Reducing edge effect of temperature-field for large area thin film deposition in hot filament chemical vapor deposition system

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DOI: 10.5185/amlett.2018.2146
www.vbripress.com/aml

Abstract

The uniformity in temperature-field of the hot filament chemical vapor deposition (HFCVD) system is of great importance since it is a critical parameter that determines the quality of the deposited films. In fact, the temperature-field is mainly filament distribution dependent. In conventional analysis method, the filament array usually has an equal-space distribution, which leads to a remarkable edge effect and consequently unable to obtain large area uniformity in temperature-field in HFCVD for high-quality thin film deposition. Here, we proposed theoretically an asymmetrical filament distribution to reduce the edge-effect of temperature field. The adjacent filament distance was optimized by using numerical simulation based on heat-transfer theory. Based the optimized condition, temperature difference as low as 13 K between the center and edge region of the filament arrays can be achieved in 100-mm substrate, which is only one tenth of the temperature difference of that in the case that the filaments were evenly distributed. Thus unequal-space distribution can be employed to enhance the uniformity in temperature field of the HFVCD system in favor of the growth of high quality thin films in large area. Copyright © 2018 VBRI Press.

Keyword: Hot filament, chemical vapor deposition, temperature-field, thin film.

Introduction

For chemical vapor deposition (CVD) technology, hot-filament CVD (HFCVD) method was one of the mostly used techniques to deposit thin films due to its simplicity, low cost and large growth area. Moreover, it permits deposition of multilayer films by introducing various gases into the system chamber in a desired sequence. During the HFCVD deposition [1-3], the uniformity of temperature field on the substrate is the most important parameter for high quality film deposition in large area. For example, for diamond thin film deposited by HFCVD, the grain nucleation [4], growth rate [5], grain size [6,7] and optical transmittance [7] are strongly dependent on the surface temperature. Higher substrate temperature will lead to grow into bigger grain size; meanwhile, with increasing the substrate temperature, the energy band gap [8] and hole mobility of the doped diamond [9-11] will decrease. Temperature field is also an important parameter that affects the quality of other materials, such as SiOx [12] and WC films [13]. Besides the temperature of the substrate, the temperature uniformity of the substrate is also very important, especially for high quality film deposition in large area.

There are two methods, finite element method and numerical simulation method that have been used to investigate the temperature field distribution in HFCVD system. The finite element method was used to simulate arbitrary complicated macroscopic system while numerical simulation method is limited to the complexity of simulated system. But the complex system can be approximate to simple mode by mathematical modeling using fundamental thermodynamic formulate. Thus, if not all the information about temperature distribution is need, we can acquire the intriguing information about temperature field by numerical simulation method. Numerical simulation method has been widely used in the research of HFCVD deposition [14, 15] to analyze the temperature field of HFCVD by optimizing the filaments distribution. However, in conventional system, filaments are evenly distributed; the temperature distribution in the substrate along the direction perpendicular to the filaments is undulatory. Numerical simulation results showed that increasing filaments number can reduce such temperature wave [16,17], but increasing filament number will lead to a drop of temperature from center region to the edge, which could result in obvious edge effect and can't be ignored, especially on the edge of a large-area substrate. It means that the edge effect and the temperature wave can't be reduced simultaneously, which limits acquiring highly uniform temperature over a large area in conventional filament array. The edge effect of temperature field is not favorable to the growth of thin films with high quality in large area. Therefore, it is very necessary to explore a method to reduce the edge effect while keeping low temperature wave.

In this work, we propose a new position distribution of filament array with an unequal-space mode to reduce the edge effect by using numerical analysis based on the heat transfer theory [18]. Our results showed that the filament array with unequal-space distribution could improve the uniformity in temperature field. We simulated the temperature field on a 100-mm substrate using unequally spaced filament array, which indicated that the difference of the temperature from the center to edge region less than 13 K, and the edge effect is weaken by the unequal-space distribution of the filaments in the HFCVD system. Therefore, the design of the filament arrays with unequal-space is an effective means to resolve the edge effect of temperature field and will give a significant guide to the uniform film deposition over large-area.

