange positions with surfactant atoms before they can become part of the stable island. Finally, only those deposited atoms that have exchanged positions can form islands, that is, islands within the surfactant layer are stable.

A brief introduction to Kinetic Monte Carlo Method

Theoretical methods to study the thin film growth process can be divided into two categories: continuity equation theory and numerical simulation. The former mainly includes Rate Equation Theory and Continuum Step Dynamics Theory; the latter includes Kinetic Monte Carlo and Molecular Dynamics.
The temporal and spatial scales of the objects studied by these methods vary.

The continuum theory adopts the continuum approximation, the essence of which is to erase atomic information or average the atomic information. This aspect makes the continuum theory more concentrated, more general, simpler and more direct than the particle model to analyze some surface macroscopic. Attributes. But its disadvantage is that microscopic information of the growth process cannot be obtained. And it is difficult to solve the problem of discreteness of atoms.

The MD method can accurately describe the dynamic evolution behavior of growing crystals, but the computational complexity is very large, and the time length and number of particles that can be simulated are limited. The actual growth process is a long and multi-particle process.

Compared with other methods, the Monte Carlo method can simulate a longer time scale, and at the same time can solve the randomness problem of the motion of a large number of atoms on the surface.

The Metropolis algorithm is equivalent to accept-reject sampling. The disadvantage is that the acceptance rate may not be high. For example, when simulated annealing, the temperature is too low, which may cause the acceptance rate to be very low, and the dynamic evolution process cannot be studied.

The research object of Kinetic Monte Carlo (KMC) method is non-equilibrium, or relaxation process. It is precisely the correctness of time evolution that is emphasized in the simulation. KMC is equivalent to the Metropolis algorithm coarse-grained in time. Instead of judging whether to accept the proposal each time, a certain accepted operation is selected by the roulette method, and the physical time required for this operation is calculated.

Since the KMC simulation only considers the reaction that causes the configuration transition, it can effectively filter out the invalid thermal vibration, so the simulation efficiency can be greatly improved.

Kinetic Monte Carlo has many variants and derived algorithms, including the most commonly used direct method (direct method), first reaction method (FRM), next reaction method (NRM), selected direct method , constant time step method (CTSM), leap frog algorithm (leap KMC), solid dynamic Monte Carlo method OKMC, KMC method based on real-time dynamic analysis (on-the-fly KMC) and so on.

The direct algorithm

The direct method is the most commonly used KMC algorithm, and its efficiency is very high. Each step only needs to generate two random numbers r_1 and r_2 equally distributed between [0,1]. where r_1 is used to select the transition path and r_2 determines the advance time of the simulation. The algorithm can be summarized as follows:

① Calculate the total transition rate when the system is in state i

$$k_{tot} = \sum_{j=1}^{N} k_{ij}$$

① Get a random number r_1;
② Find the path $\mathrm{i} \rightarrow j_k$, let

$$\sum_{n=1}^{j_k-1} k_{ij} \leq r_1 k_{\mathrm{tot}} \leq \sum_{n=1}^{j_k} k_{ij}$$

④ The system moves to the state j_k while simulating time advancement,

$$\delta t = -\frac{1}{k_{\mathrm{tot}}} \ln(r_2) \text{ 或 } \frac{1}{k_{\mathrm{tot}}}$$

⑤ Repeat the above process.

A personal understanding to the direct method

The essence of KMC is that all configuration transitions of the system are analogized to the decay of atoms, and its rate is the decay constant in the decay law. Atomic decay itself is also a complex dynamic process, and we observe that its probability of occurrence conforms to the law of decay. So this analogy follows the laws of nature, so KMC can simulate the real time of the reaction.

For the simplest example, let the rates of events A and B be $\mathrm{R_A}$ and $\mathrm{R_B}$respectively.

- Starting from time $\mathrm{t} = 0$, the time when A and B occur all obey the exponential distribution (independent of each other) :

$$p(t = t_A) = \mathrm{R_A} e^{-\mathrm{R_A} t}$$
$$p(t = t_B) = \mathrm{R}_B e^{-\mathrm{R}_B t}$$

- Using the method of probability theory, we can calculate the probability that A/B happens first and the time is δt

$$p(t_A < t_B \& t_A = \delta t) = \frac{\mathrm{R_A}}{\mathrm{R_A} + \mathrm{R}_B} \times (\mathrm{R_A} + \mathrm{R}_B) e^{-(R_\mathrm{A} + R_B)\delta t}$$

$$p(t_B < t_A \& t_B = \delta t) = \frac{\mathrm{R}_B}{\mathrm{R_A} + \mathrm{R}_B} \times (\mathrm{R_A} + \mathrm{R}_B) e^{-(R_\mathrm{A} + R_B)\delta t}$$

To extend to multiple events, change $\mathrm{R_A} + \mathrm{R}_B$ to $\mathrm{R_{tot}}$. Therefore, we only need two random numbers to determine which event occurs and when.

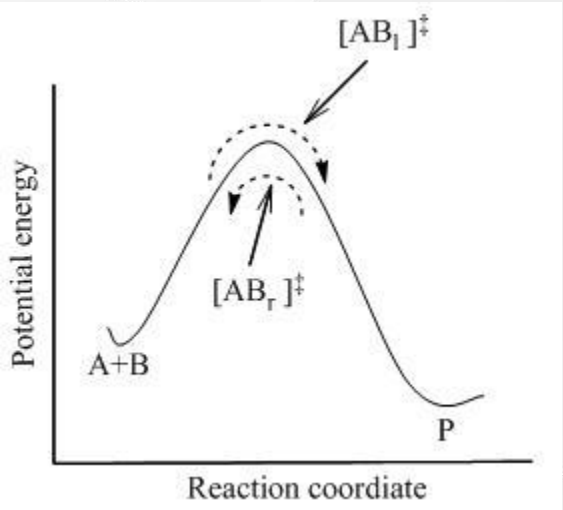
$$\delta t = -\frac{1}{R_{\mathrm{tot}}} \ln(r_2) \text{ 或} E(\delta t) = \frac{1}{R_{\mathrm{tot}}}$$

- After an event occurs, the event table and corresponding rate change. But since the exponential distribution has no memory, we can still do the same operation, which is no problem in probability.

The results of KMC simulations largely depend on the selection of kinetic processes (configurations) in the model and the accuracy of the rates. Many theoretical calculations can provide support in this regard, including first principles methods, molecular mechanics methods, and transition state theory (TST). The former includes the Hartree-Fock (HF) method based on wave functions, as well as electron density functional theory (DFT).

The transition state theory under the harmonic approximation (hTST) gives:

$$k_{ij} = \frac{\prod_{i=1}^{3N} \nu_{i,i}^{0}}{\prod_{i=1}^{3N-1} \nu_{ij}^{sad}} \exp\left(-\frac{\Delta E_{i,j}}{k_B T}\right)$$



In most calculations, the pre-factor (phonon spectrum) is set as a constant, which does not change with the transition process. The potential barrier can be calculated in combination with other methods.

When it is not necessary to accurately calculate the dynamic evolution process of the system, some semi-empirical parameters and approximate models are often used. For example, when determining the migration activation energy, the bond-count KMC is often used, that is, the migration activation energy is determined by the number of the nearest neighbors of the initial position and the final position of the migration atom.

03 Designed a simple deposition-diffusion-aggregation model based on KMC method

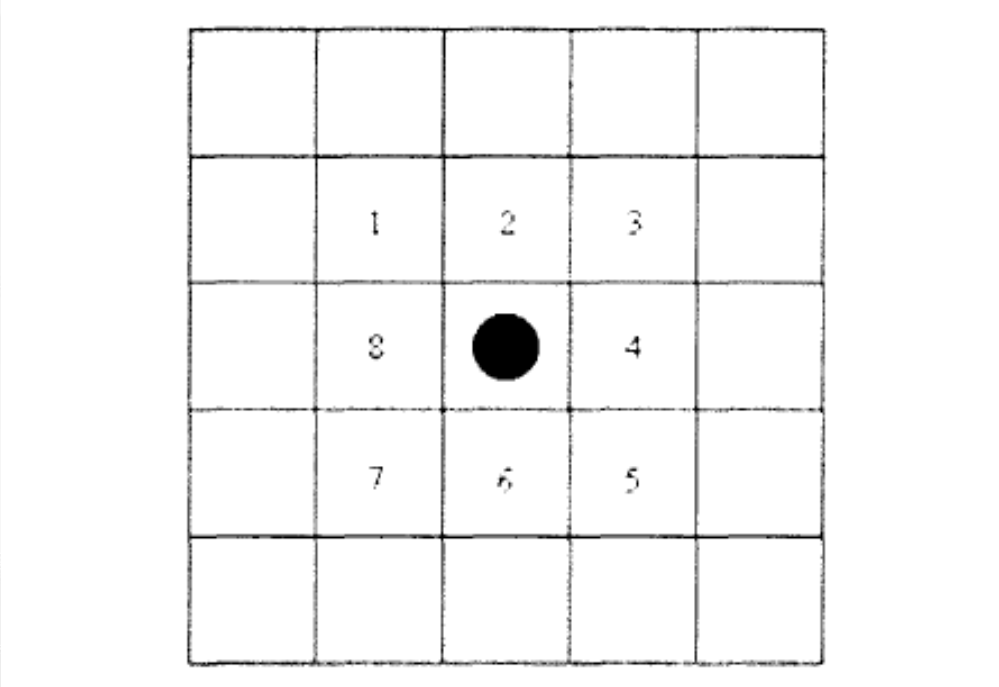
(1) Model description

A square grid is used as an ideal substrate surface for thin film growth, regardless of defects and residual kinetic energy of atoms. And the base material is the same as the film material.

①Deposition

The deposition rate R_d (the number of deposited atoms per unit time) is given before every simulation.

During the simulation process, if the deposition process occurs, a random number is generated by the computer to randomly select a lattice coordinate (i, j) on the surface of the substrate as the initial deposition position of the incident atoms on the substrate. If this position is a vacancy, it will be occupied; if this position is already occupied by other atoms, it will continue to search for vacancies in the 8 adjacent grids, and it is considered that the process of finding vacancies does not require time (equivalent to a very small ES barrier).

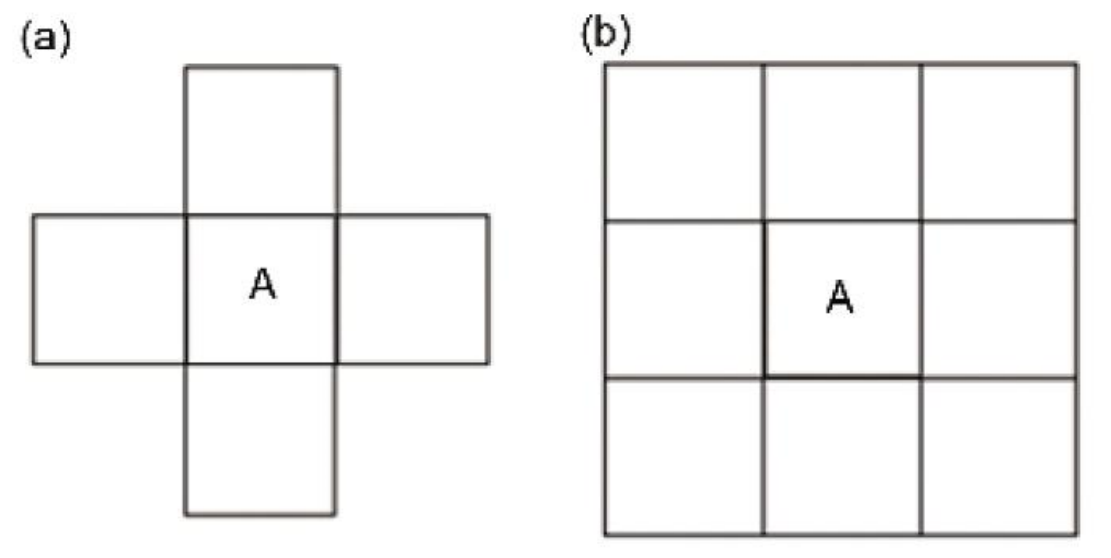


②Diffusion

It is assumed that adatoms can only diffuse into vacancies, and the direction of diffusion is their four nearest neighbors (at 2, 4, 6, and 8). Instead of diffusing to the next nearest neighbors: 1, 3, 5, and 7 that need to overcome higher energy barriers. If one of these positions is already occupied by atoms, no diffusional movement will occur in that direction. The diffusion rate of adatoms during the diffusion process is calculated using the following equation:

$$R_h = V_h \exp\left(-E_{ijkl}/K_B T\right)$$

$$E_{ijkl} = E_{fs} \times \left(m_{kl} - m_{ij}\right)$$



E_{fs} represents the interaction energy between adatoms and substrate atoms, m_{ij} and m_{kl} represent the number of neighbors at the beginning and end, respectively.

③Desorption

One atom of the substrate surface is randomly selected for removal, and the desorption rate can be expressed as

$$R_e = V_e \exp\left(-E_{ij}^{e}/K_B T\right)$$

where V_e is a constant factor, E_{ij}^{e} is the energy barrier that needs to be overcome for the desorption of adatoms from the substrate, which can be expressed as:

$$E_{ij}^{e} = E_{ff} + E_{fs} \times m_{ij}$$

where E_{ff} represents the interaction energy between adatoms and substrate atoms.

In summary, the algorithm flow is as follows:

i. All diffusion and desorption events and their corresponding rates are calculated.

ii. Generate random numbers r_1 and r_2 to judge the event X and the required time δt respectively.

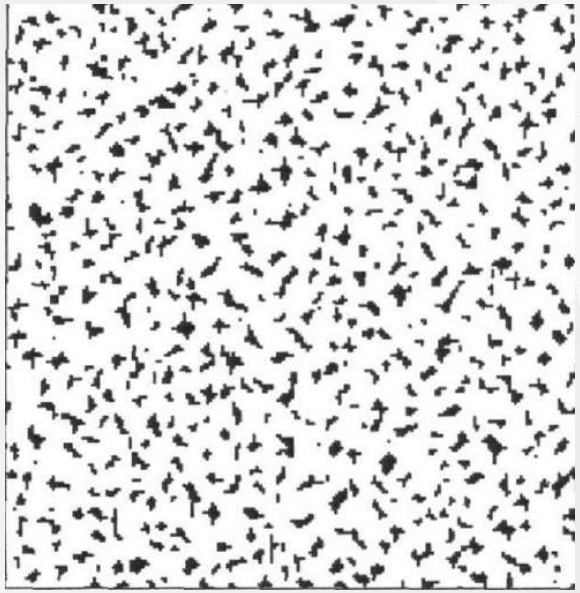
iii. If δt is less than the arrival time of the next depositional event $\Delta t_d(next)$, event X occurs, and $\Delta t_d(next)$ decreases by δt; if δt is greater than the arrival time of the next depositional event $\Delta t_d(next)$, then a depositional event occurs.

iv. Back to the first step.

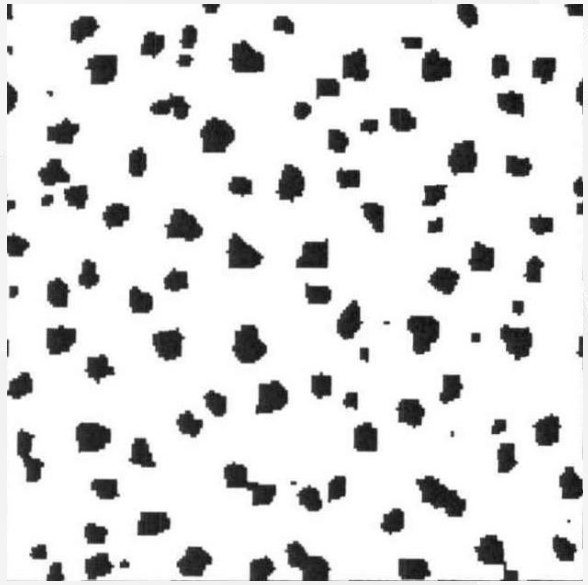
(2) Simulation results

Grid MxM=200x200, The deposition rate of incident atoms is 0.05ML/s, and the substrate coverage is 0.15.

