Nucleation in Vapor phase deposition

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What is Nucleation?

- Thin film has two kinds of material: amorphous and crystals (long-rang order).
- First step in crystallization is nucleation. (Time for new phase to appear)
Classical Nucleation Theory

- Nucleation rate = $\rho Z j exp(-\Delta F/kT)$
  - $\rho$ is the number of possible nucleation sites per unit volume
  - $Z$ is the Zeldovich factor
  - $j$ is grow rate
  - $T$ is nucleation temperature
  - $\Delta F$ is the energy cost for nucleus, at the top of barrier
  - $\Delta F = -\frac{4\pi}{3} R^3 \rho \Delta \mu + 4\pi R^2 \gamma$
  - $R$ is radius of nucleus sphere, critical size from highest free energy
  - $\Delta \mu$ is the chemical potential of nucleus
  - $\gamma$ is the interfacial tension
Temperature dependence

- The higher the temperature, the larger probability of nucleation.

![Graph showing the relationship between 1/T and grain numbers with a fitted exponential decay model. The model parameters are listed in a table.]

<table>
<thead>
<tr>
<th>Model</th>
<th>ExpDec1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Equation</td>
<td>( y = A_1 \exp\left(-\frac{x}{t_1}\right) + y_0 )</td>
</tr>
<tr>
<td>Reduced Chi-Sqr</td>
<td>69.6021</td>
</tr>
<tr>
<td>Adj. R-Square</td>
<td>0.9996</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Standard Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>( y_0 )</td>
<td>9.68681</td>
<td>5.28081</td>
</tr>
<tr>
<td>( A_1 )</td>
<td>4.72387E6</td>
<td>1.1728E6</td>
</tr>
<tr>
<td>( t_1 )</td>
<td>4.83199E-4</td>
<td>1.4031E-5</td>
</tr>
<tr>
<td>( k )</td>
<td>2069.53994</td>
<td>60.09482</td>
</tr>
<tr>
<td>( \tau )</td>
<td>3.34928E-4</td>
<td>9.72557E-6</td>
</tr>
</tbody>
</table>
Discussion

- The temperature cannot go to very high, since evaporation will be very fast at high temperature.

-150°C

-30°C

30°C
Conclusion

• For well crystallized thin film, the growth temperature cannot be too high or too low. Too high will form large crystals, while too low will form poorly crystallized islands.
• The crystal size depend on growth temperature.
• Growth rate, pressure and substrate condition also affect crystallized thin film.