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Calculation of growth process of nanostructured materials

W. Li

School of Physics and Electronic Information, Baicheng Normal Universtity 137000 JiLin Baicheng，China

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It nanometer is today one of the hot areas of research, through electro deposition method manufacturing Orderly structure With metal and semiconductor properties, Micron from the magnitude of nanotechnology potential direct impact on the distribution of morphology, So conductive pushing the situation on the potential distribution is particularly important. This means using mathematical derivation of the potential distribution of analytical expressions, A reasonable explanation of the prospective growth of 2 dimensional nanostructures structure morphology, The theoretical analysis for the future laid the foundation.

Keywords: Nanostructural Materia，The electricity deposite，The calculator imitate， Grow head，The electricity certainly distributes

AIMS AND BACKGROUND

Preparation of mesoscopic, nano-scale of the microstructure is a concern in recent years. In the many methods used, it is one of the hot spots to study the ordered structure of micrometer to nanometer order with metal and semiconducting properties by electrodeposition. In this paper, the electrosteposition method is used to prepare the ordered array pattern of copper nanostructured material with certain microstructure in the quasi-two-dimensional electrochemical crystallization process. Therefore, the growth characteristics and the growth mechanism are analyzed Is necessary. At present, the preparation of copper nanowires under non-oscillation conditions has been very perfect, but the research on the characteristics and properties of nanostructured materials under different external conditions is relatively few. This paper is to study the growth characteristics and growth mechanism of nanostructured materials under different controlled growth conditions. Different control of growth conditions mainly refers to the input growth voltage amplitude is the same and the frequency is different. It is very meaningful to make a basic study of its vast application space[1].

EXPERIMENTAL

Mathematical model of growth mechanism in one - dimensional case

Crystal growth can be considered to be caused by stable electrical oscillation, assuming that the growth of the container length is l , voltage is $v_0 \sin \omega t$, the problem can be described as:

$$E_{tt} - a^2 E_{XX} = 0 \qquad (1)$$

$$E|_{X=0} = v_0 \sin \omega t \qquad (2)$$

$$E|_{X=l} = 0 \qquad (3)$$

Because the use of complex numbers to calculate more convenient, Therefore, the boundary condition $v_0 \sin \omega t$ is rewritten as $v_0 e^{i\omega t}$, that is, the imaginary part of the complex number $\mathrm{Im}(v_0 \sin \omega t)$. When the calculation is completed, the imaginary part of the result is the solution of the equation. Since the steady oscillation is caused by the AC power supply, the cycle is the same as the AC power cycle[2]:

$$E(x,t) = X(x) e^{i\omega t} \qquad (4)$$

Substituting equation (4) into the ordinary differential equation of X yields: $X'' + (\omega / a)^2 X = 0$

Solving the ordinary differential equation of X: $X(x) = Ae^{\frac{i\omega x}{a}} + Be^{-\frac{i\omega x}{a}}$, and so:

$$E(x,t) = \left[Ae^{\frac{i\omega x}{a}} + Be^{-\frac{i\omega x}{a}} \right] e^{i\omega t} \qquad (5)$$

Substituting equation (5) into equation (2) yields:

$$[A+B] e^{i\omega t} = v_0 \sin \omega t \qquad (6)$$

* To whom all correspondence should be sent:
E-mail: liweiliwei77@163.com

Substituting equation (5) into equation (3) yields:

$$\left[Ae^{\frac{i\omega l}{a}} + Be^{-\frac{i\omega l}{a}} \right] = 0 \quad (7)$$

The imaginary part of expression $E(x,t)$ is the final solution of the equation:

$$E(x,t) = v_0 \frac{\sin \frac{\omega(l-x)}{a} \sin \omega t}{\sin\left(\frac{\omega l}{a}\right)} \quad (8)$$

Mathematical model of growth mechanism in three - dimensional case

Assuming that there is an initial perturbation in region Ω, at time at, the region affected by this disturbance can be described as a sphere with the center of M as the radius and the sphere as the inner envelope and the outer The surface of the surface is the area where the fluctuation has been conveyed, and the outer envelope is the area where the disturbance has not yet been conveyed. The above process is described by the following equation[3]:

Wave equation：

$$E_{tt} - a^2 \Delta E = 0 \quad (9)$$

The equation is implemented by separating the variable method

$$E(r,t) = T(t)v(r) \quad (10)$$

Equation (10) is substituted into equation (9):

$$\frac{T''}{a^2 T} = \frac{\Delta v}{v}$$

Equation on the left is a function of t ,the right side of the equation is a function of r, the equation to be established, must be equal to the same constant, the constant as $-k^2$, then get two equations:

$$T'' + k^2 a^2 T = 0 \quad (11)$$

$$\Delta v + k^2 v = 0 \quad (12)$$

The solution of Eq. (11) is:

$$\begin{cases} T(t) = C\cos kat + D\sin kat & (k \neq 0) \\ T(t) = C + Dt & (k = 0) \end{cases}$$

In the spherical coordinate system, the solution of Eq. (12) is:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(\frac{r^2 \partial v}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial v}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 v}{\partial \varphi^2} + k^2 v = 0 \quad (13)$$

Separate variables on variable V：

$$v(\rho,\varphi,z) = R(\rho)Y(\theta,\varphi)$$

Substituting equation (13)，Equation (13) is divided by $\left(\frac{r^2}{RY}\right)$ at both ends：

$$\frac{1}{R}\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) + k^2 r^2 = \frac{-1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial Y}{\partial \theta}\right) - \frac{R}{Y \sin^2\theta}\frac{\partial^2 Y}{\partial \varphi^2}$$

The left side of the equation is a function of r, and the right side of the equation is a function of θ and φ. If the equation holds, the equation needs to be equal to a constant Let the constant be $l(l+1)$:

$$\frac{1}{R}\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) = \frac{-1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial Y}{\partial \theta}\right) - \frac{R}{Y \sin^2\theta}\frac{\partial^2 Y}{\partial \varphi^2} = l(l+1)$$

Get two equations：

$$\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) + \left[k^2 r^2 - l(l+1)\right]R = 0 \quad (14)$$

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial Y}{\partial \theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial \varphi^2} + l(l+1)Y = 0 \quad (15)$$

Equation (14) is not a standard Bessel equation, and the equation (14)is transformed so that: $x = kr$， Substituting equation (14)

$$x^2 R'' + 2xR' + \left[x^2 - l(l+1)\right]R = 0$$

Let $R = \frac{\omega}{\sqrt{x}}$, substitute equation (14)

$$x^2 \omega'' + x\omega' + \left[x^2 - \left(l + \frac{1}{2}\right)^2\right]\omega = 0$$

Let $v = \left(l + \frac{1}{2}\right)$，substitute equation (14)

$$x^2 y'' + xy' + (x^2 - v^2)y = 0 \quad (16)$$

$x_0 = 0$ is the first order pole of $p(x) = (1/x)$, the second order pole of $q(x) = \left(1 - v^2/x^2\right)$, so: $x_0 = 0$ is the regular singularity of the equation

Determine the equation：$s(s-1) + s - v^2 = 0$

Determine the two roots of the equation: $s_1 = v, s_2 = -v$;（$s_1 - s_2 = 2$ or v is an integer)

$$y(x)=a_0x^S+a_1x^{S+1}+a_2x^{S+2}+...+a_Kx^{S+K}...(a_0\neq 0)$$

The recursive formula for the coefficients is: $\left[(s+k)^2-v^2\right]a_k+a_{k-2}=0$

$$a_k=\frac{-a_{k-2}}{(s+k)^2-v^2}=\frac{-a_{k-2}}{(s+k+v)(s+k-v)\ -v^2}$$

The general solution of the equation is:

$$y(x)=\sum_{k=0}^{\infty}\frac{(-1)^k}{\Gamma(v+k+1)}\left(\frac{x}{2}\right)^{v+2k}+\sum_{k=0}^{\infty}\frac{(-1)^k}{\Gamma(-v+k+1)}\left(\frac{x}{2}\right)^{-v+2k} \quad (19)$$

The other party said finishing

$$\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+l(l+1)\sin^2\theta=\frac{-1}{\Phi}\frac{d^2\Phi}{d\varphi^2}$$

The left side of the equation is a function of θ, and the right side of the equation is a function of φ [4]. If the equation is to be established, it should be equal to a constant λ:

$$\Phi''+\lambda\Phi=0 \quad (20)$$

$$\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left[l(l+1)\sin^2\theta-\lambda\right]\Theta=0 \quad (21)$$

Eigenvalue problem of solution equation: $\lambda=m^2 \quad (m=0,1,2...)$

Eigenfunction:

$$\Phi(\varphi)=A\cos m\varphi+B\sin m\varphi \quad (22)$$

Substituting $\lambda=m^2$ into equation (21):