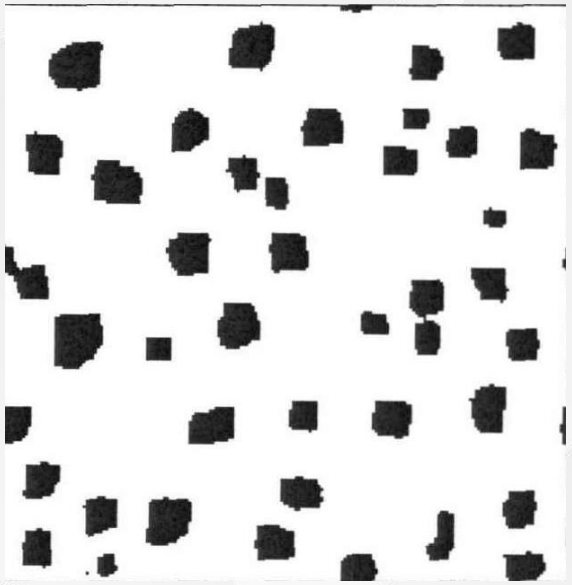
$V_e = V_{\mathrm{h}} = 10^{12} Hz$, $E_{fs} = 0.5\mathrm{eV}$, $E_{ff} = 0.9\mathrm{eV}$



$T = 300K$



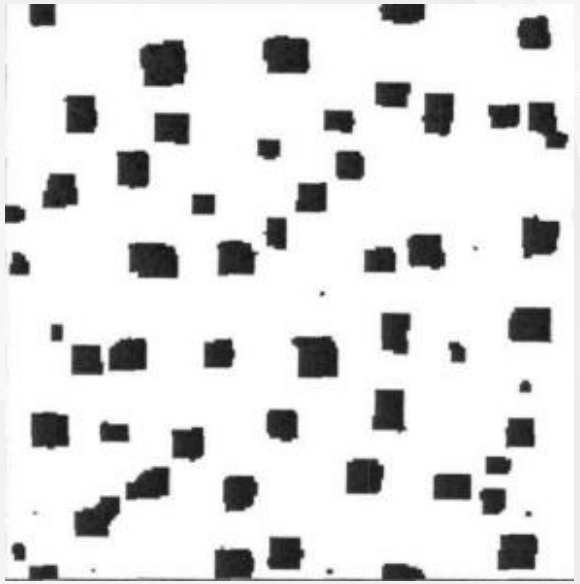
$T = 400K$



$T = 500K$

Grid MxM=200x200, The substrate temperature was 400K, and the substrate coverage was 0.15.

$V_e = V_{\mathrm{h}} = 10^{12} Hz, \quad E_{fs} = 0.5\mathrm{eV}, \quad E_{ff} = 0.9\mathrm{eV}$



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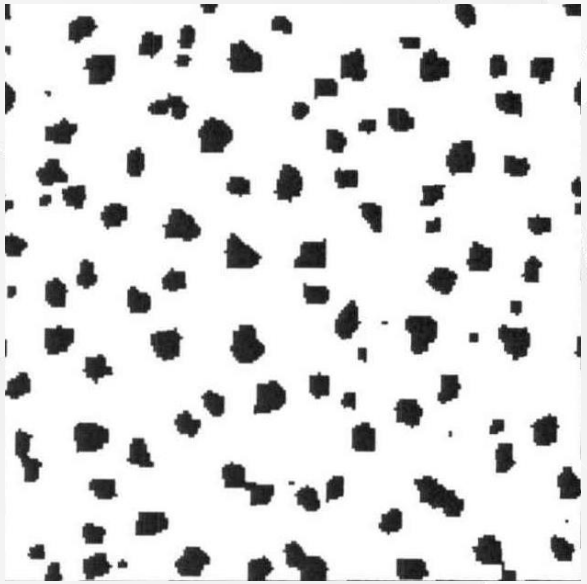

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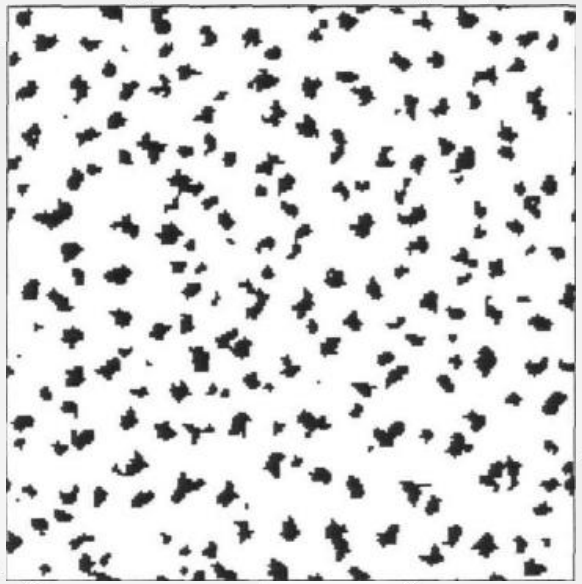

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(3) Analysis of the results

When the deposition rate is constant, with the continuous increase of substrate temperature, the morphology of islands gradually changes from dispersed growth to dense cluster growth. When the temperature is low (200K), "due to the low diffusion rate of atoms, the deposited atoms are dispersed on the surface of the substrate. When the temperature was raised to 300K, atomic bonding and small clusters appeared, but were still very dispersed. When the temperature continues to rise, from rising to 400K, the clusters have been clearly seen, and the atomic clusters have fractal arms extending out, which are typical fractal islands. As the temperature continues to increase (500K), due to the increase in the diffusion rate of atoms, the more the number of atomic neighbors, the lower the energy, so the atoms can gather together more fully, the fractal arms gradually become thicker, the morphology of the island It gradually becomes a compact island, while the island density gradually decreases. When the temperature continued to rise, the growth of the island completely changed to compact growth, and basically showed the morphology of a square base. This is in good agreement with the experimental observation of the effect of substrate temperature changes on the island morphology.

When the substrate temperature is constant, with the increase of the deposition rate, the relative diffusion time of the deposited atoms decreases, and new atoms are deposited on the random vacancies before it has time to aggregate, so the morphology of the islands evolves from compact growth to fractal growth. The density increases accordingly.

02

Case TWO

Transition metal dichalcogenides

中国科学技术大学
University of Science and Technology of China

An unusual morphological phase transition in the growth of MoSe2 nanoribbons

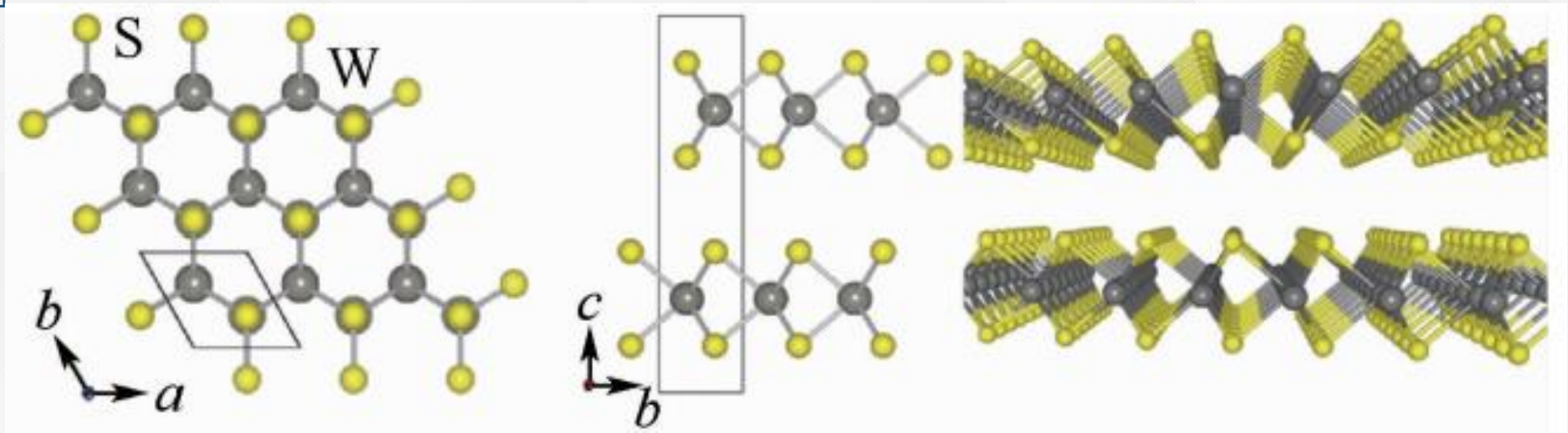
MoSe2 纳米带生长中不寻常的形态相变

02 Works

01 Reviewed the research progress of various aspects of TMDs materials

02 Interpretation of an unusual 2D-to-1D morphological phase transition of TMD in MBE growth using kinetic Monte Carlo method simulations (under trial)

01 Reviewed the research progress of various aspects of TMDs



The chemical formula of transition metal dichalcogenides (TMDs) is generally MX2, where M is a transition metal atom, and X is a chalcogen (S, Se, or Te). More than 40 materials of different elemental compositions have been discovered.

The transition metal sulfide layered material contains three atomic layers, and the transition metal layer is embedded in the middle of two sulfur atomic layers. Each transition metal sulfide layer has a hexagonal lattice structure. Accordingly, the bulk material is constructed by stacking monolayers of transition metal sulfide materials. The layers are connected by chemical bonds, and the layers are connected by van der Waals forces.

Transition metal sulfide layered materials are semiconducting, semi-metallic, magnetic, and superconducting, and thus are widely used in optoelectronics, spintronics, catalysts, lubricants, chemical and biological sensors, supercapacitors, solar cells, and lithium batteries middle.

Conclusion of material properties of TMDs

1 Electronic performance

The band structure of transition metal sulfide layered materials depends on the number of layers. When the thickness of the bulk material is reduced to a multilayer or a single layer, the electronic properties of the layered material change significantly. Due to quantum effects of transition metal sulfide materials, the band gap changes with the number of layers.

2 Optical properties

Transition metal sulfide materials have excellent optical properties and are widely used in the fields of photodetection and photoluminescence.

3 Mechanical performance

Similar to graphene, 2D transition metal sulfide material is also a thin mechanical material with inherent flexibility, thus showing good prospects in the field of mechanics.

4 Energy storage performance

Binding materials are introduced in lithium-sulfur batteries to improve the performance of the battery, and some studies have found that transition metal sulfide materials can be used as binding materials.

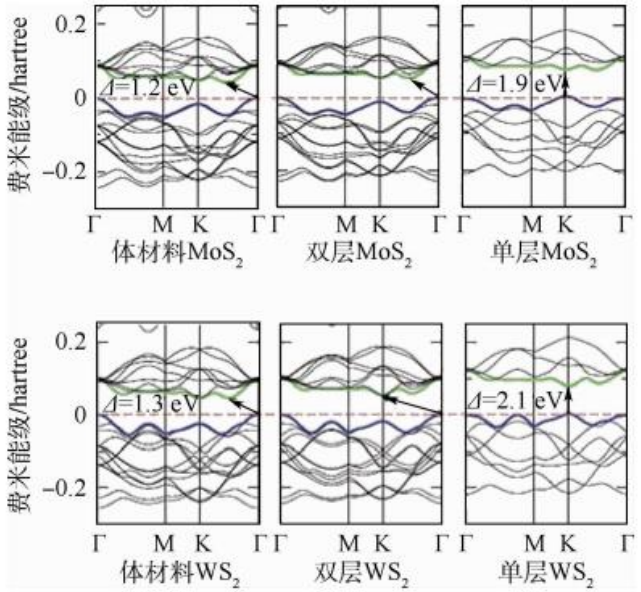
5 Thermal properties

The transition metal sulfide material has excellent thermal stability and can still maintain good thermal stability at high temperature without decomposition, so it can be used in high temperature devices. In addition, transition metal sulfide materials have excellent thermodynamic conductivity and are promising thermoelectric materials.

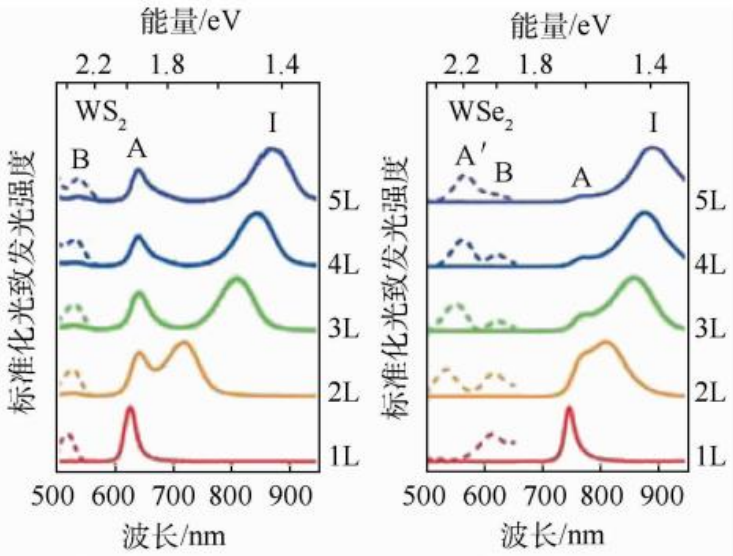
6 Valley Electronics Performance

Transition metal sulfides such as molybdenum disulfide have spin-orbit coupling and symmetry breaking, resulting in the selective absorption of left- and right-handed circularly polarized light in the K valley and K' valley, so they are useful in spintronics and valleys. It has a wide range of applications in electronics and other fields.

Recent researches on properties of TMDs



Γ,M,K—布里渊区的高对称性点。



(a) 二硫化钨层数n=1,2,…,5时的标准化光致发光性光谱

(b) 二硒化钨层数n=1,2,…,5时的标准化光致发光性光谱

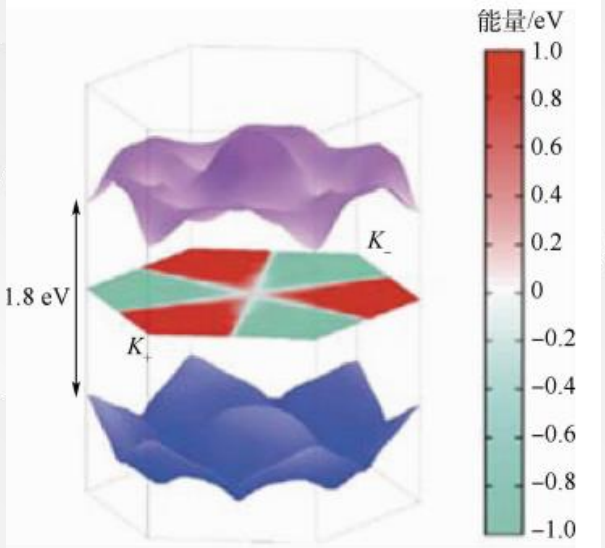
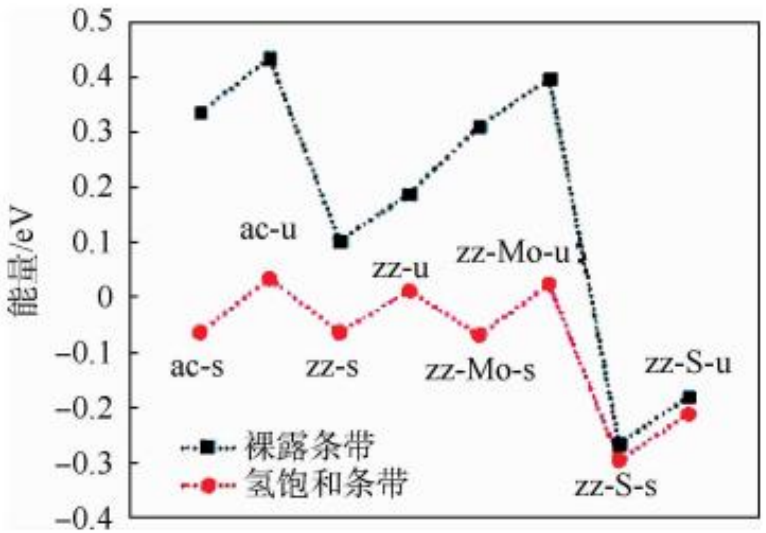
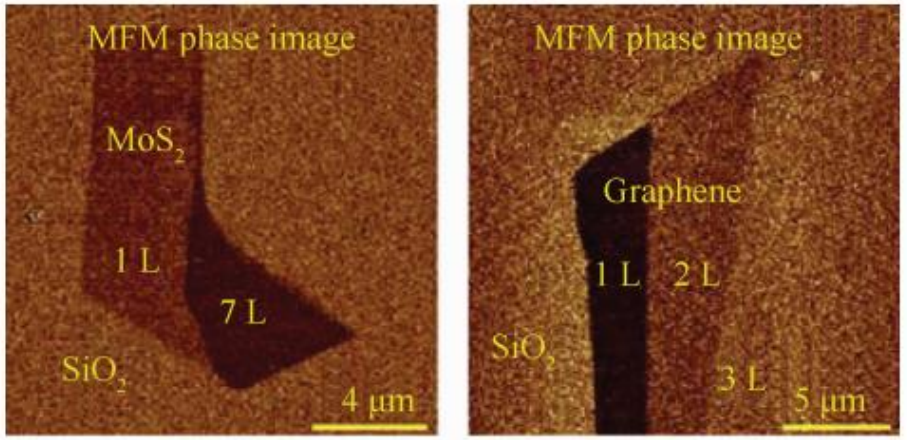


图 4 价带顶和导带底[51]

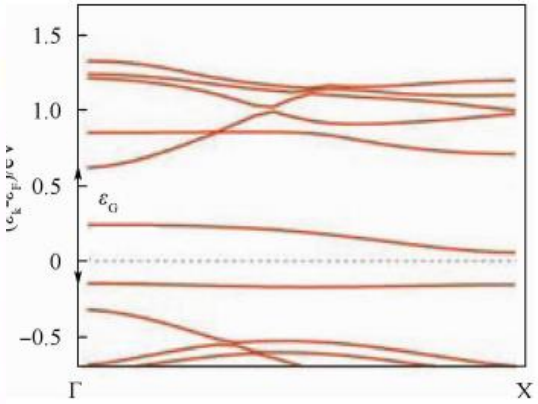
Top valence band and bottom conduction band