Foundation of temperature-field equation in the HFCVD system

During HFCVD deposition, generally the total pressure in the chamber is much lower than the atmospheric pressure, and thus the conduction heat through gases can be ignored. The substrate temperature is mainly affected by thermal radiation and heat exchange between the substrate and the cooling water. In order to acquire large-area uniform temperature field in the HFCVD system, firstly, we consider a long filament design that parallel to the substrate, as shown in **Fig. 1**. Here, the Cartesian coordinates (x, y, z) are adopted, where the origin of coordinates is in the center of the substrate, the x axis is parallel to the substrate and filament, and the y axis is perpendicular to the filament and parallel to the substrate.

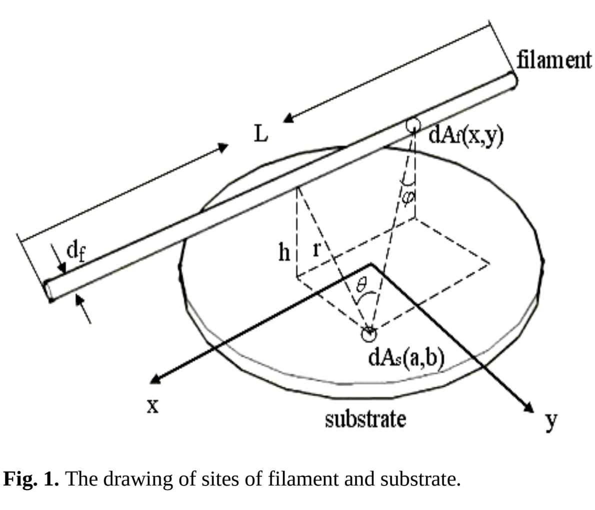


Fig. 1. The drawing of sites of filament and substrate.

The temperature of the filament is denoted as T_f. According to Stefan-Boltzmann's law, the radiant heat energy, E, emitted from the filament is:

$$E = \varepsilon_f \sigma T_f^4 \tag{1}$$

Here, ε_f is the emissivity of filament surface, and σ is the Boltzmann constant. The radiation intensity of filament is I and can be given as:

$$E = \pi I \tag{2}$$

We consider the quantity of heat radiation from a microprofile dA_f nearby point (x, y, z) on the filament to a microprofile dA_s nearby point (a, b, 0) on the substrate. The solid angle of dA_f dA_f to dA_s is given by

$$\omega = \frac{dA_s \cos\theta}{(b-y)^2 + H^2 + (a-x)^2} \tag{3}$$

Here, H is the distance from the filament to the substrate, θ is the angle between the vertical and the radiation direction of dA_f . If the absorptivity of substrate is α_s, the angle between z axis and the radiation direction is φ . In that, the heat which dA_s acquired from dA_f can be given by

$$dQ_{in} = \alpha_s I \cos\varphi \cdot dA_f \omega \tag{4}$$

Assuming the diameter of filament is d_f, so the active area of dA_f is $d_f dx$. From equations (1) - (4), we can acquire:

$$dQ_{in} = \frac{\alpha_s \varepsilon_f \sigma T_f^4 d_f \cos\theta \cos\varphi}{\pi[(b-y)^2 + H^2 + (a-x)^2]} dA_s dx \tag{5}$$

The total heat energy that dA_s acquired from outside is integral with respect to dQ_{in}. So the total heat energy dA_s absorbed, Q_{in}, is described by

