Nucleation in Vapor phase deposition

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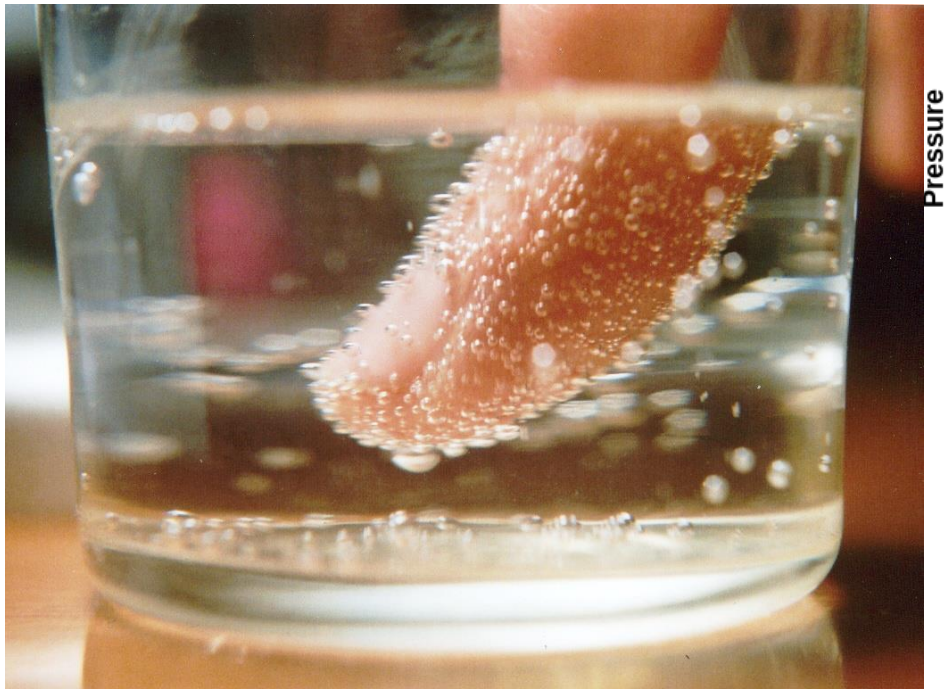
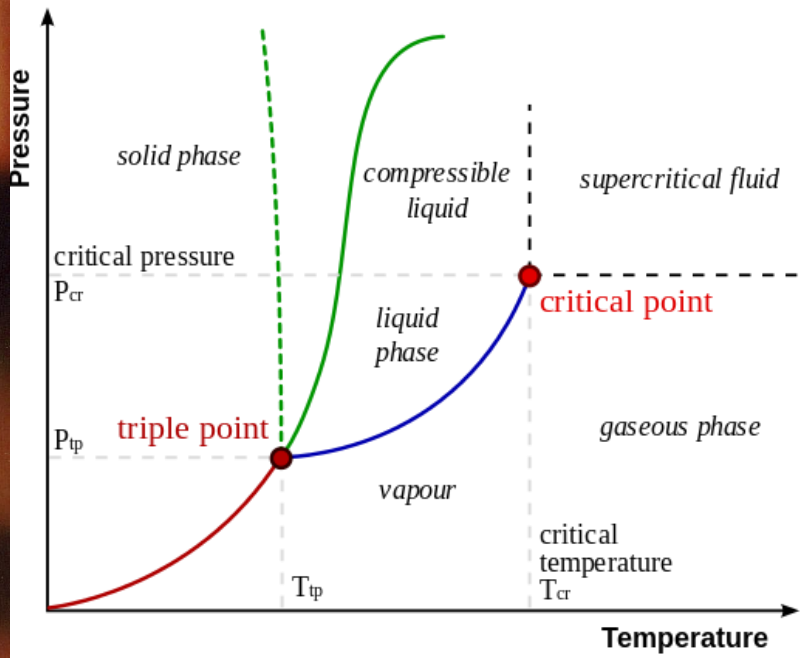
What is Nucleation?