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left[l(l+1)-\frac{m^2}{\sin^2\theta}\right]\Theta=0 \quad (23)$$

Let $\begin{cases}\theta=\mathrm{acr}\cos x\\ x=\cos\theta\end{cases}$, replace θ with x: $\frac{d\Theta}{d\theta}=\frac{d\Theta}{d\theta}\frac{dx}{d\theta}=-(\sin\theta)\frac{d\Theta}{dx}$

so:

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)=\frac{1}{\sin\theta}\frac{dx}{d\theta}\frac{d}{dx}\left(-\sin^2\theta\frac{d\Theta}{dx}\right)=\frac{d}{dx}\left[(1-x^2)\frac{d\Theta}{dx}\right]$$

Equation (23) can be organized as:

$$\frac{d}{dx}\left[(1-x^2)\frac{d\Theta}{dx}\right]+\left[l(l+1)-\frac{m^2}{1-x^2}\right]\Theta=0 \quad (24)$$

To be further organized as:

$$(1-x^2)\frac{d^2\Theta}{dx^2}-2x\frac{d\Theta}{dx}+\left[l(l+1)-\frac{m^2}{1-x^2}\right]\Theta=0 \quad (25)$$

It is difficult to solve equations by conventional methods (25), Next, we discuss the relationship between equation (25) and equation (26):

$$(1-x^2)y''-2xy'+l(l+1)y=0 \quad (26)$$

According to Leibniz formula:

$$\frac{d^n}{dx^n}\left[A(x)B(x)\right]=\sum_{k=0}^{n}\frac{n!}{(n-k)!k!}\frac{d^{n-k}}{dx^{n-k}}\left[A(x)\right]\frac{d^k}{dx^k}\left[B(x)\right]$$

m times the equation (26), we can get:

$$(1-x^2)u''-2x(m+1)u'+(l-m)(l+m+1)u=0 \quad (27)$$

It can be seen that the equation (25) is obtained by the differential equation (26), if the general solution of the equation (26)

$$y(x)=d_0y_0+d_1y_1$$

Then the general solution of equation (25) is:

$$y(x)=c_0y_0^m+c_1y_1^m$$

among them:

$$\begin{cases}y_0^m=(1-x^2)^{\frac{m}{2}}\frac{d^m}{dx^m}y_0\\ y_1^m=(1-x^2)^{\frac{m}{2}}\frac{d^m}{dx^m}y_1\end{cases}$$

Next, the series solution is used to solve the equation (26) in the neighborhood of $x_0=0$,

$$y''-\left(\frac{2x}{1-x^2}\right)y'+\left[\frac{l(l+1)}{1-x^2}\right]y=0$$

among them:

$$p(x)=\left(\frac{-2x}{1-x^2}\right),q(x)=\frac{l(l+1)}{1-x^2}$$

The solution of the equation is[5]:

$$y(x)=a_0+a_1x+a_2x^2+...+a_kx^k+...$$

Further recursion can be:

$$y'(x)=a_1+2a_2x+3a_3x^2+...+(k+1)a_{k+1}x^{k+1}+...$$

$$y''(x)=2a_2+3\cdot 2a_3x+4\cdot 3a_4x^2+...+(k+2)(k+1)a_{K+2}x^{K+2}+...$$

Put these expressions into the equation, the power of the same project merger, you can get:

$$\begin{array}{l|l} 2\cdot 1a_2 + l(l+1)a_0 = 0 & 3\cdot 2a_2 + (l^2+l-2)a_1 = 0 \\ 4\cdot 3a_4 + (l^2+l-6)a_2 = 0 & 5\cdot 4a_5 + (l^2+l-12)a_3 = 0 \\ \ldots\ldots & \ldots\ldots \end{array}$$

$$(k+2)(k+1)a_{K+2} + (l^2+l-k^2-k)a_K = 0$$

Recursive formula for the induction coefficient[6]:

$$a_{K+2} = \frac{(k^2+k-l^2-l)}{(k+2)(k+1)}a_K = \frac{(k-l)(k+l+1)}{(k+2)(k+1)}a_K$$

and so:

$$\begin{cases} y_0(x) = 1 + \dfrac{(-l)(l+1)}{2!}x^2 + \dfrac{(2-l)(-l)(l+1)(l+3)}{4!}x^4 + \ldots \\ \quad \dfrac{(2k-2-l)(2k-4-l)\ldots(2-l)(-l)(l+1)\ldots(l+2k-1)}{(2k)!}x^{2k} + \ldots \\ y_1(x) = x + \dfrac{(1-l)(l+2)}{3!}x^3 + \dfrac{(3-l)(1-l)(l+2)(l+4)}{5!}x^5 + \ldots \\ \quad \dfrac{(2k-1-l)(2k-3-l)\ldots(1-l)(l+2)\ldots(l+2k)}{(2k+1)!}x^{2K+1} + \ldots \end{cases}$$

The general solution of equation (26) is: $y(x) = d_0 y_0(x) + d_1 y_1(x)$.