$$\begin{aligned}
Q_{in} &= \int_{-L/2}^{L/2} \frac{\alpha_s \varepsilon_f \sigma T_f^4 d_f \cos\theta \cos\varphi}{\pi[(b-y)^2 + H^2 + (a-x)^2]} dA_s dx \\
&= \frac{\alpha_s \varepsilon_f \sigma T_f^4 d_f dA_s}{\pi} \int_{-L/2}^{L/2} \frac{\sqrt{(b-y)^2 + H^2}}{\sqrt{(b-y)^2 + H^2 + (a-x)^2}} \\
&\times \frac{H}{\sqrt{(b-y)^2 + H^2 + (a-x)^2}} \frac{1}{(b-y)^2 + H^2 + (a-x)^2} dx \\
&= \frac{\alpha_s \varepsilon_f \sigma T_f^4 d_f H \sqrt{(b-y)^2 + H^2}\, dA_s}{\pi} \\
&\times \int_{-L/2}^{L/2} \frac{1}{[(b-y)^2 + H^2 + (a-x)^2]^2} dx \\
&= \frac{\alpha_s \varepsilon_f \sigma T_f^4 d_f H dA_s}{2\pi r} \left(\frac{l-a}{(l-a)^2 + r^2} + \frac{l+a}{(l+a)^2 + r^2}\right) \\
&+ \frac{\alpha_s \varepsilon_f \sigma T_f^4 d_f H dA_s}{2\pi r^2} \left(\arctan\frac{l-a}{r} + \arctan\frac{l+a}{r}\right)
\end{aligned} \tag{6}$$

where

$$l = L/2 \qquad r = \sqrt{H^2 + (b-y)^2}$$

respectively, and y is the ordinate value of filament, standing for filament's horizontal position.

When many filaments are placed parallel to each other and to the substrate, the total heat energy should be the sum of heat energy acquired from each filament. If the filaments number is *N*, then equation (6) can be described by

$$Q_{in} = \sum_{i=1}^{N} \frac{\alpha_s \varepsilon_f \sigma T_f^4 DHdA_s}{2\pi r_i} \left(\frac{l-a}{(l-a)^2 + r_i^2} + \frac{l+a}{(l+a)^2 + r_i^2} \right) + \sum_{i=1}^{N} \frac{\alpha_s \varepsilon_f \sigma T_f^4 DHdA_s}{2\pi r_i^2} \left(\arctan\frac{l-a}{r_i} + \arctan\frac{l+a}{r_i} \right) \quad (7)$$

Here, $r_i = \sqrt{H^2 + (b - y_i)^2}$. y_i is the ordinate value of filament *i*, and accordingly, we can obtain the spaces between any arbitrary two filaments.

Assume the heat energy which dA_s released, Q_{out}, contains the radiant heat and the heat transfer by cooling water. So Q_{out} can be described by

$$Q_{out} = \varepsilon_s \sigma T_{ab}^4 dA_s + \alpha (T_{ab} - T_0) dA_s \quad (8)$$

Here, T_{ab} is the temperature of point (*a, b, 0*), and T_0 is the temperature of cooling water.

It gives that the former term of equation (6) is proportional to the biquadrate of temperature, farther bigger than latter term. Therefore, the latter term can be ignored.

According to thermal balance equation $Q_{in} = Q_{out}$, it can be inferred from equations (7) and (8) that:

$$T_{ab} = \left[\sum_{i=1}^{N} \frac{\varepsilon_f d_f H}{2\pi r_i} \left(\frac{l-\mathrm{a}}{(l-a)^2 + r_i^2} + \frac{l+a}{(l+a)^2 + r_i^2} \right) + \sum_{i=1}^{N} \frac{\varepsilon_f DH}{\pi r_i^2} \left(\arctan\frac{l-a}{r_i} + \arctan\frac{l+a}{r_i} \right) \right]^{0.25} T_f \quad (9)$$

Equation (9) is the temperature field equation of substrate. If we know the filaments length *L*, height *H*, number *N* and the ordinate y_i of each filament, the temperature of arbitrary point (*a*, *b*) on substrate can be computed by using equation (9).

From equation (9) we can know that the temperature of point (*a*, *b*) on the substrate is proportional to filaments temperature T_f and the quarter squares of filament diameter d_f. When the filaments length is very long so that $[H^2 + (b - y_i)^2]/l$ is farther smaller than *l*, the equation (9) can be approximate to the following form:

$$T_{ab} = \left(\sum_{i=1}^{N} \frac{\varepsilon_f d_f H}{r_i^2} \right)^{0.25} T_f = \left[\sum_{i=1}^{H} \frac{\varepsilon_f d_f H}{H^2 + (b - y_i)^2} \right]^{0.25} T_f \quad (10)$$

Equation (10) is irrelevant to the abscissa of point (*a*, *b*), which means that when the filaments length is enough long, the temperature distribution along x-direction on substrate can be regarded as accordant and the varying of temperature is mainly along y-direction.