- 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=$\rho Z j exp(-\Delta F/kT)$

  ρ is the number of possible nucleation sites per unit volume

  Z is the Zeldovich factor

  j is grow rate

  T is nucleation temperature

  ΔF is the energy cost for nucleus, at the top of barrier

  $\Delta F = -\frac{4\pi}{3} R^3 \rho \Delta\mu + 4\pi R^2 \gamma$

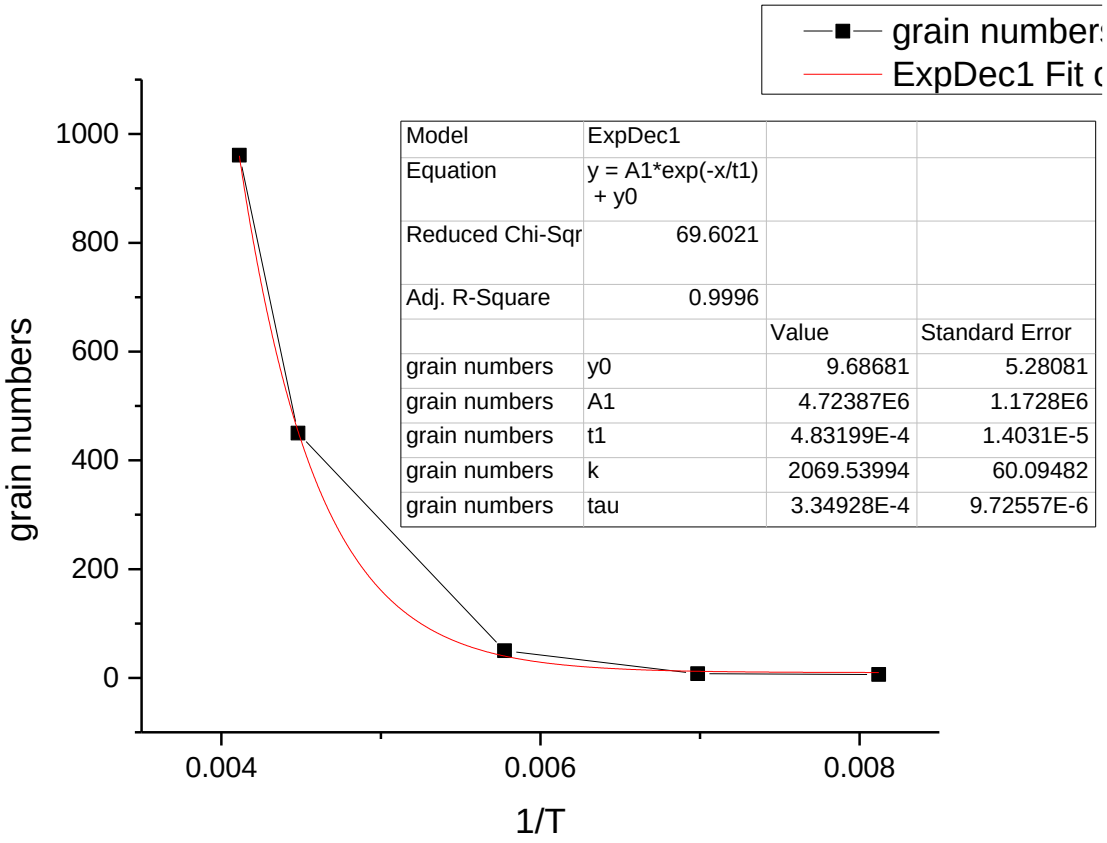
  R is radius of nucleus sphere, critical size from highest free energy

  Δμ is the chemical potential of nucleus

  ϒ is the interfacial tension

Temperature dependence

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



Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	69.6021		
Adj. R-Square	0.9996		
		Value	Standard Error
grain numbers	y0	9.68681	5.28081
grain numbers	A1	4.72387E6	1.1728E6
grain numbers	t1	4.83199E-4	1.4031E-5
grain numbers	k	2069.53994	60.09482
grain numbers	tau	3.34928E-4	9.72557E-6