The general solution of equation (25) is: $y(x) = c_0 y_0^m + c_1 y_1^m$

In summary, the potential distribution in the whole space is: $E = \{T\cdot R\cdot\Theta\cdot\Phi\}$

$$(1)\, T(t) = C\cos kat + D\sin kat \qquad (k = 0,1,2\ldots)$$

$$(2)\, R = \begin{cases} \displaystyle\sum_{k=0}^{\infty}\frac{(-1)^k}{\Gamma(v+k+1)}\left(\frac{r}{2}\right)^{v+2k} + \sum_{k=0}^{\infty}\frac{(-1)^k}{\Gamma(-v+k+1)}\left(\frac{r}{2}\right)^{-v+2k} & (v \neq \text{Integer}) \\ \displaystyle\left[\frac{2}{\pi}\left(\ln\frac{r}{2} + 0.577216\right) + 1\right]\sum_{k=0}^{\infty}\frac{(-1)^k}{k!(v+k)!}\left(\frac{r}{2}\right)^{v+2k} & (v = \text{Integer}) \end{cases}$$

$$(3)\, \Theta = c_0 y_0^m + c_1 y_1^m$$

The solution of the equation is:

$$\begin{cases} y_0(x) = 1 + \dfrac{(-l)(l+1)}{2!}x^2 + \dfrac{(2-l)(-l)(l+1)(l+3)}{4!}x^4 + \ldots \\ \quad \dfrac{(2k-2-l)(2k-4-l)\ldots(2-l)(-l)(l+1)\ldots(l+2k-1)}{(2k)!}x^{2K} + \ldots \\ y_1(x) = x + \dfrac{(1-l)(l+2)}{3!}x^3 + \dfrac{(3-l)(1-l)(l+2)(l+4)}{5!}x^5 + \ldots \\ \quad \dfrac{(2k-1-l)(2k-3-l)\ldots(1-l)(l+2)\ldots(l+2k)}{(2k+1)!}x^{2K+1} + \ldots \end{cases}$$

Where: c_0, c_1, l are constants, and $k = 0,1,2\ldots$.

$$(4)\, \Phi(\varphi) = \cos m\varphi + \sin m\varphi \qquad (m = 0,1,2\ldots).$$

RESULTS AND DISCUSSION

The MATLAB language is the most influential and dynamic software in the world today. It is based on matrix operations and has evolved into a highly integrated computer language. It provides powerful scientific computing, flexible programming flow, high-quality graphical visualization and interface design. The following uses MATLAB 6.0, the third chapter of the mathematical formula derived in the specific boundary conditions were simulated, the following computer simulation and experimental data comparison:

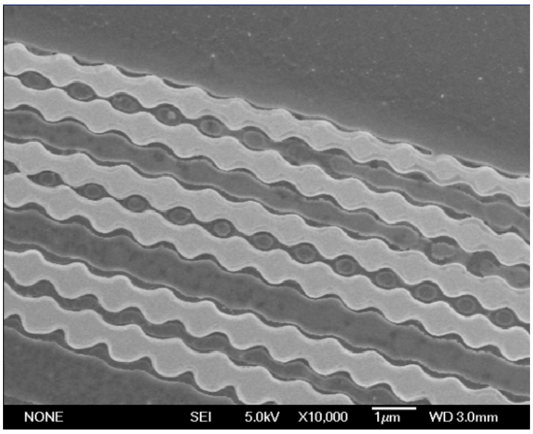

Fig. 1. Water bath temperature:-4.15˚C, PH:4.444(Survey temperature: 18.7˚C),Density: 50mmol/l CuSO4 Input voltage oscillation amplitude: 0.72V,Frequency:0.8 Hz growth appearance.