In conventional filaments distribution, the space of adjacent filaments is equal. The ordinate of filament y_i can be described by

$$y_{i+1} = y_i + d \quad (11)$$

Here, *d* is the space of adjacent filaments. But this equal-space distribution would lead to serious edge effect. In order to reduce this defect, we optimized filaments parameters with unequal-space distribution method. This method abandons the restriction that the space of adjacent filaments is equal. So the ordinate of filament y_i should be described by

$$y_{i+1} = y_i + d_{\mathrm{i}} \quad (12)$$

Here, d_i is the space of filament *i* and *i+1*. With this distribution method, the spaces of adjacent filaments are uncertain.

In order to acquire the relation of the temperature distribution with filaments length, height and number, numerical simulation method was used. Every y_i was permitted to vary from -150 mm to 150 mm on 100-mm substrate, and the temperature of arbitrary point on substrate was computed using temperature field equation (9). In order to optimized filaments sites, $\{y_i\}$, a content optimization function is need. After exploring many optimization functions, we found that the temperature variance along X axis can be simply decreased by means of extending the length of filaments. In view of this cause, the optimization was chosen:

$$f = \int_{-50}^{50} (T_{0y} - p)^2 dy \quad (13)$$

Here, $T_{0\ y}$ is the temperature of point (*0, y, 0*) on 100-mm substrate, *p* is the average temperature of substrate.

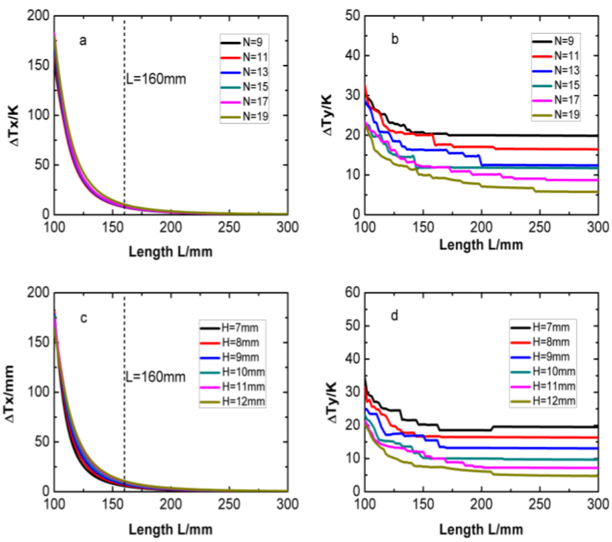
According to equation (13), the relation between optimized filaments sites { y_i } and filaments height *H*, length *L*, and number *N* can easily be confirmed. After this, optimized *H*, *L*, *N* can be effortlessly acquired.

Results and discussion

According to above numerical simulation model, the effects of different filament parameters (filament length *L*, filament height *H* and filament number *N*) on the temperature field in HFCVD system were investigated, in which temperature field can be characterized by the difference between the minimum and maximum temperature along X axis (ΔTx) and Y axis (ΔTy) and the mean-square deviation of substrate temperature (*Ts*). *Ts* is the authentic reflex of the uniformity of temperature field.

The dependences of ΔTx and ΔTy on the filament length *L* at different filament numbers *N* and different filament heights *H* are shown in **Fig. 2**. From **Fig 2 (a)** and **(b)**, we can see that when the filament height *H* is kept as a constant, the filament number is changed , the curves of ΔTx varying with the filament length *L* is nearly coincident, while the curves of ΔTy show a greatly difference in changed trend with different filament number *N*. This indicates that filament number *N* mainly affects the temperature distribution along y-direction while exhibits negligible influence on that along the x-direction. Further, the dependence of ΔTx and ΔTy on the filament length with different filament heights are shown in **Fig. 2(c)** and **(d)**. When the filament number N was firstly chosen as 15, we observed the change in the curves of ΔTx and ΔTy with