(a) MoS_2

(b) 石墨烯

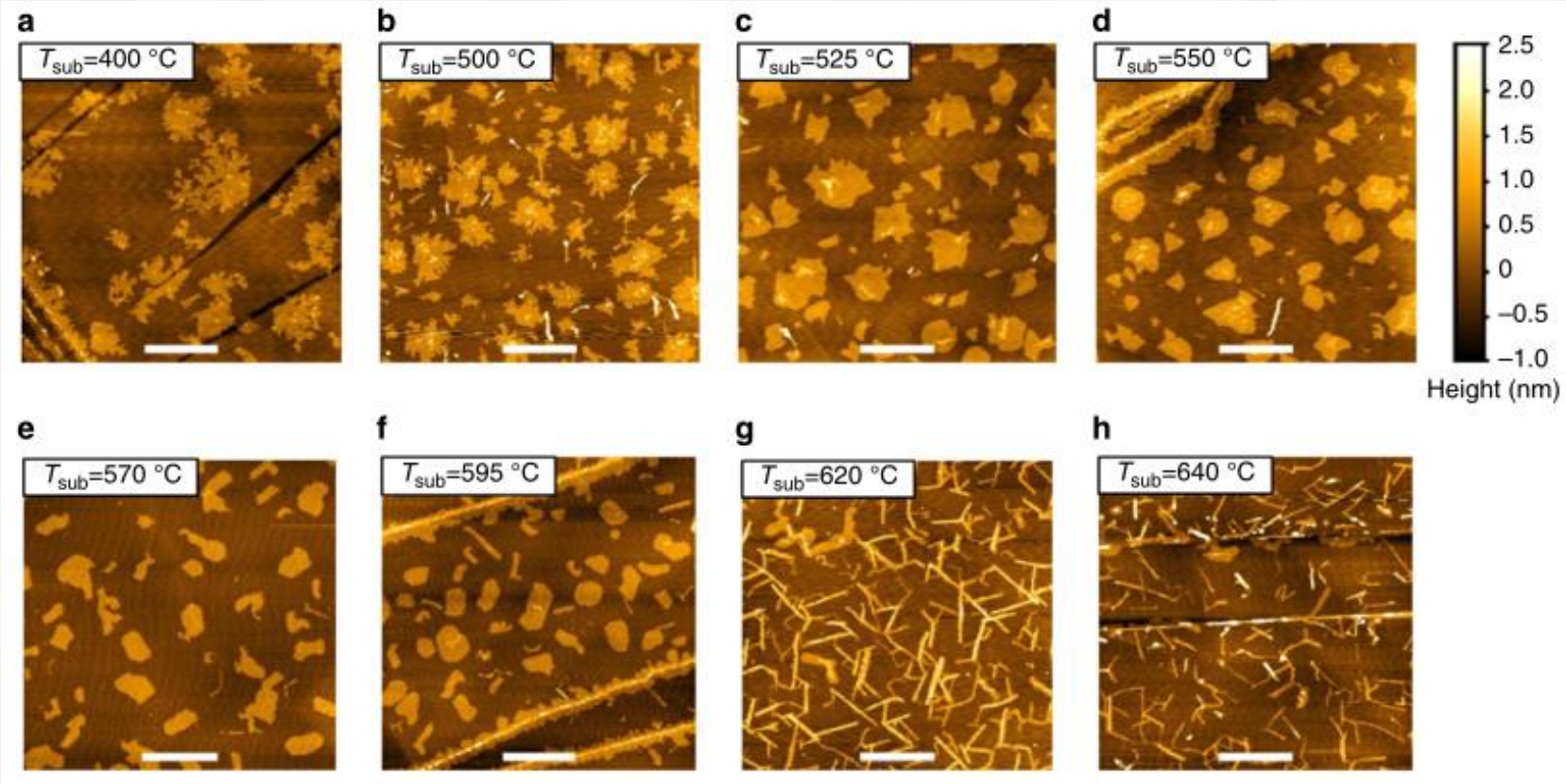


ε_G—禁带宽度;ε_k—动能;ε_F—费米能。

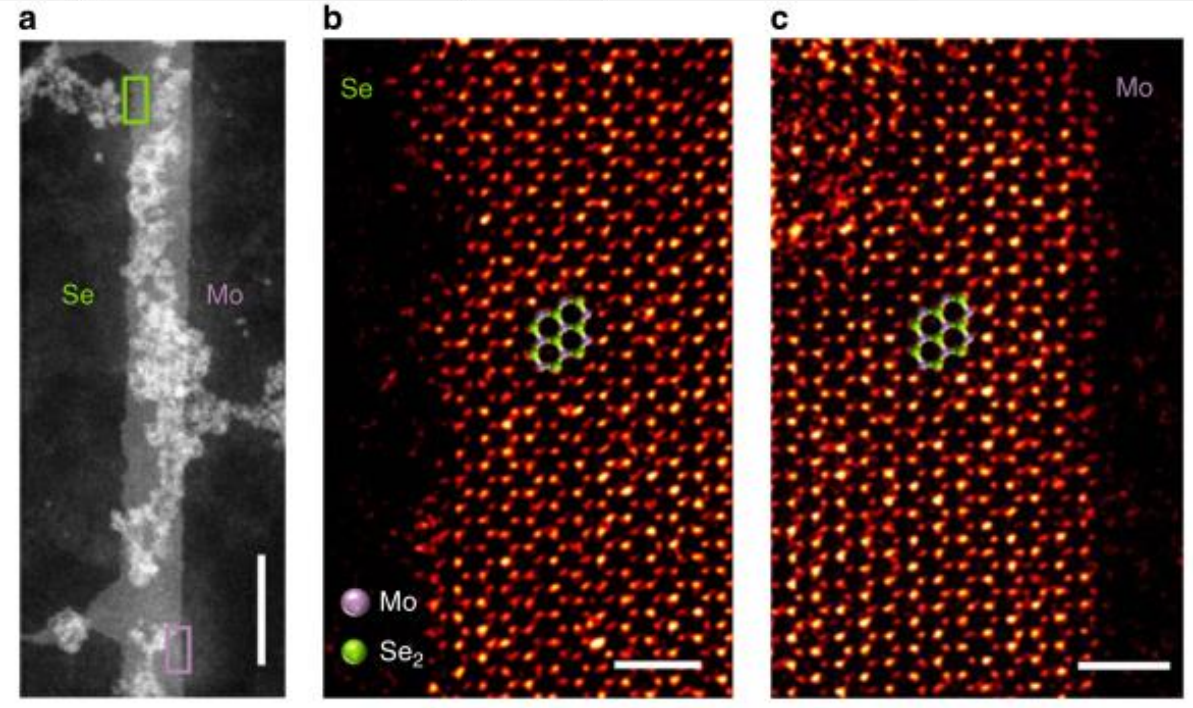
4 二硫化钼条带钼边缘吸收硫单体的费米能附近电子能带结构[37]

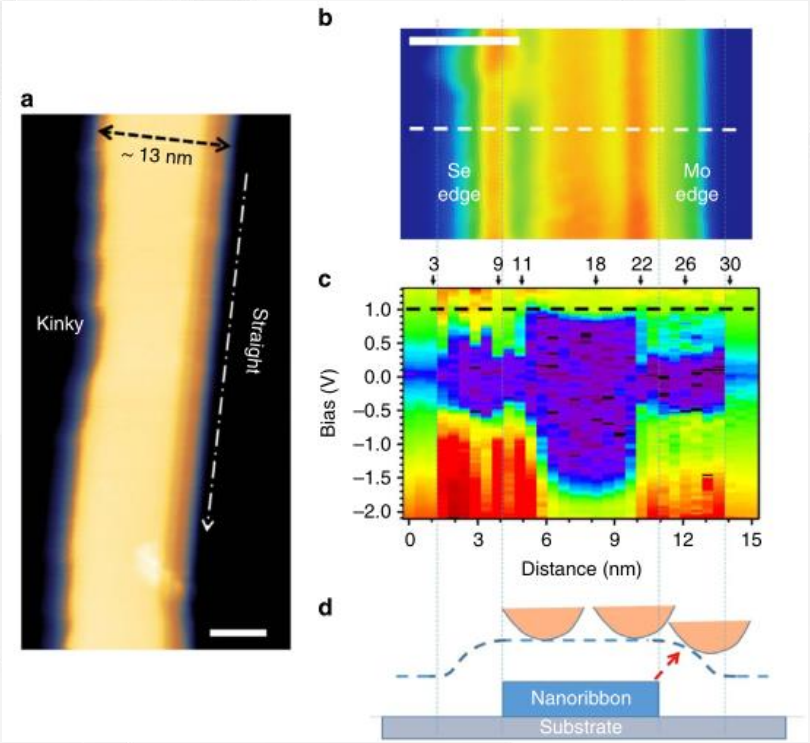
02

An unusual 2D-to-1D morphological phase transition of TMDs in MBE growth



An unusual pattern of nanoribbon growth has been discovered in the molecular beam epitaxy (MBE) growth of MoSe2 (molybdenum selenide) on a graphite substrate. With proper control of substrate temperature and Se overpressure, the MoSe2 atomic layer undergoes a three-stage shape transition: from fractals to compact 2D nanoislands, and finally to nanoribbons, which is in contrast to the traditional two-stage growth behavior involving only transitions (from fractal to compact) different.





The lattice structure of MoSe2 nanoribbons is still stable 1H phase instead of metastable 1T or 1T0 phase. This observation indicates that there is no structural phase transition accompanied by a morphological phase transition that leads to the formation of nanoribbons. Furthermore, inferred from the atomic registration, which is determined by the brightness of the atoms, the long sides of the strips are all zigzag edges, the straighter edges are molybdenum edges, and the more curved edges are selenium edges

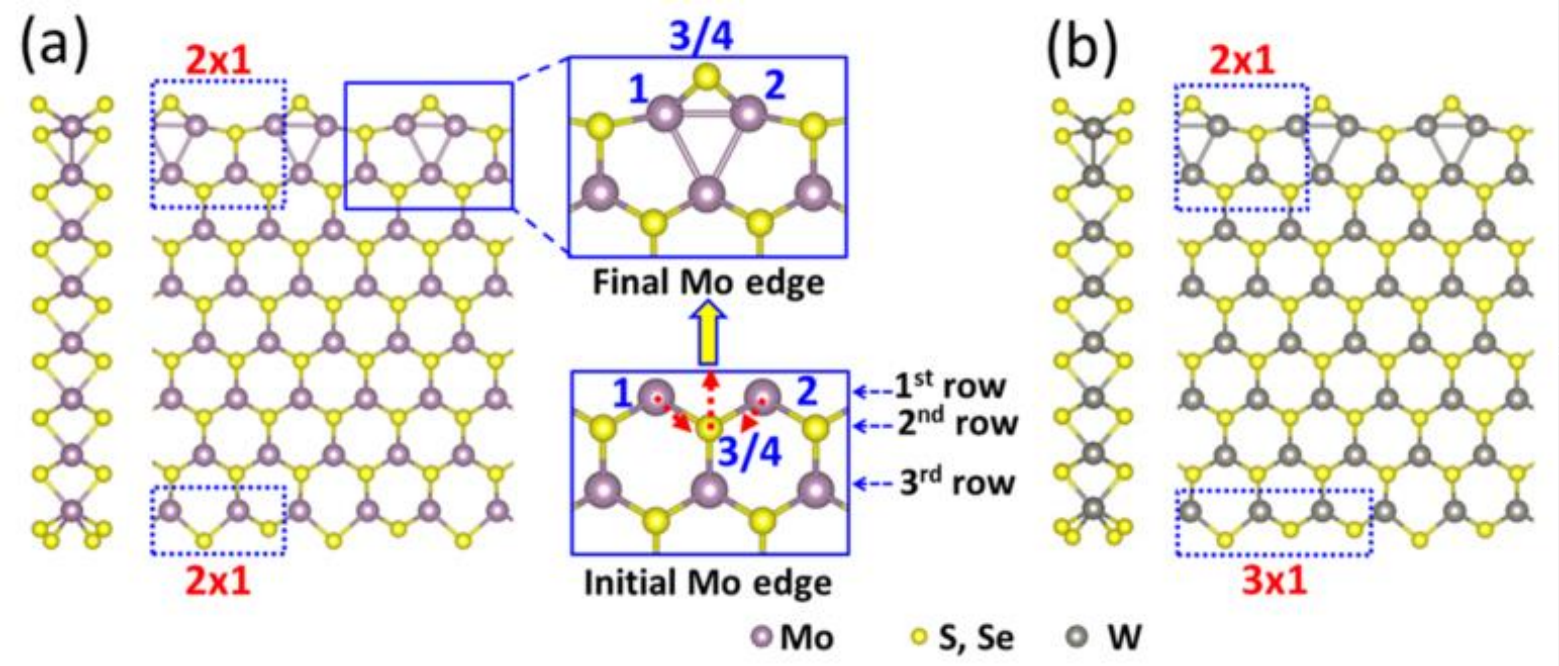
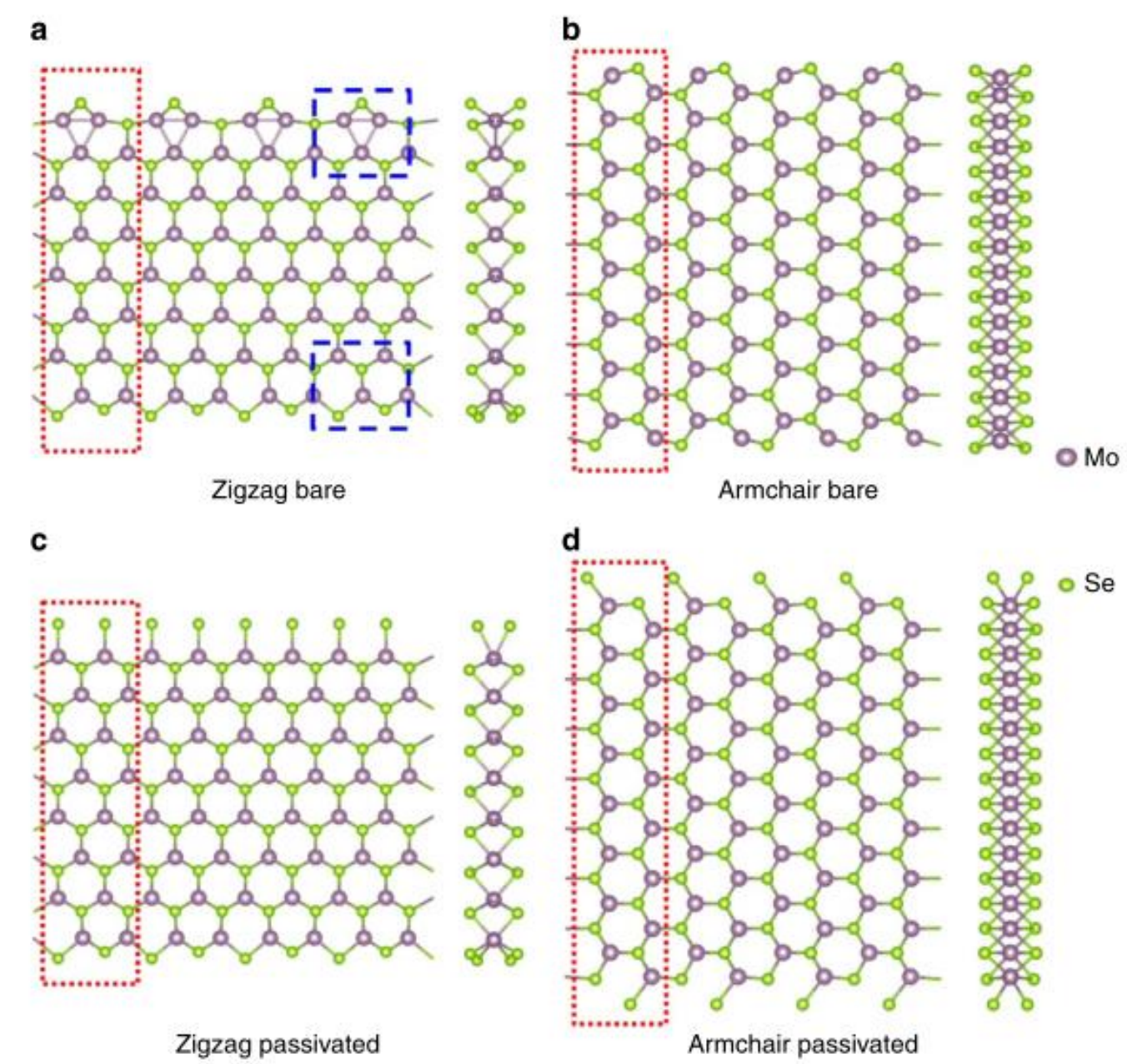


Table 1. Energy Change (ΔE) Due to Edge Reconstruction[a]