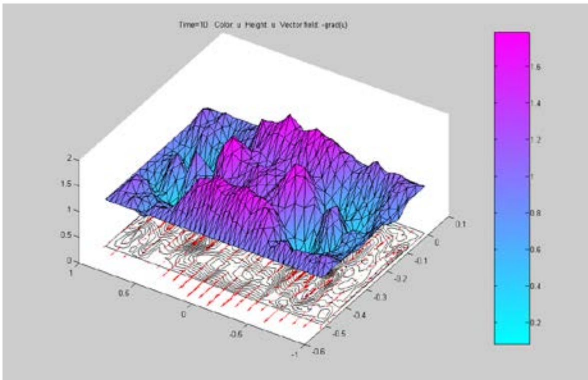

Fig. 2. The potential distribution of the growth front is simulated by MATLAB

The simulation results show that the image is consistent with the crystal growth morphology in the experiment, which verifies the correctness of the mathematical formula. In this paper, the physical model of the nanostructured materials grown by electro deposition was established. Some basic work has been done to study the growth of nanostructured materials[7].

CONCLUSIONS

This text more and completely introduced research general situation, making method and token method of the Na rice structure material[8]. The making mechanism which counteracts to aim at the structure material of the electricity deposition method making Na rice carried on mathematics to deduce with the emulation of calculator. Make use of the accurate control of the in addition growth electricity power in the quasi- two-dimensional electricity crystallize the process, the making submits to have must the copper Na rice structure material of microstructural have the preface array the pattern, and to grow a characteristics and grew a mechanism to carry on analysis[9]. Finally put forward signal and crystal of the in addition electric voltage to grow the mathematical formula that the sophisticated electricity certainly distributes, counteracted Matlab to carry on emulation to play to show, mainly include a contents:

1.Under the one dimensional circumstance：

$$E(x,t) = v_0 \frac{\sin \frac{\omega(l-x)}{a} \sin \omega t}{\sin\left(\frac{\omega l}{a}\right)}$$

2.Under the one dimensional circumstance, the distribute of electricity power satisfies $E = \{T \cdot R \cdot \Theta \cdot \Phi\}$

Detailed contents：

$(1)\, T(t) = C\cos kat + D\sin kat \qquad (k = 0,1,2...)$

$$(2)\, R = \begin{cases} \sum_{k=0}^{\infty} \frac{(-1)^k}{\Gamma(v+k+1)} \left(\frac{r}{2}\right)^{v+2k} + \sum_{k=0}^{\infty} \frac{(-1)^k}{\Gamma(-v+k+1)} \left(\frac{r}{2}\right)^{-v+2k} & (v \neq \text{Integral}) \\ \left[\frac{2}{\pi}\left(\ln\frac{r}{2} + 0.577216\right) + 1\right] \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(v+k)!} \left(\frac{r}{2}\right)^{v+2k} & (v = \text{Integral}) \end{cases}$$

$(3)\, \Theta = c_0 y_0^m + c_1 y_1^m$

The continuation is the definition of y_0^m and y_1^m:

$$\begin{cases} y_0^m = (1-x^2)^{\frac{m}{2}} \frac{d^m}{dx^m} y_0 \\ y_1^m = (1-x^2)^{\frac{m}{2}} \frac{d^m}{dx^m} y_1 \end{cases}$$

$$\begin{cases} y_0(x) = 1 + \frac{(-l)(l+1)}{2!} x^2 + \frac{(2-l)(-l)(l+1)(l+3)}{4!} x^4 + ... \\ \qquad \frac{(2k-2-l)(2k-4-l)...(2-l)(-l)(l+1)...(l+2k-1)}{(2k)!} x^{2K} + ... \\ y_1(x) = x + \frac{(1-l)(l+2)}{3!} x^3 + \frac{(3-l)(1-l)(l+2)(l+4)}{5!} x^5 + ... \\ \qquad \frac{(2k-1-l)(2k-3-l)...(1-l)(l+2)...(l+2k)}{(2k+1)!} x^{2K+1} + ... \end{cases}$$

c_0, c_1 and l is constants, $k = 0,1,2....$

$(4)\, \Phi(\varphi) = \cos m\varphi + \sin m\varphi \qquad (m = 0,1,2...)$

3.The usage Matlab carried on emulation to play to show, crystal growth in its picture and experiment the facial look be basic to fit together and verified the accuracy that the mathematical formula deduce thus and further[10].

Comprehensive say, this text built up an electricity deposition a method a growth the Na rice structure material of physical model. Did some foundation a work for the growth that the research controls the Na rice structure material.

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