Fig. 2. The dependence of ΔTx and ΔTy of the temperature field on 100-mm substrate on the filaments length with different filament numbers and heights. (a) The temperature difference between center



and edge along X axis and (b) Y axis at H=9.4 mm. (c) The temperature difference between center and edge along X axis and (d) Y axis at N=15.

the filament height H. It is found that as same as the trend of ΔTx and ΔTy shown in **Fig. 2(a)** and **(b)**. The curves of ΔTy have a great change with the filament height H but the curves of the ΔTx are almost the same. Above results proves that the filament number N or the filament height H are the mainly parameters that determine the temperature uniformity along y-direction, though little influence on that along x-direction. In addition, it can be seen from **Fig. 2(a)** and **(c)** that the plots of ΔTx drop fleetly with filament increasing, which gives a sharp contrast to the plots of ΔTy shown in **Fig. 2(b)** and **(d)** varying slowly with L increasing. This proves that filament length L mainly affects the temperature uniformity along x-axis but has a little influence on that along y-axis, which is in contrast to the trend of the filament number and the filament height.

Therefore, the influence of filament length on temperature distribution is independent on the influence of filament number and height. As filament length increasing, ΔTx has a small change and decreases slowly. In that case that the filament is indefinitely long, the influence of filaments on substrate along x-direction can be ignored and the temperature distribution along x-direction will be a constant. Such assumption is in perfect consistence with equation (10). **Fig. 3** shows the curves of Ts with the filament length at different filament numbers and different heights. We can see that when filament length increases gradually, Ts decreases rapidly and then begins to become smooth at filament length exceeding 160 mm. Therefore, when the filament length is more than 160 mm, the variation of Ts curves can be ignored. Thus to save filament material, wan optimized filament length about 160 mm is suggested with improved temperature distribution.

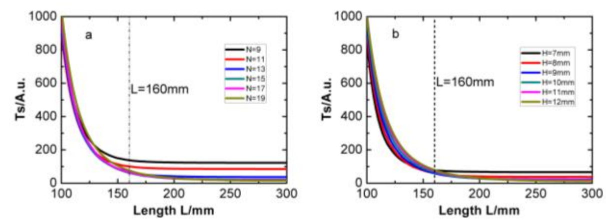


Fig. 3. The influence of filament length (L) on mean-square deviation of substrate temperature (Ts) at different filament numbers (a) and different filament heights (b).

In order to acquire optimized filament number N, we studied the influence of filament height H on ΔTy with difference N at L=160 mm as shown in **Fig. 4**. With increasing the filament height H, ΔTy drops rapidly first and then reaches a constant value. On the other hand, by increasing the filament number N favors ΔTy to reach a constant value. It can be seen easily that the curve of ΔTy at N = 9 is obviously different from other curves, but from N = 11, the curves of ΔTy become coincident and have little change with the filament height H. The reason of above changed trend is because that when the filament number is 9, the effect of unequal-space distribution of filaments on the temperature field is not very obvious, but when N is larger than 11, the trend of ΔTy with H become coincident. Therefore, N = 11 is aleast and optimized value for uniform temperature field.

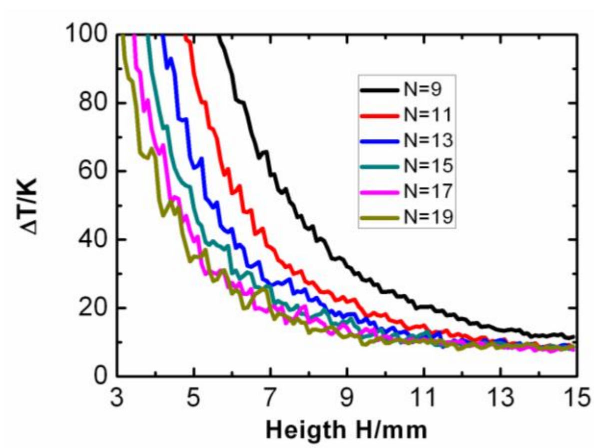


Fig. 4. The influence of filament height (H) on ΔTy at difference filament numbers when filament length L is 160 mm.