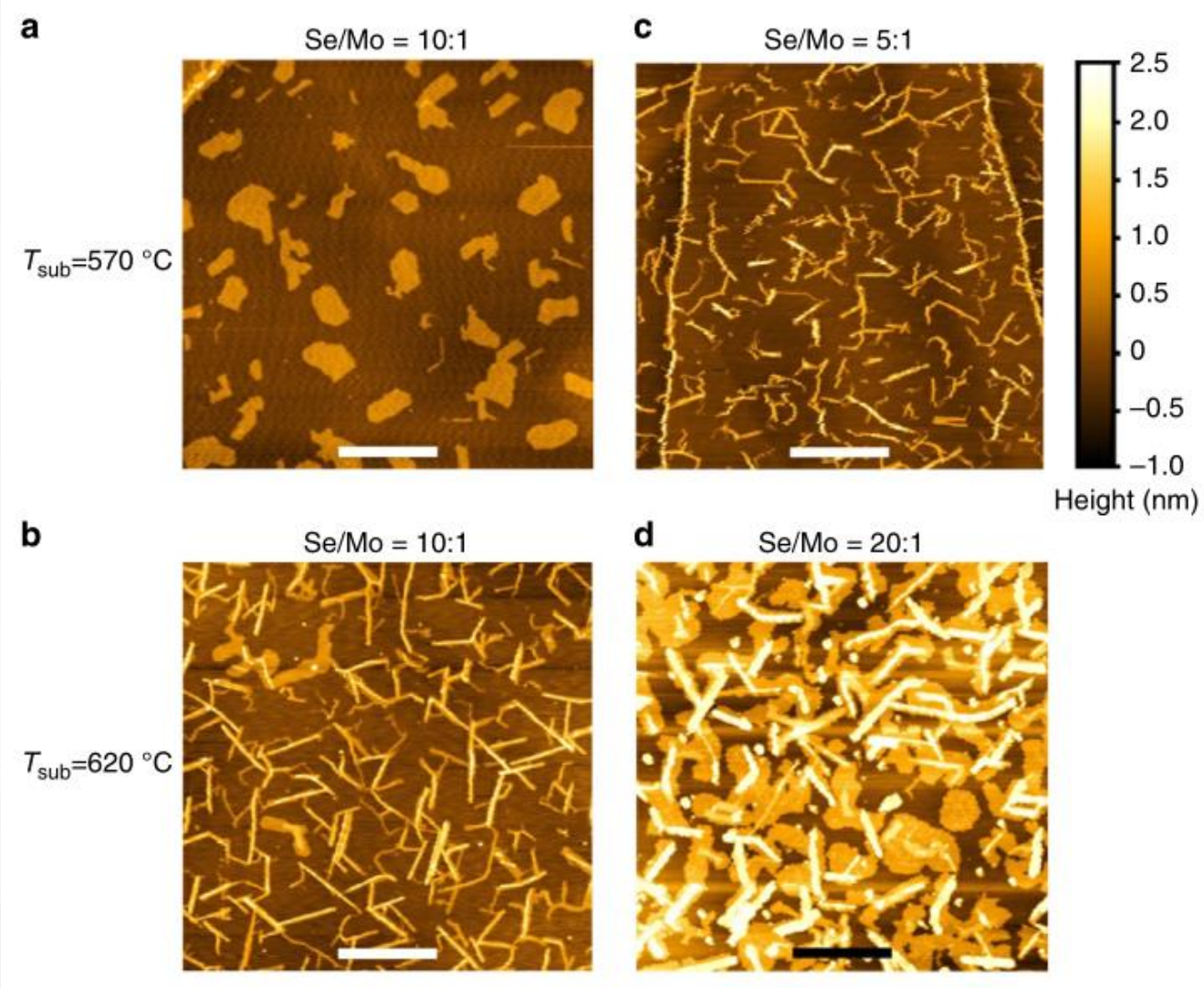
	MoS_2		$MoSe_2$		WS_2		WSe_2	
	2 × 1	3 × 1	2 × 1	3 × 1	2 × 1	3 × 1	2 × 1	3 × 1
M edge	**0.261**	−0.014	**0.823**	0.515	**0.807**	0.531	**1.012**	0.690
X edge	**0.320**	0.259	**0.158**	0.115	0.120	**0.172**	0.009	**0.046**

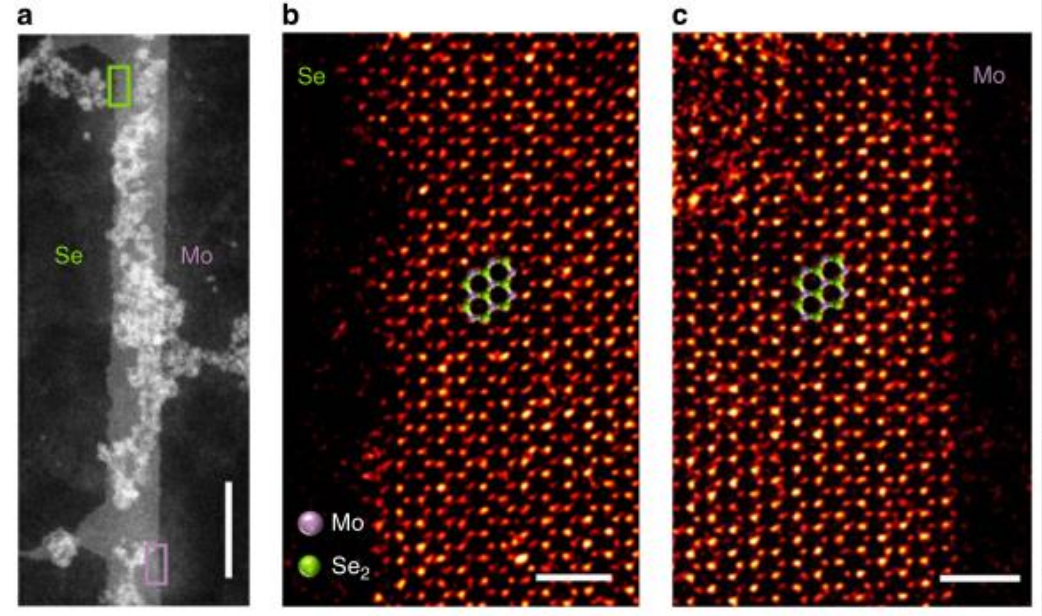
The most likely reason is that the relative energies and growth rates between different edges have changed at the transition temperature, including bare zigzag (molybdenum and selenium edges) and armchair edges and their passivated counterparts.

At a constant selenium flux, the higher substrate temperature actually means a lower concentration of available selenium adatoms at the 2D island growth front, since the binding energy of selenium is much lower than that of molybdenum. Therefore, we speculate that the available selenium concentration on the surface must have played a key role in changing the bonding configuration of the different edge structures, thereby changing their relative energies and growth rates.

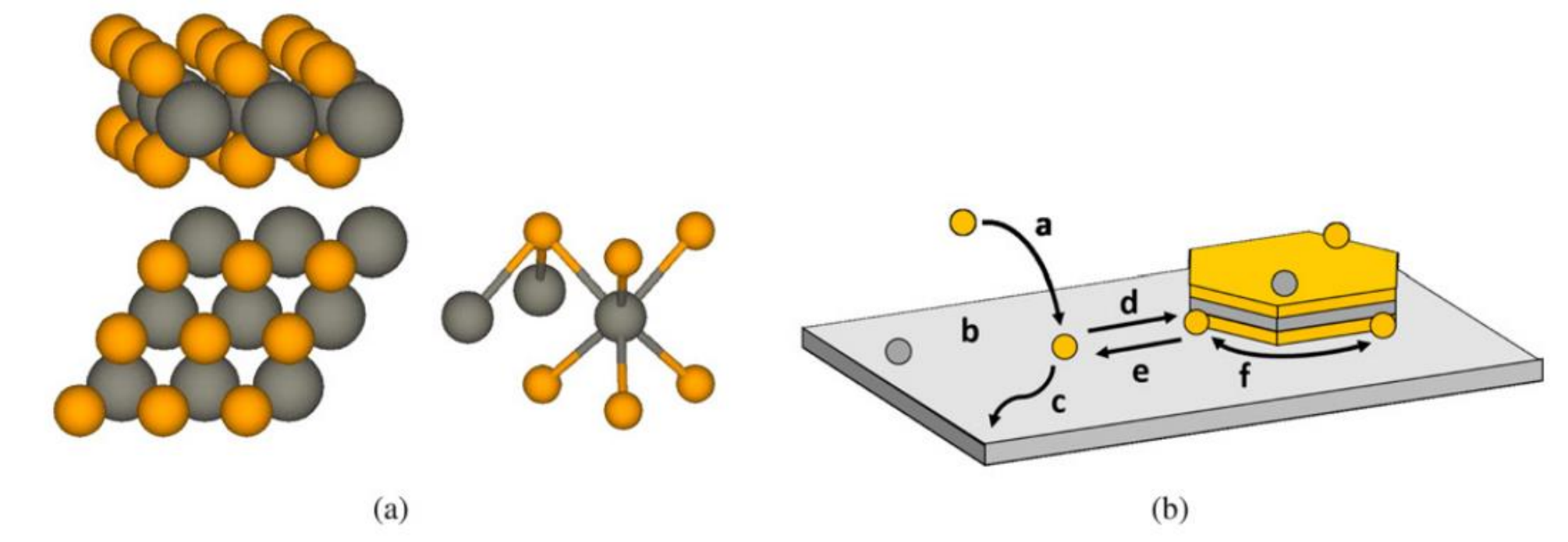


The energy gain along the reconstructed Mo edge is 0.82 eV per cell, while the energy gain along the reconstructed Se edge is 0.16 eV per formula cell. In particular, the more stable reconstructed Mo edges become straighter, while the less stable Se edges contain more kinks. Conversely, under Se-enriched conditions, excess Se adatoms can effectively passivate molybdenum atoms at the edge, and the total energy of fully passivated zigzag and armchair nanoribbons is found to be closer, with the former only 0.10 eV lower per unit. In this case, the growth rates of the zigzag and armchair edges are also expected to be almost the same, thus favoring the compact structure of the MoSe2 islands.





This theory is confirmed experimentally: the temperature from 2D (or compact) to 1D (or elongated) growth mode can indeed be changed by the nominal Se:Mo flux ratio, confirming that Se adatoms play a role in triggering the The important role in the morphological transition, the lower selenium concentration is favorable for the growth of nanoribbons



I wish to develop a kinetic Monte Carlo model based on diffusion on a lattice to describe vdW nucleation and growth of low-dimensional TMDs. The combination of KMC simulations with first-principles calculated parameters and advanced algorithms makes it possible to accurately simulate and effectively describe the competing factors that lead to many phenomena important to the growth process and atomic-scale mechanisms of TMD materials. This model will provide insight into the fine-grained control of vdW epitaxy of TMDs, providing a quantitatively accurate model for MBE growth of TMDs.

03

Case THREE

Electrochromic films

中国科学技术大学
University of Science and Technology of China

NiO/ WO3 based Electrochromic films

电致变色玻璃

03 What did I do

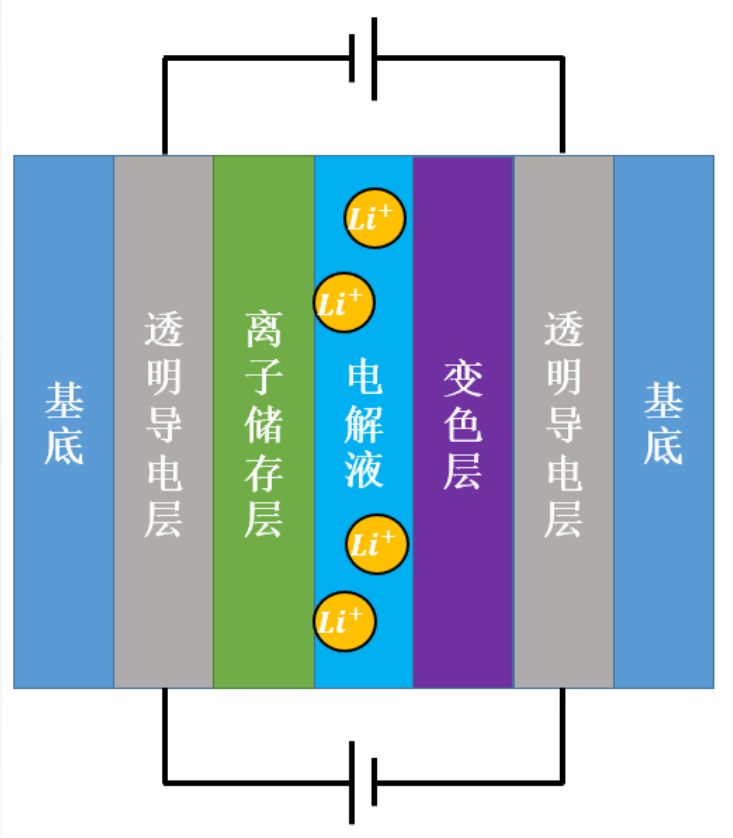
01 Prepared NiO and WO3 color-changing glasses under different sputtering conditions

02 Compared the discoloration and cycle performance of glasses and optimized parameters by means of characterization

01 Prepared NiO and WO3 color-changing glasses under different sputtering conditions

The mechanism of electrochromic

Electrochromic phenomenon refers to the phenomenon that the material undergoes reversible discoloration under the action of redox reaction under the condition of applying voltage or current.



Fuaghnan Model:

$$WO_3 + x\,M^+ + x\,e^- \leftrightarrow M_x\,WO_3$$

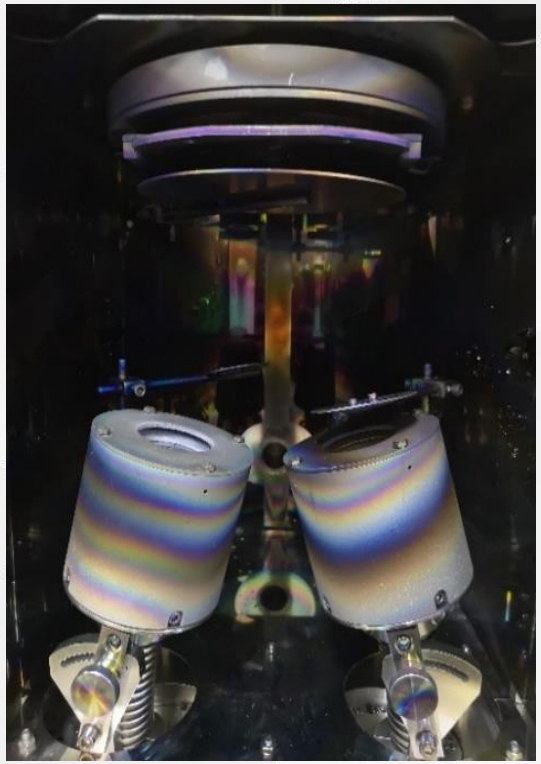
$$\mathrm{NiO}(bleached\ state) + \mathrm{OH}^- \leftrightarrow \mathrm{NiOOH}(colored\ state) + e^-$$

$$\mathrm{Ni(OH)_2}(bleached\ state) \leftrightarrow \mathrm{NiOOH}(colored\ state) + \mathrm{H}^+ + e^-$$

$$\mathrm{NiO_X}(initial\ deposition) + \mathrm{yM}^+ + \mathrm{ye}^- \leftrightarrow \mathrm{M_yNiO_X}(bleached\ state)$$

$$\mathrm{M_yNiO_X}(bleached\ state) \leftrightarrow \mathrm{M_{y-z}NiO_X}(colored\ state) + \mathrm{zM}^+ + \mathrm{ze}^-$$

Magnetron Sputtering Coating



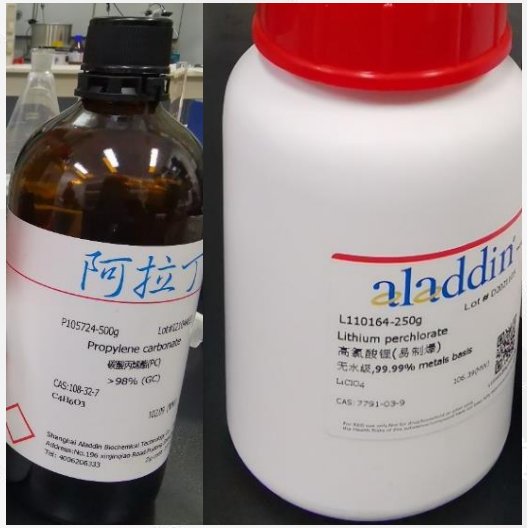
The target is placed in the cathode and the vacuum coating chamber is filled with process gas. The process gas is a mixture of argon (Ar) and oxygen in a certain proportion; then a high voltage is applied in two stages to cause a glow discharge. At this time, Ar is ionized to generate Ar positive ions and new electrons; the new electrons fly to the substrate, and the Ar ions are accelerated to the cathode target under the action of the electric field, and bombard the target surface with high energy, causing the target to sputter.