Discussion

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

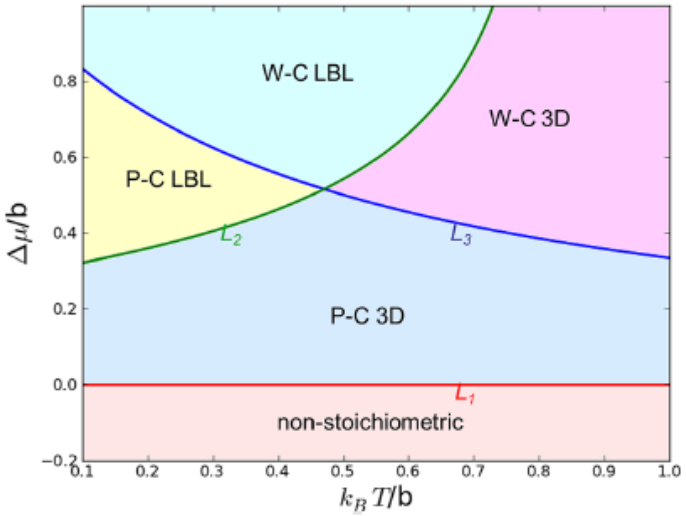
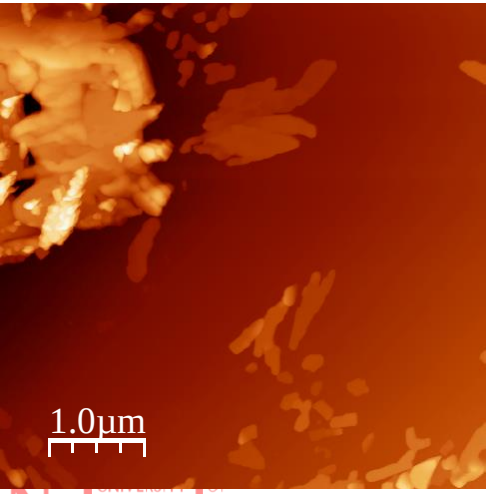
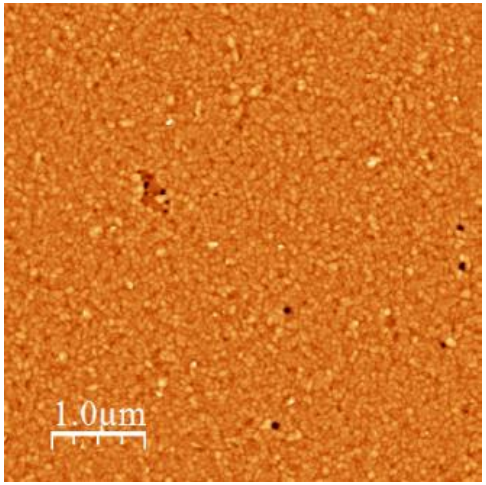


FIG. 6. The theoretically constructed growth diagram. L_1 (red): boundary between stoichiometric and non-stoichiometric growth; L_2 (green): boundary between 2D layer-by-layer (LBL) and 3D growth; L_3 (blue): boundary between the P-C and W-C growth.

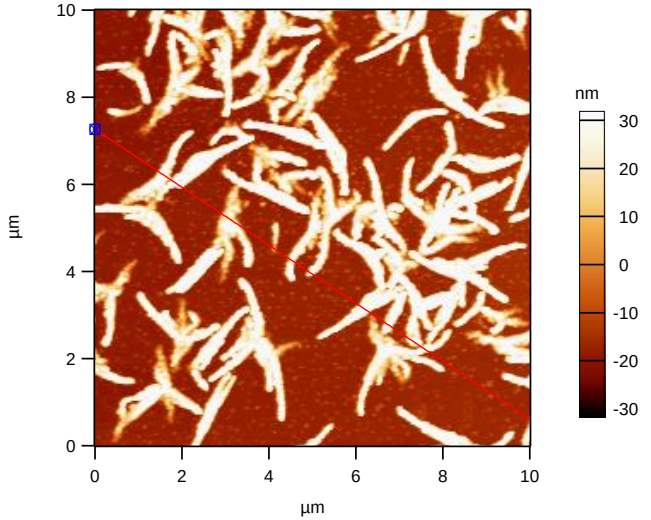
-150C



-30C



30C



Nebraska Lincoln

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.