Fig. 5 shows the influence of filament height H on ΔTx, ΔTy and Ts when keeps the filament length L equal to 160 mm and filament number N of 11. As H increasing, ΔTy decreases rapidly but ΔTx increases slowly. On the other hand, Ts decreases firstly and then to increase, and H equal to 11.5 mm is a conversion point of *Ts*. It means that when *H* is 11.5 mm, the curve of Ts reaches the minimum value, and the temperature field reaches the most uniform condition, correspondingly, ΔTx is 9.6K and ΔTy is 12.9K,

According to above analysis, we can conclude that filaments length *L* is a main factor that affects the temperature uniformity along x-direction, but *H* and *N* are the main reason for temperature uniformity along y-direction. Combining above discussion and considering saving filament material at the greatest extent, the optimized filament parameters are *L* = 16+0 mm, *H* = 11.5 mm, and *N* = 11.

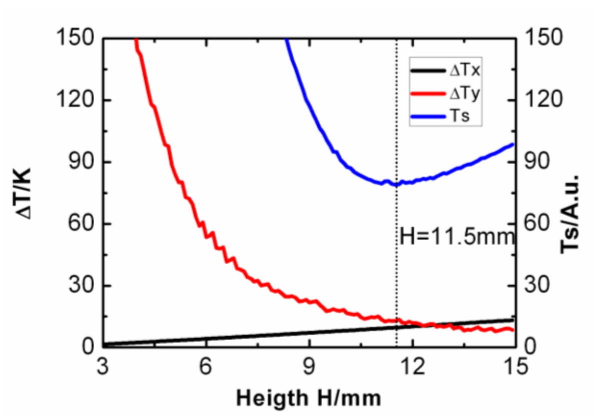


Fig. 5. The influence of filaments height (H) on ΔTx, ΔTy and Ts when *L*=160 mm and N=11.

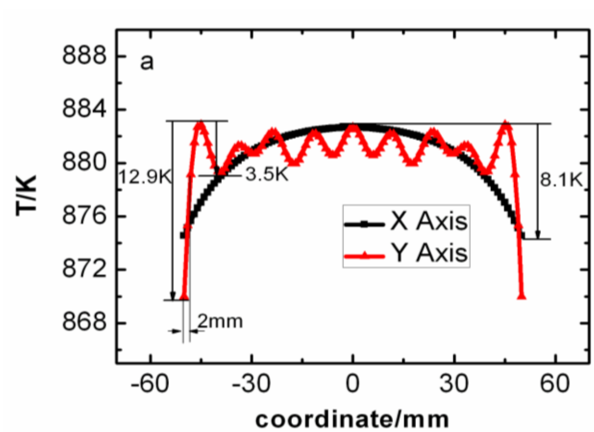


Fig. 6. The temperature field distribution on 100-mm substrate at *L*=160 mm, *H*=11.5 mm and *N*=11. The difference between maximum and minimum temperature is less than 13K, and the average temperature is 879.8K.

Fig. 6 gives the distribution of temperature field on a 100-mm substrate at the optimized filament parameters: *L* = 160 mm, *H* = 11.5 mm, and *N* = 11. We can find that the difference between the minimum and maximum temperature on substrate is less than 13 K and the average temperature is 879.8.K. The variation of temperature along Y axis mostly is less than 3K and there is only a drop of 10K at the edge with 2 mm wide, which can be attributed to the optimization of filaments interspace. The space distribution of adjacent filaments, d_i, under this optimized configure is listed in **Fig. 7**. The spaces between two most fringe filaments, d_1 and d_{10}, are very small. This optimized result prevents a rapid drop of the temperature in the edge. But this is likely to make the temperature of edge region is much higher than that of center region. Therefore, the space between the second and third filament is optimized to be about 0.012, which is the biggest space. The spaces between middle filaments are nearly the same. This unequal-space distribution extremely ensures the uniformity of temperature field.