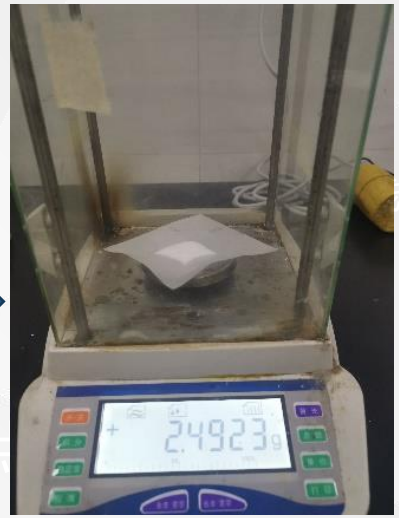
Preparation of thin films

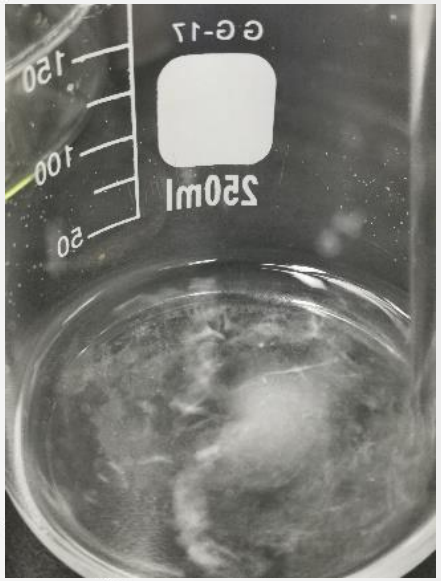
Preparation of thin films

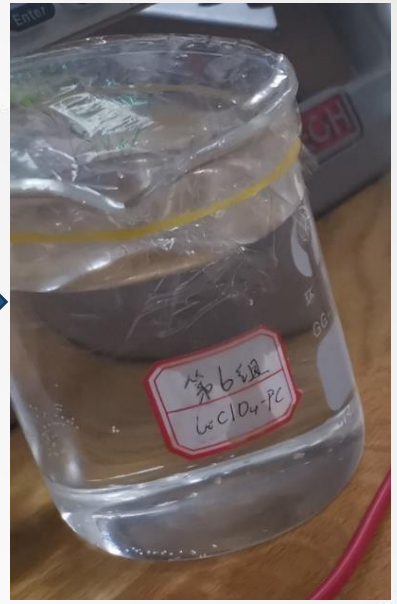
material	Sputtering temperature（℃）	Ar:O2（sccm）	Sputtering power（W）	Sputtering time (h)
WO3	25	15:15	150	1
WO3	25	15:15	100	2
WO3	200	10:20	100	1
WO3	200	15:15	100	1.5
WO3	200	15:15	100	1
WO3	200	15:15	100	0.5
NiO	200	15:15	100	1
NiO	200	10:20	100	1
NiO	25	10:20	100	1

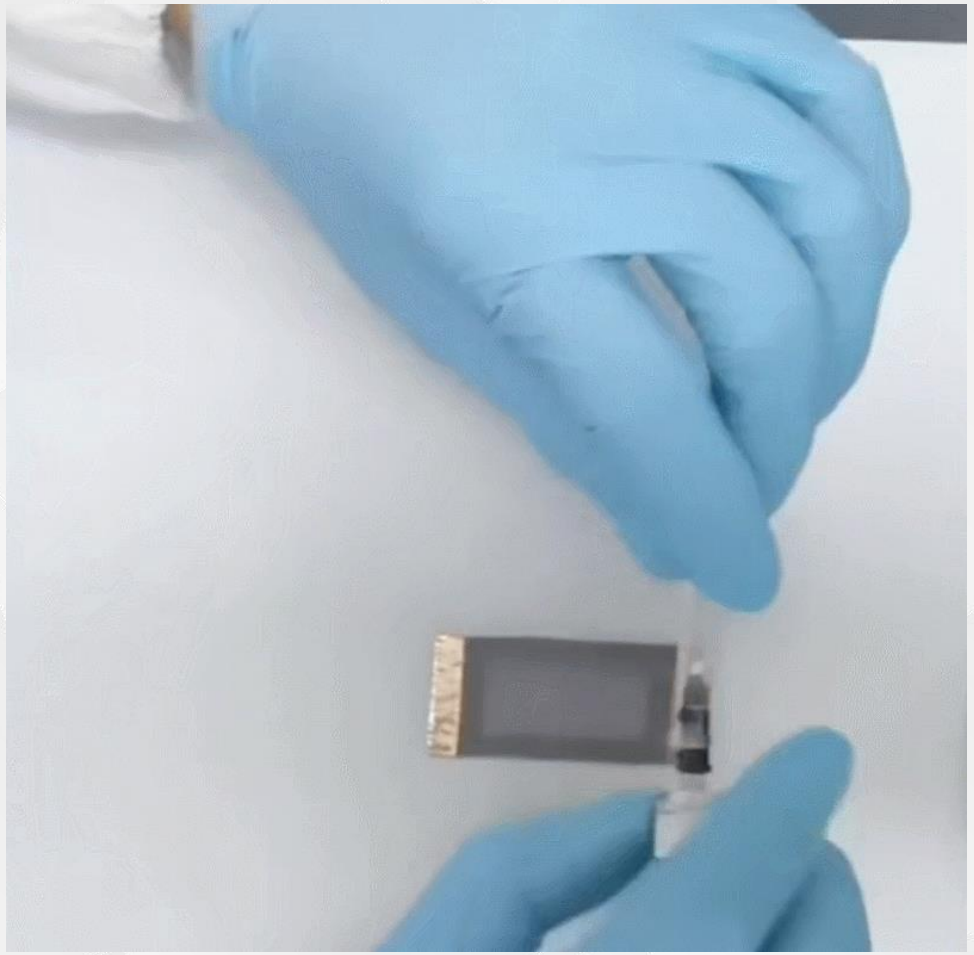
Preparation of Liquid Electrolytes



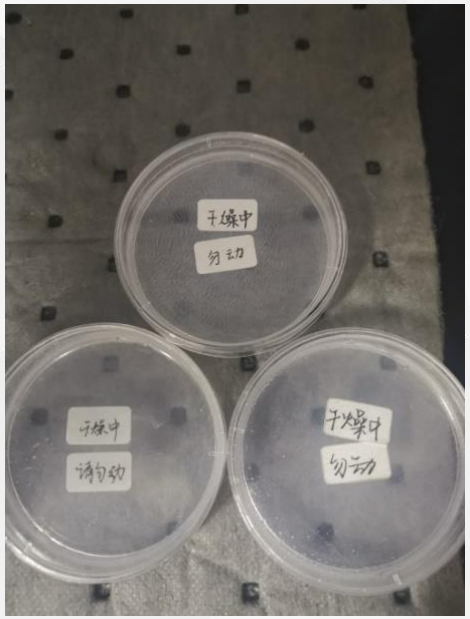




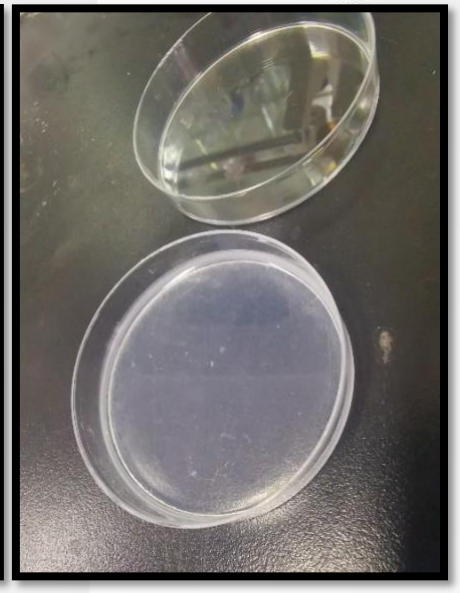




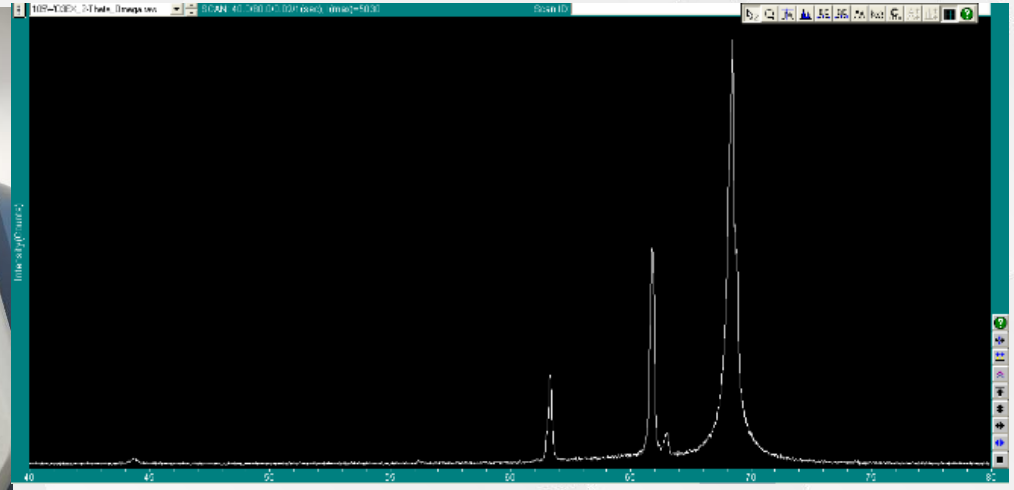
Preparation of Solid Electrolytes

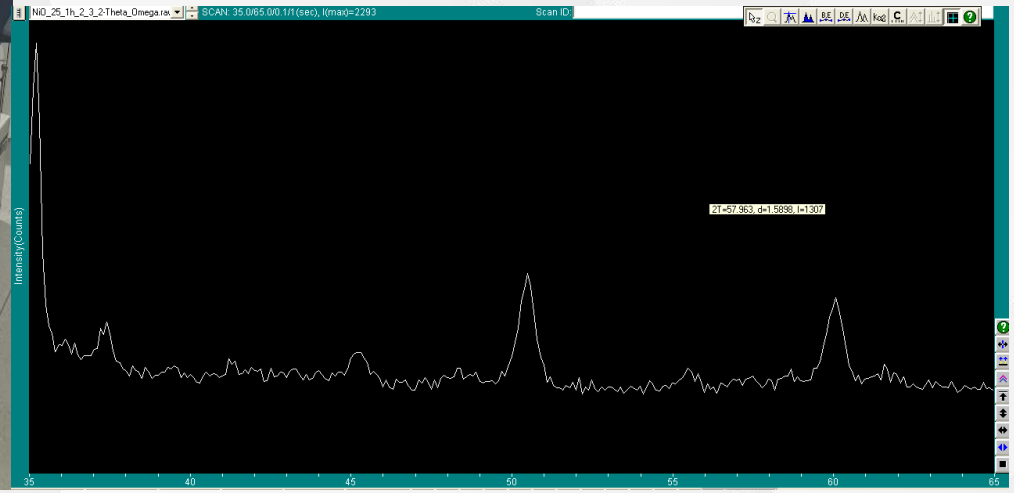


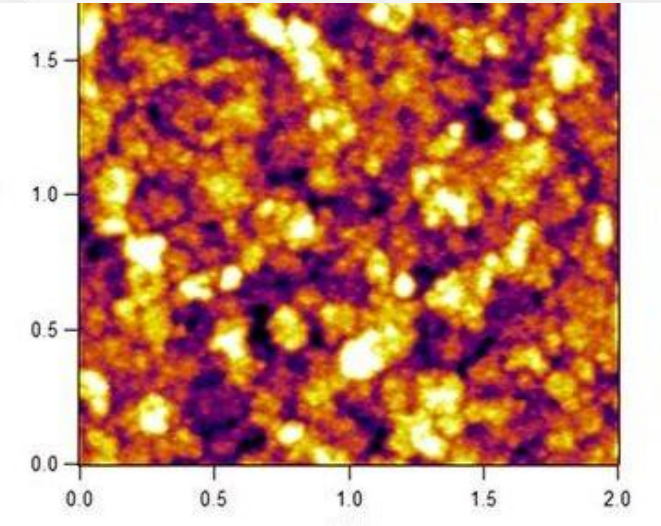
实践难点

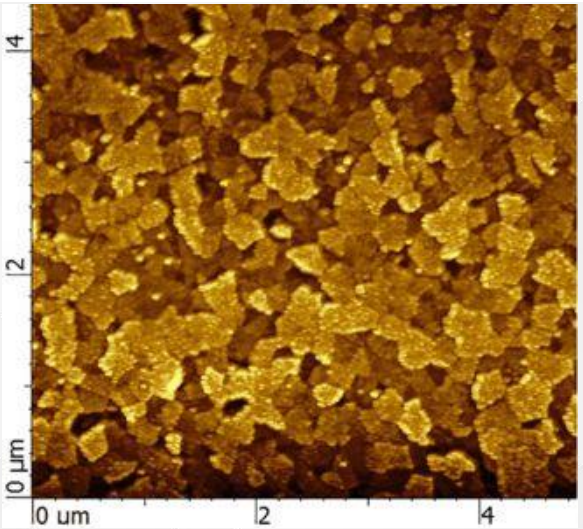


Characterization of film composition and morphology

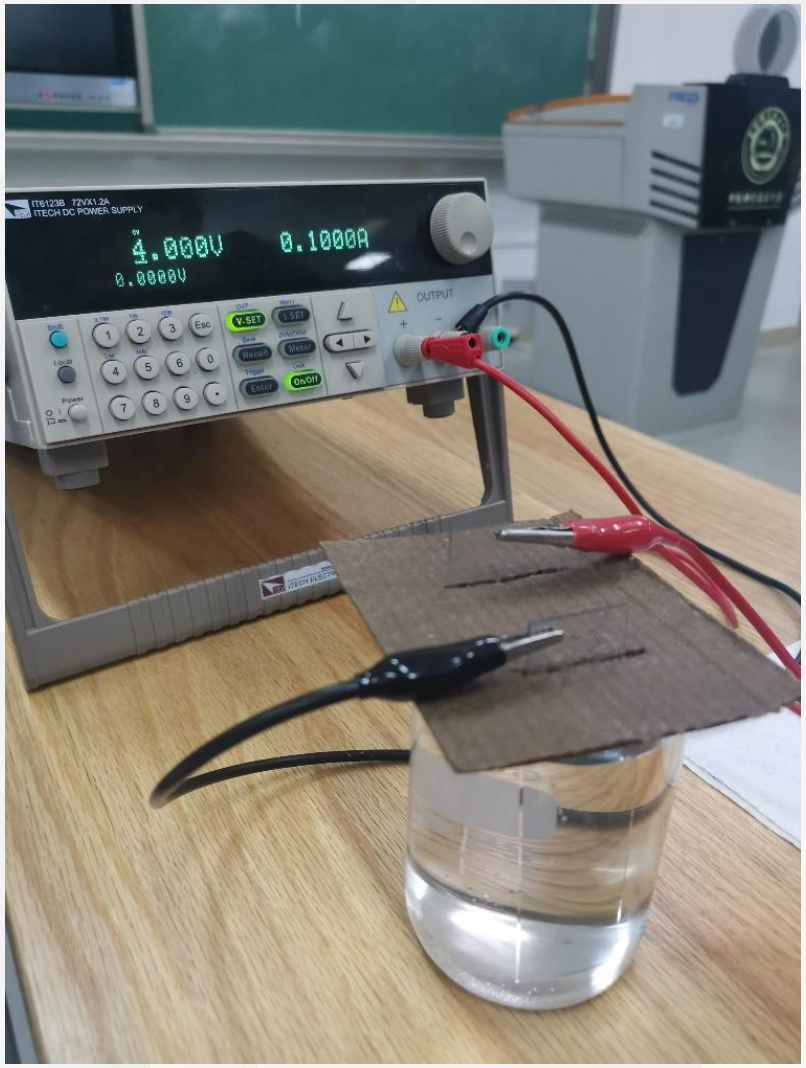




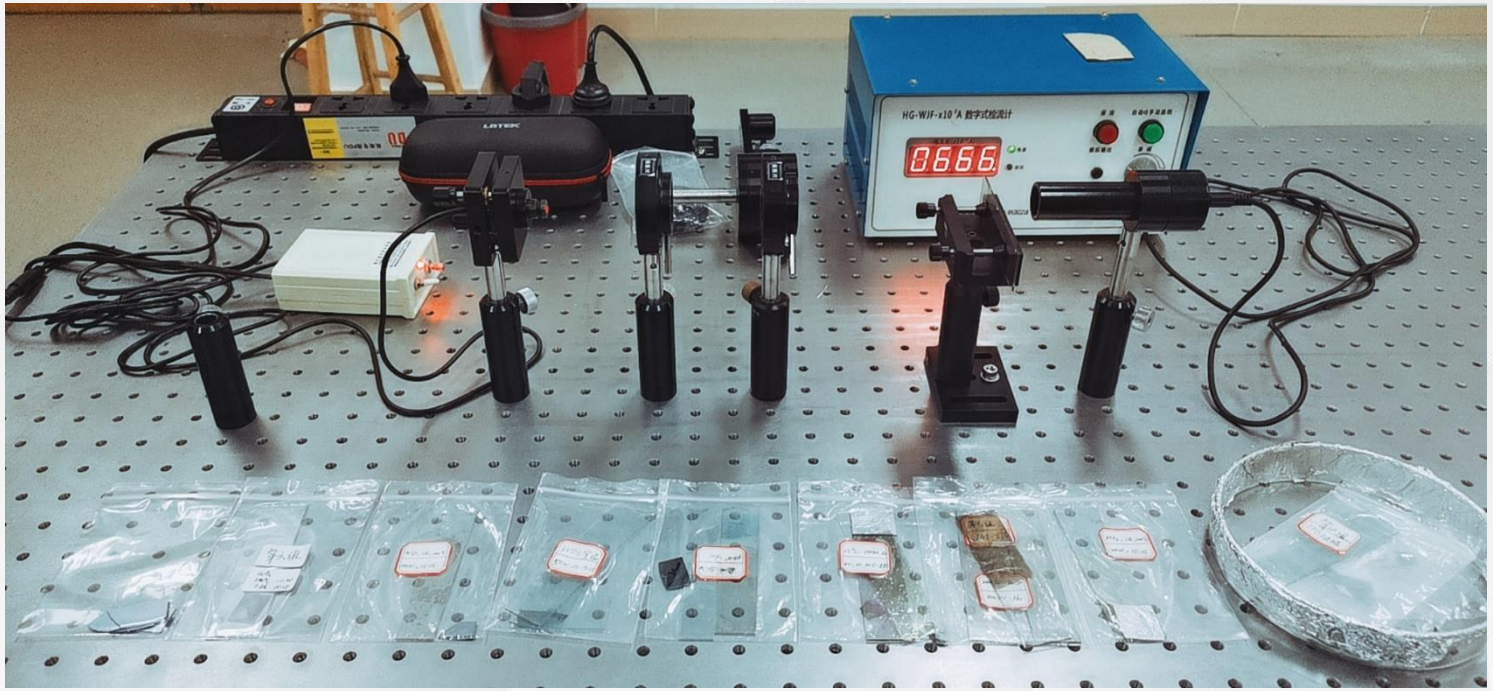




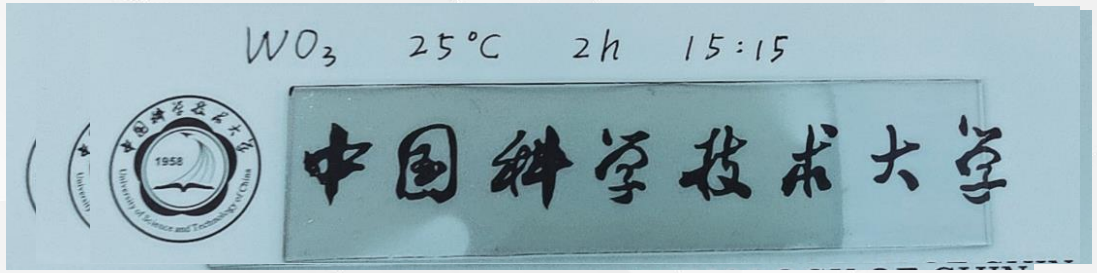
02 Compared the discoloration and cycle performance of glasses and optimized parameters by means of characterization

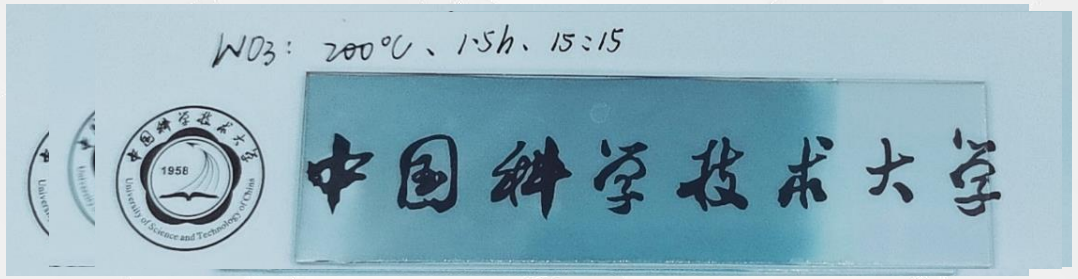


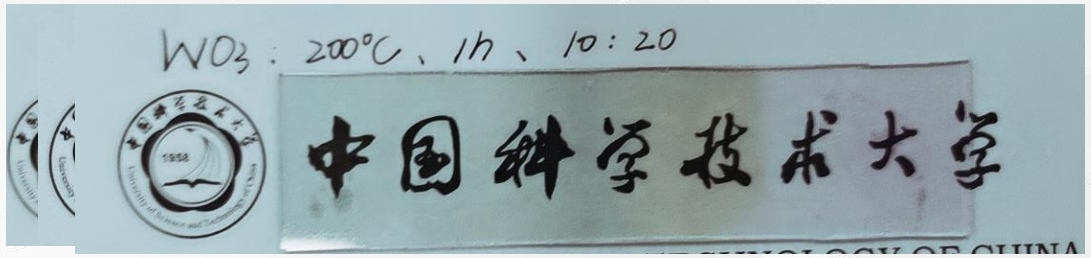
Color changing device and light path for measuring changes in light intensity

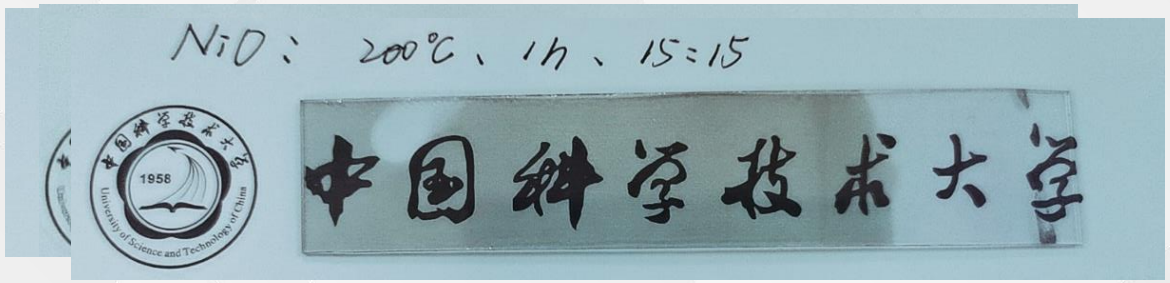


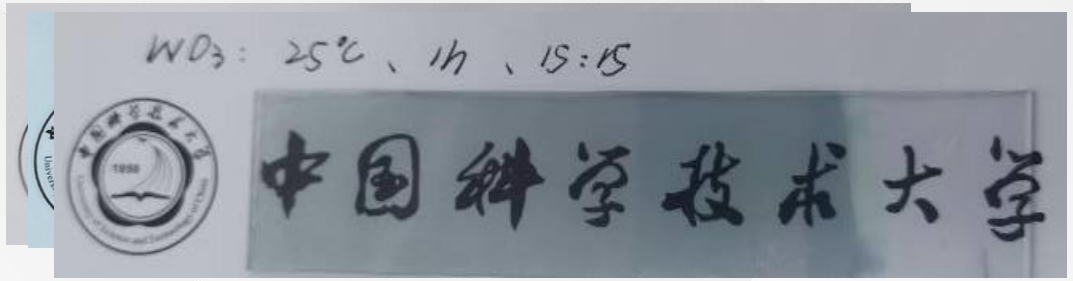
Color change and cycle effect

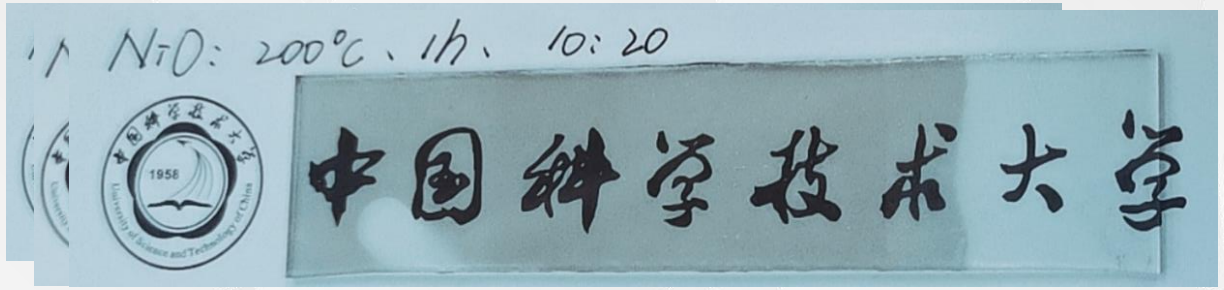




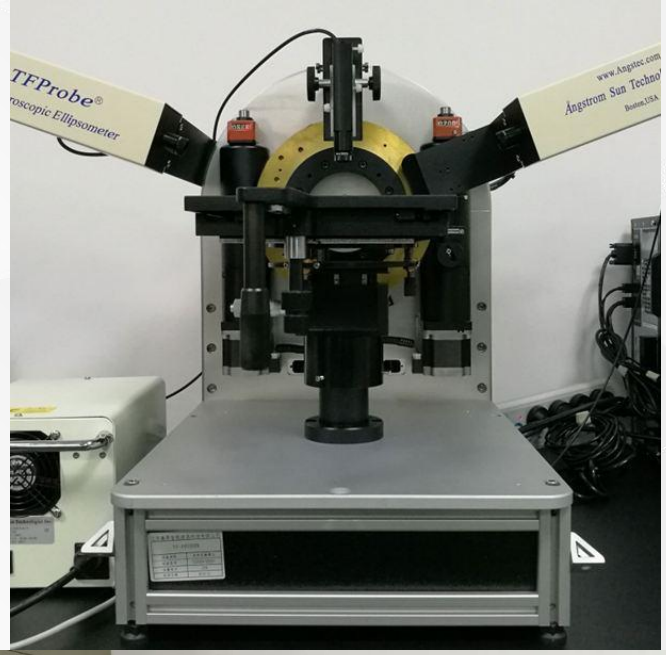


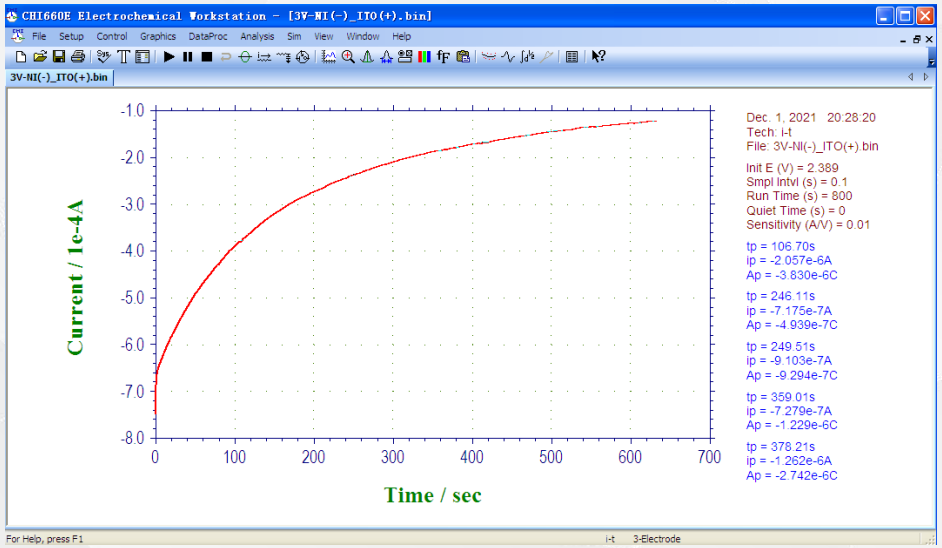


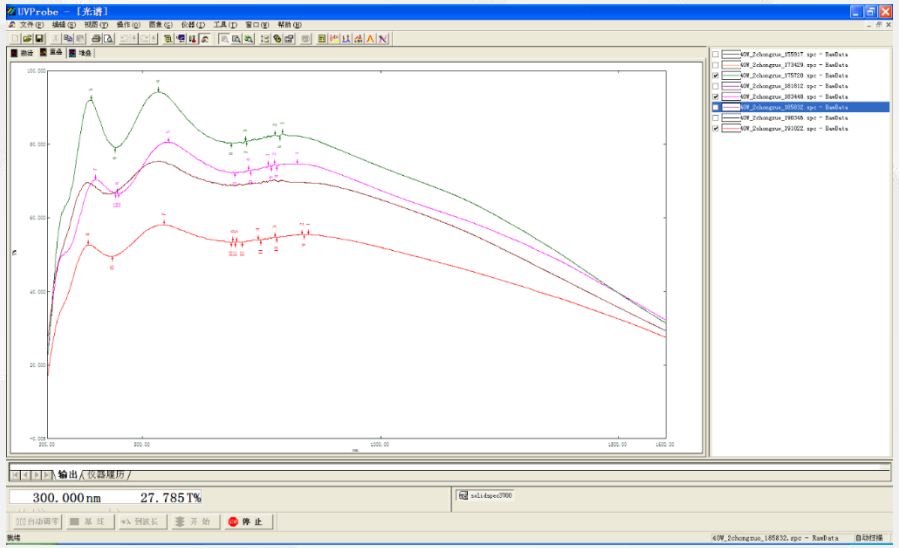


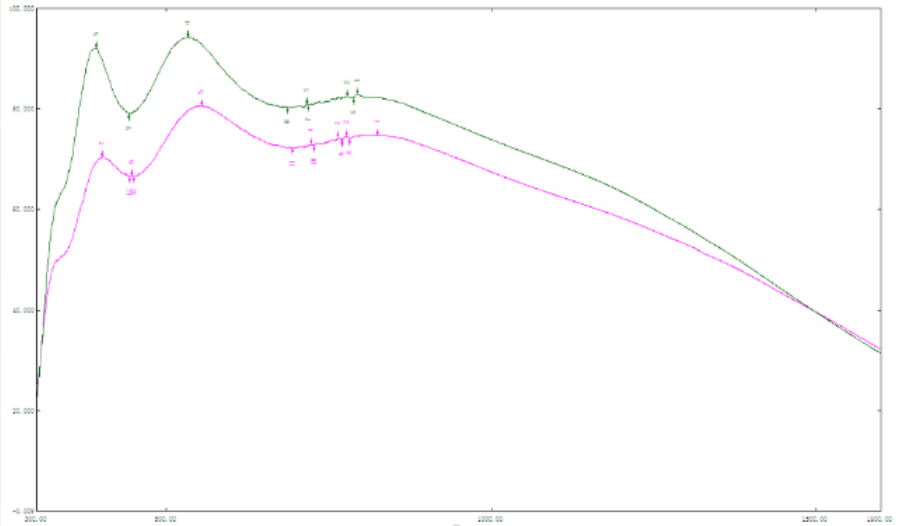


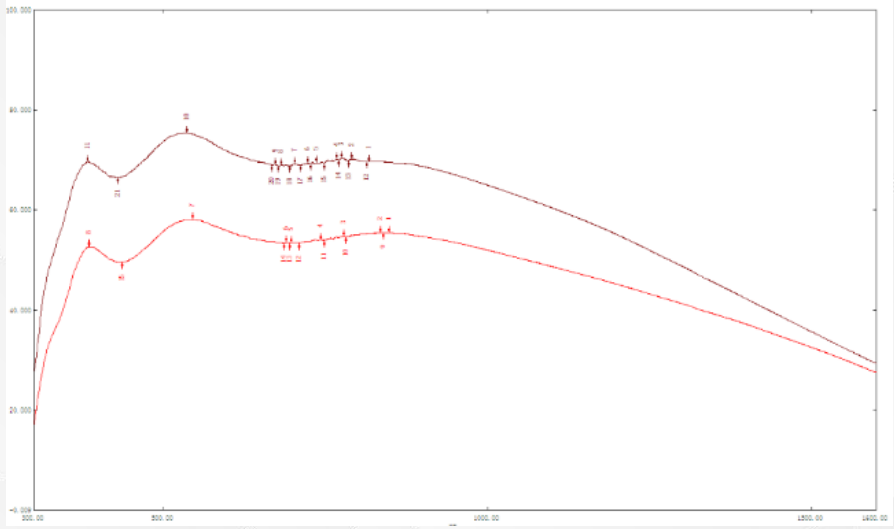
Measurement of current, film thickness and transmission spectra











Analyze of the result

Parameters	Film thickness/nm	Light Intensity (change divided by color state)	Circulation coefficient
W03-25℃-1h-15:15（150W）	64.53±0.709	0.9471	0.77427
W03-25℃-2h-15:15	57.00±0.184	0.3959	0.65775
W03-200℃-1h-10:20	50.77±0.559	0.2384	0.50943
W03-200℃-1.5h-15:15	58.04±0.175	0.5731	0.85374
W03-200℃-1h-15:15	54.91±0.194	0.3088	0.57868
W03-200℃-0.5h-15:15	46.57±0.335	0.1903	0.48182
Ni0-200℃-1h-15:15	53.85±0.105	0.3379	0.79070
Ni0-200℃-1h-10:20	52.62±0.060	0.2264	0.64567

Temperature will affect the roughness and looseness of the film;
Within a certain range, the thicker and looser the structure of the film, the stronger the ability to inject and extract ions, and the better the discoloration effect and cyclability.