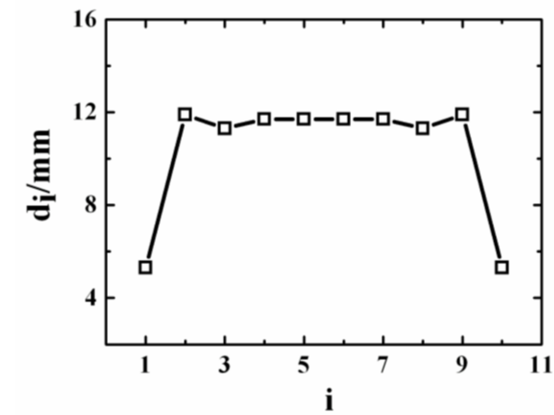


Fig. 7. The space distribution between each two adjacent filaments when *L* is 160 mm H is 11.5 mm and *N* is 11.

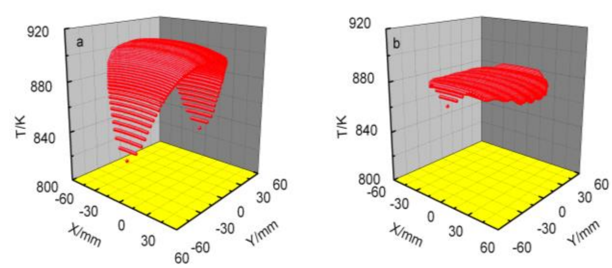


Fig. 8. The temperature field distribution of 100-mm substrate at equal-space (a) and unequal-space filament arrays (b). Filament array parameters are chosen as *L*=160 mm, *H*=11.5 mm, *N*=11. Here, "X" stands for the direction parallel to filaments, and "Y" stands for the direction perpendicular to filaments.

A comparison of temperature fields between equal-space and unequal-space for filament arrays is shown in **Fig. 8**. It is easy to observe from **Fig. 8 (a)** and **(b)** that an optimized filament array with unequal-space has much better uniformity than un-optimized filament array with equal-space. When *L* is 160mm, *H* is 11.5mm, and *N* is 11, the difference between the minimum and maximum temperature is more than 100K before optimizing filament inter space **(Fig.8(a))** but it only is less than 13 K after the optimization of the filament inter space **(Fig.8(b))**, which was about one tenth of temperature-difference for equal-space filaments distribution. Therefore, no doubt that optimized unequal-space filament array is very significant to obtain a large area of uniform temperature field, which is much better than conventional equal-space filament distribution with a same filament number. In addition, it can be deduce based on the temperature filed equation (9) that if the optimized filaments parameters: *L* =160 mm, *H* =11.5 mm, and *N* = 11 are increased, the superiority in uniformity of temperature field for unequal-space filament array will be enlarged, and meanwhile, the uniformity of temperature field for equal-space filament arrays will become worse. Therefore, this unequal-space filaments design can reduce the edge-effect of temperature field largely and hence obtain the steady and uniform temperature field for a large area of high-quality films deposition.

Conclusion

The filaments distribution with equal-space will lead to edge-effect, which limits acquiring large-area uniform temperature field in HFCVD. We proposed an unequal-space distribution of the filament arrays to reduce this effect greatly. Numerical simulation results indicate that by optimizing adjacent filaments space, large-area highly uniform temperature field less than 13K can be obtained on a 100-mm substrate under the optimized filament parameters: filaments length L = 160 mm, height H = 11.5 mm and number N = 11. Under otherwise identical filaments parameters, the difference between the minimum and maximum temperature for unequal-space filament arrays is only one tenth of that for the equally -spaced filament arrays. This highly uniform temperature field induced by unequal-space distribution of the filament arrays will play an important role in highly quality thin films deposition over a large area.

Acknowledgements

This work was supported by the National Natural Science Foundation of China (Grand No. 11574369，61390503，11674387), the financial support from the Ministry of Science and Technology of China (Grant No. 2016YFA0200800, 2016YFA0200400), Key Research Program of Frontier Sciences of CAS (Grant No.QYZDJ-SSW-SLH042) and the “Strategic Priority Research Program” of CAS (Grant No. XDB07020200).

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