04

Case FORE

X-rays

中国科学技术大学
University of Science and Technology of China

Comparison of the mechanisms of X-ray generation(literature research)

X射线产生的机制的比较(文献调研)

Mechanism	Nucleus-nucleus Bremss-trahlung	Secondary Electron Bremss trahlung	Transition Radiation	Channeling X- radiation	Two-electron One- photon Atomic Transition	Radiative Electron Capture	Inverse Compton Radiation	Synchrotron Radiation
Physical nature	Ion collision with target nucleus	Collision of ejected electrons	Particle-Media Interface Collision	Energy Level Transition of Crystal Plane Potential Wells	Two electrons transition at the same time	impact ion trapping target electron	High-energy particles enhance photons	Circular motion of high-energy electrons
Features	asymmetric, big difference, high energy	The experimental environment is sensitive, small share	determined by the medium distribution	High radiation intensity, good monochromaticity, directional and polarized	characteristic spectral line, the energy spectrum is wider, low probability	The target electron momentum needs to meet the conditions, and there is a sharp peak	Uneven distribution of angles	High power, wide energy spectrum, good directivity and polarization
Application direction	generate electron-positron pairs	Background noise, try to control	Measure media properties, record high-energy particles	Crystal fine structure measurement	Elemental identification	Momentum distribution of electricity in solids	Particle deceleration, X-ray source	Particle and Nuclear Physics Research

05

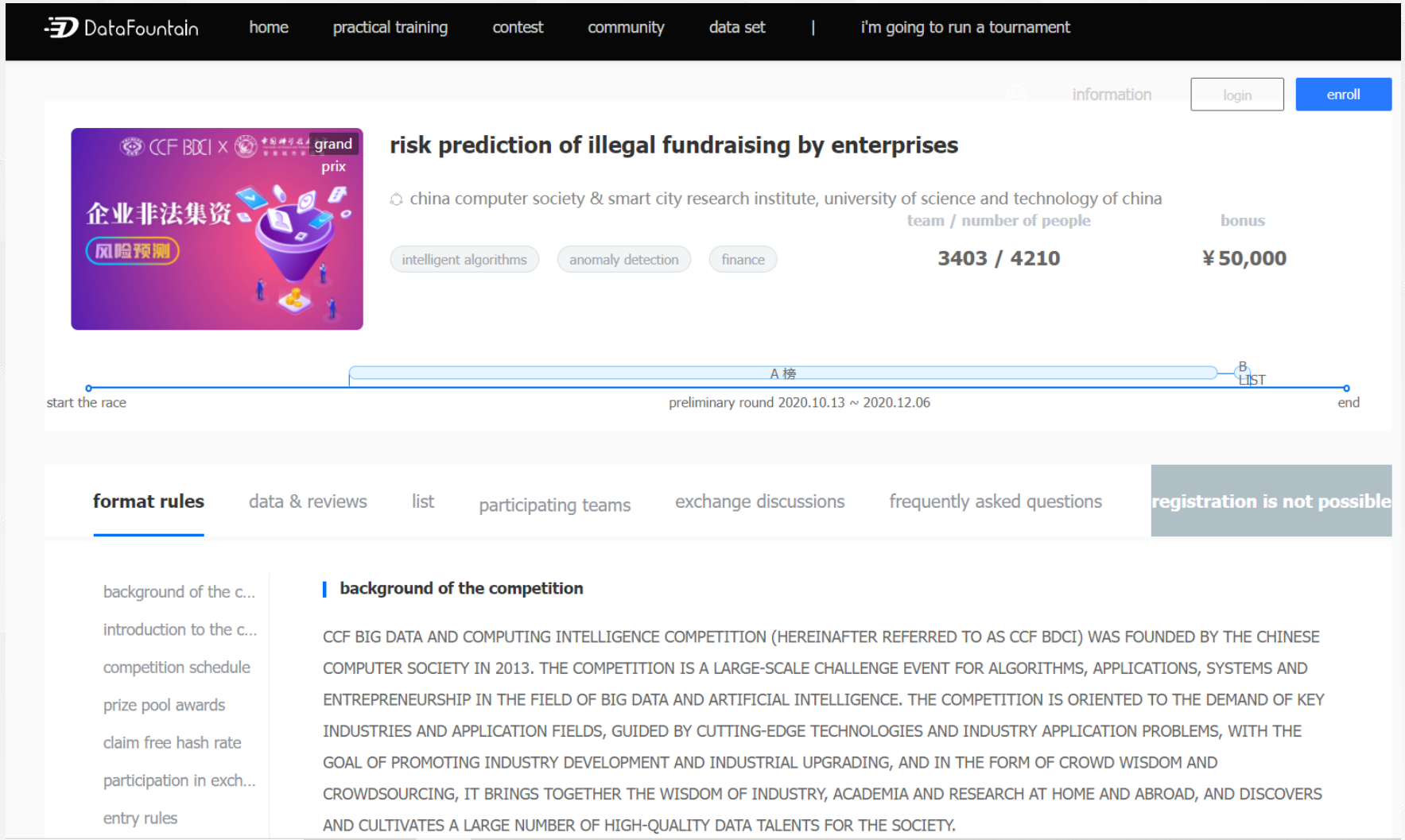
Case FIVE

Big data science

中国科学技术大学
University of Science and Technology of China

Prediction of the risk of illegal fundraising by enterprises (2020 CCF Competition Questions)

企业非法集资风险预测（2020CCF大数据与计算智能大赛赛题）



Using machine learning, deep learning and other methods to train a predictive model, the model can learn relevant information about the enterprise to predict whether the enterprise has the risk of illegal fundraising. The difficulty of the competition is that the data set includes a large amount of enterprise-related information, and how to extract effective features from it and make risk predictions becomes the key issue of this competition.

My Solution and Score

I. Preprocessing and statistical sorting
II. Building features
III. Use the cross-validation method to cyclically train the model, and use LightGBM+gridsearchcv to automatically find better parameters
IV. Predict the results, then calculate the accuracy

```python
def k_fold_serachParmaters(model,train_val_data,train_val_kind, test_kind):
    mean_f1=0
    mean_f1Train=0
    n_splits=5

    cat_features = ['oplocdistrict', 'industryphy', 'industryco', 'enttype',
            'enttypeitem', 'enttypeminu', 'enttypegb',
           'dom', 'oploc', 'opform']

    sk = StratifiedKFold(n_splits=n_splits, shuffle=True, random_state=2020)
    pred_Test = np.zeros(len(test_kind))
    for train, test in sk.split(train_val_data, train_val_kind):
        x_train = train_val_data.iloc[train]
        y_train = train_val_kind.iloc[train]
        x_test = train_val_data.iloc[test]
        y_test = train_val_kind.iloc[test]

        model.fit(x_train, y_train,
                  eval_set=[(x_test, y_test)],
                  categorical_feature = cat_features,
                 early_stopping_rounds=100,
                 verbose=False)

        pred = model.predict(x_test)
        fper_class = eval_score(y_test,pred)

        pred_Train = model.predict(x_train)
        pred_Test += model.predict_proba(test_kind)[:, 1]/n_splits
        fper_class_train = eval_score(y_train,pred_Train)

        mean_f1 += fper_class['f1']/n_splits
        mean_f1Train+=fper_class_train['f1']/n_splits
```

ranking	ranking changes	the name of the team	maximum score submission time	highest score
1	↑ 1	SLBBGC	2020-12-06 16:16	0.84933501
2	-	phantom day	2020-12-06 00:13	0.84835288
3	-	wu fan is not ordinary	2020-12-06 00:13	0.84777421

The highest accuracy of our model is 0.84520188762562878.

06

Case Six

Simulation of fusing

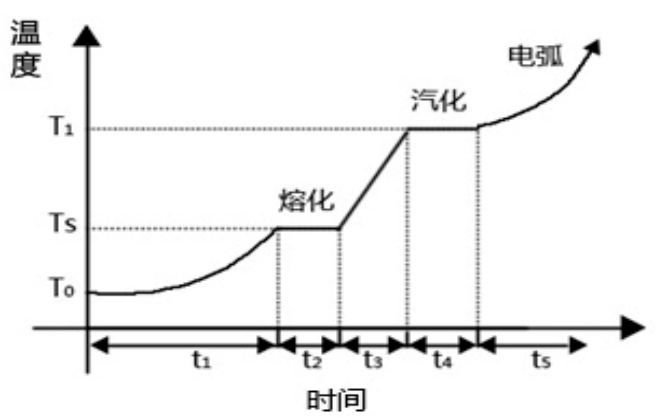
中国科学技术大学
University of Science and Technology of China

Influencing factors of fuse blowing

（2021 CUPT Competition Questions）

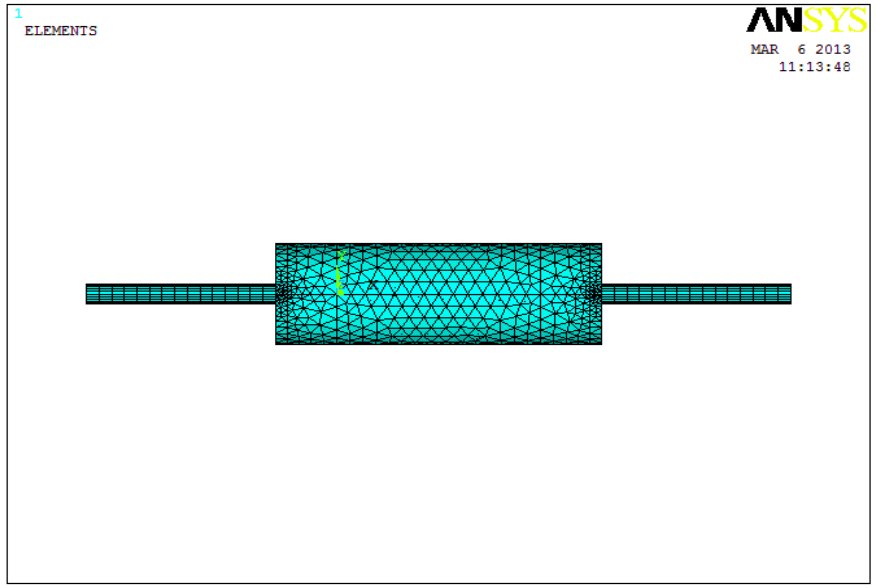
保险丝熔断因素（2021全国大学生物理竞赛赛题）

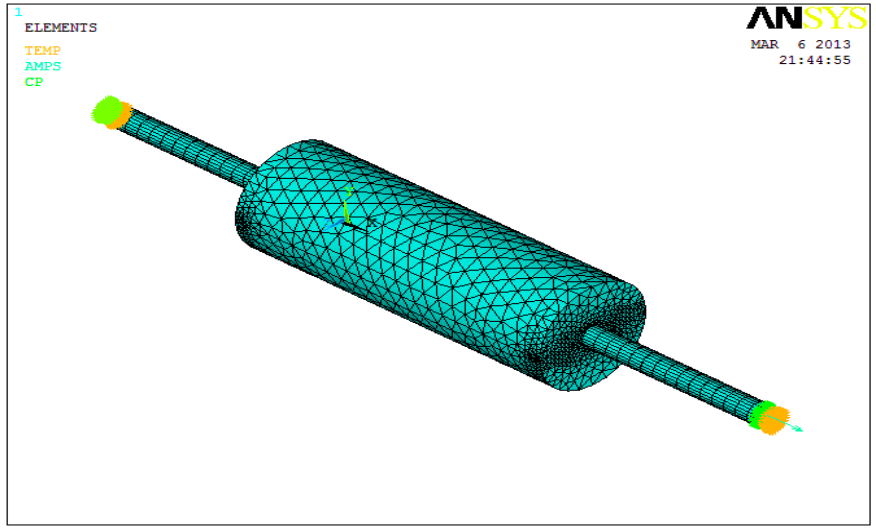
A short length of wire can act as an electrical fuse. Determine how various parameters affect the time taken for the fuse to ‘blow’.



This is the entire fuse process of the melt, and the total time required is t_1, t_2, t_3, t_4 and time. In fact, the temperature of each part of the melt is not uniform. The node with the highest temperature reaches the melting point and gas point first. Since the local liquid and gas state heat up very quickly, and the arc generation is also completed instantaneously, the main part is t_1

Theoretical Analysis and Modeling





A thermoelectrically coupled model

$$q_w + k\nabla^2 T = \rho c \frac{\partial T}{\partial t} \qquad t > 0 \quad (x, y, z) \in V$$

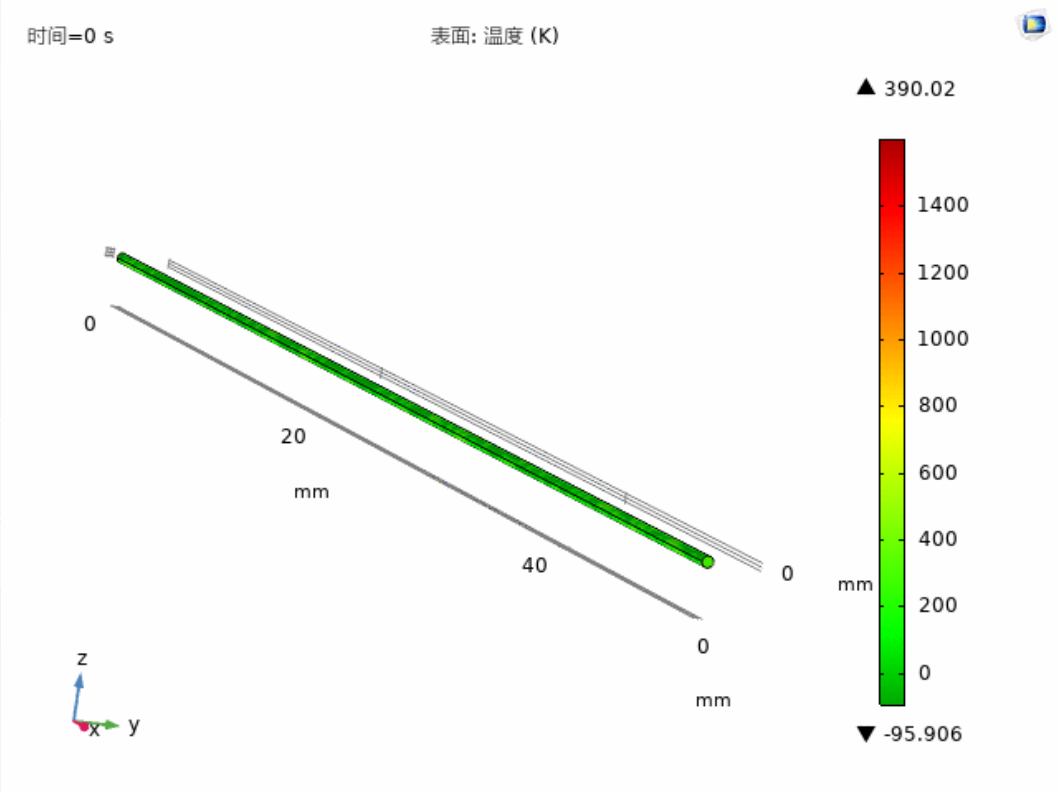
$$T(t, x, y, z) = T_{\mathrm{f}} \qquad (x, y, z) \in \text{Cylinder bottom}$$

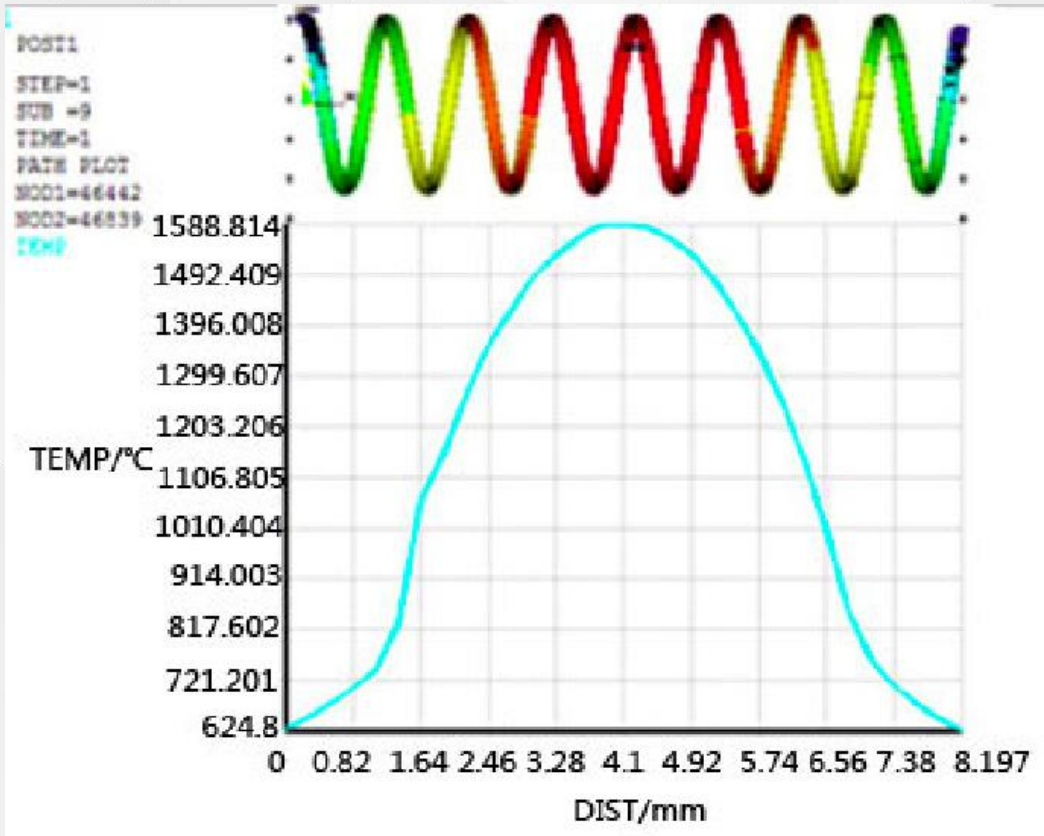
$$q_a + q_{\mathrm{t}} + q_{\mathrm{e}} = 0 \qquad (x, y, z) \in \text{Cylinder side}$$

$$T(0, x, y, z) = T_{\mathrm{f}}$$

$$q_a = -k \frac{\partial T}{\partial n} \qquad q_t = h(T_i - T_{\mathrm{f}}) \qquad q_e = \varepsilon \sigma T^4$$

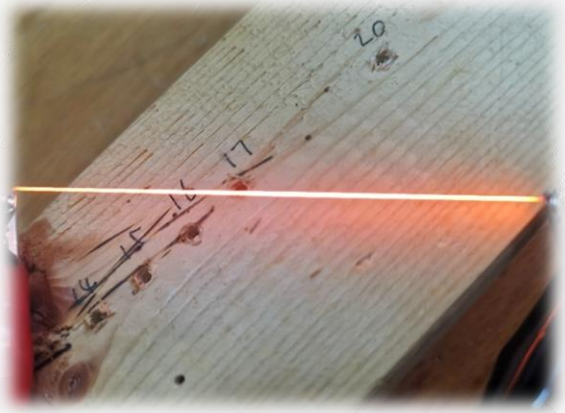
Analog simulation with COMSOL





Symmetrical distribution of temperature, with the highest temperature in the middle

Experimental measurement



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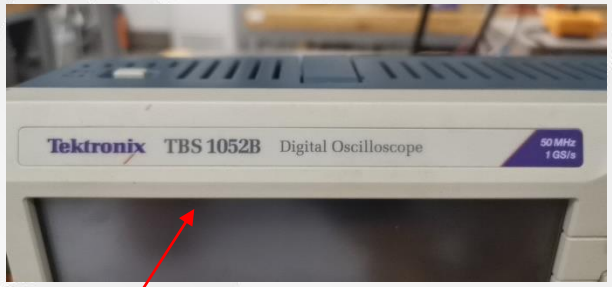
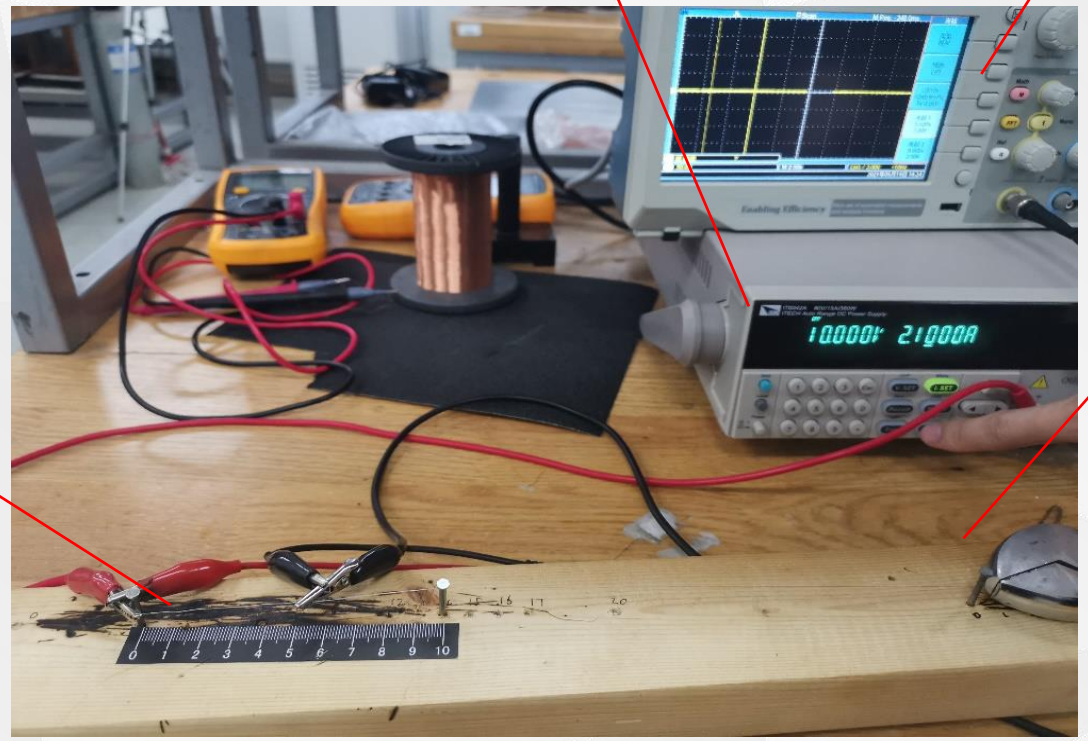
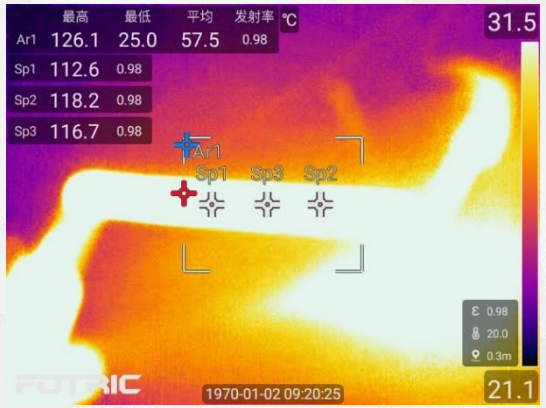


Three wire materials of various wire diameters

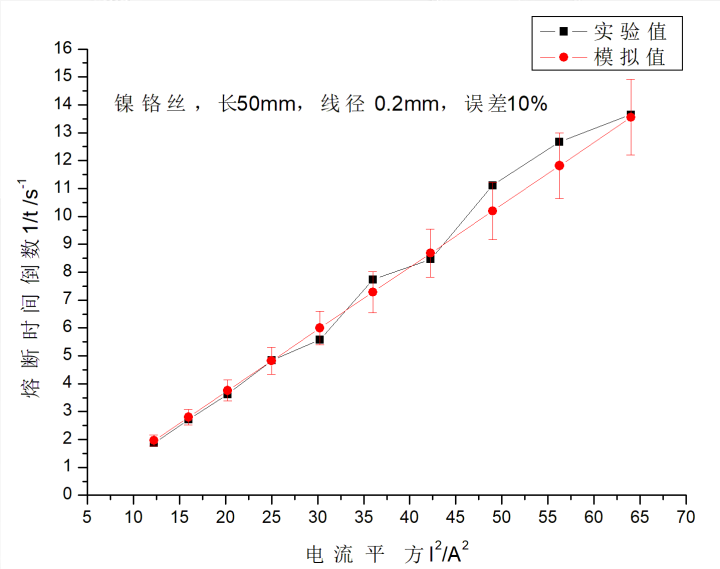
Cr20Ni80 nickel-chromium wire, constantan wire, nickel-iron wire

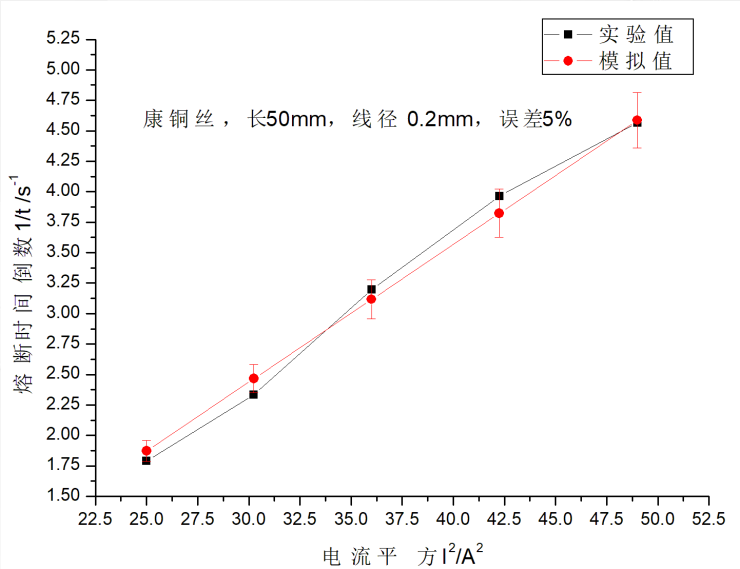


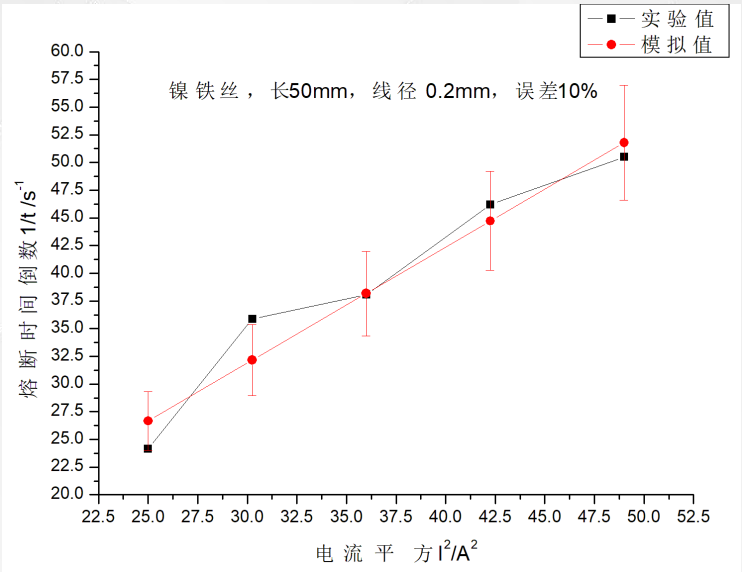
Wooden boards, vernier calipers, wires, etc.

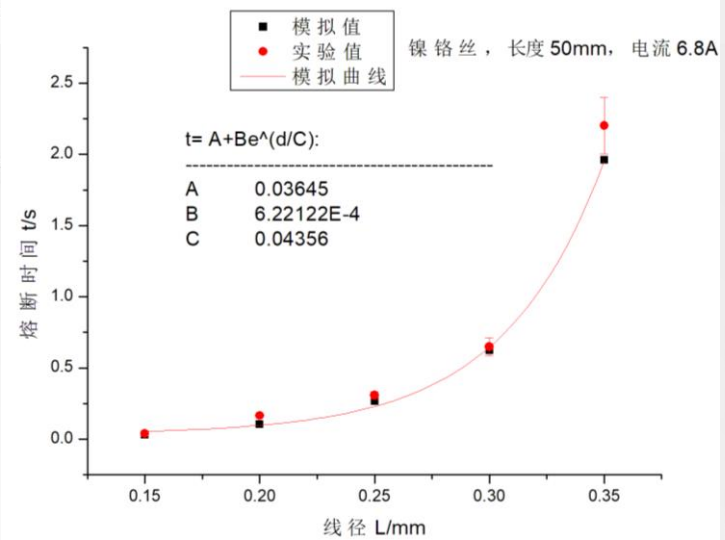


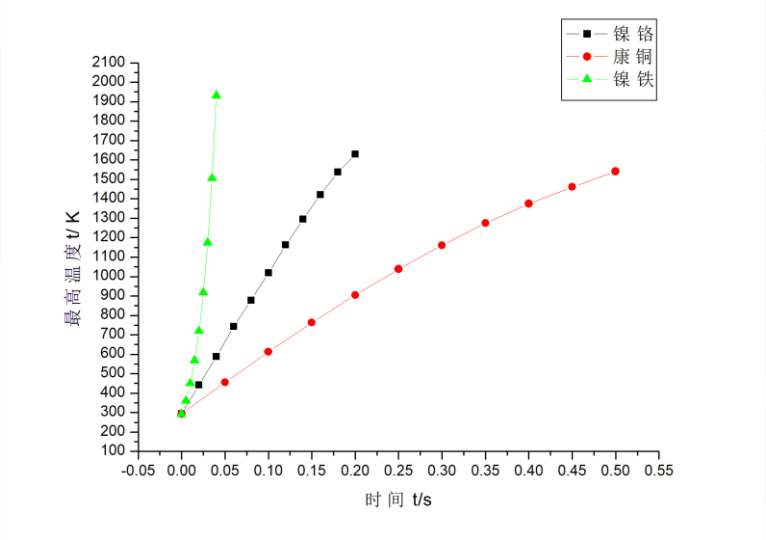
Comparison of simulation and experimental data (different variables)

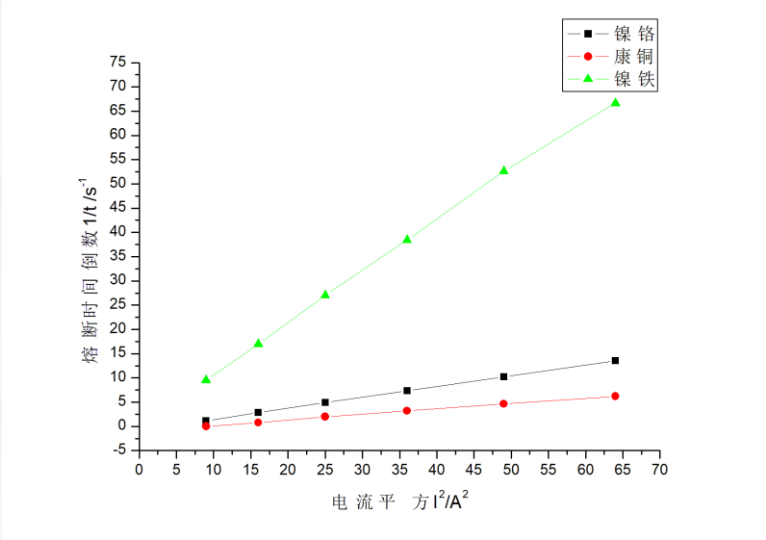






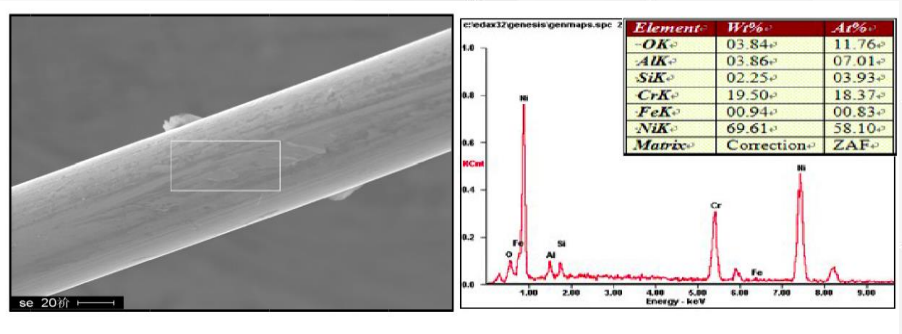


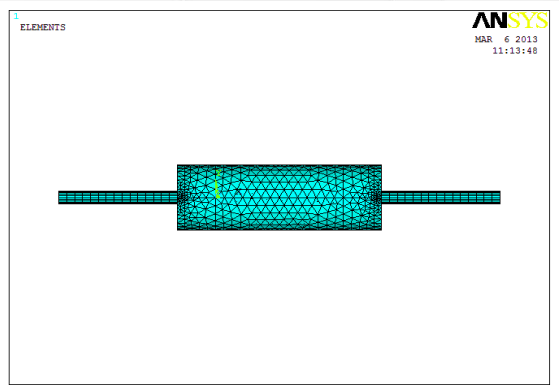


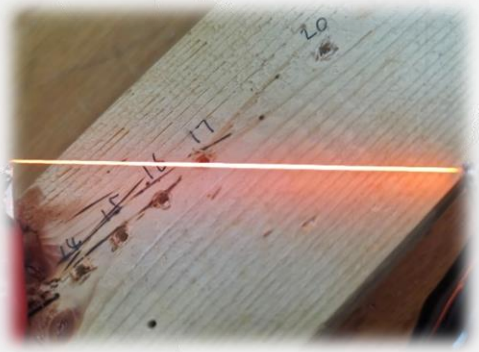


Conclusions

A short length of wire can act as an electrical fuse. Determine how various parameters affect the time taken for the fuse to ‘blow’.







→ various parameters

- electric current: $\frac{1}{t} \propto I^2$
- wire material: The greater the resistivity, the greater the temperature coefficient of resistance, and the faster the temperature rise
- diameter: $t \propto e^{kd}$
- length: Only has little effect
- flow rates: The larger the flow rate, the stronger the convection heat dissipation and the slower the fusing.
- bend or add enameled wire: Obstruct convection heat dissipation and slow down fusing

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THANKS!

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