Molecular Beam Epitaxy

09/26/2008

MSE 576: Thin Films

Deepak Rajput

Graduate Research Assistant
Center for Laser Applications
Materials Science & Engineering
University of Tennessee Space Institute
Tullahoma, Tennessee 37388-9700
Email: drajput@utsi.edu
Web: http://drajput.com

Outline

- Epitaxy
- Molecular Beam Epitaxy
- Molecular Beam
- Problems and Diagnostics

Epitaxy

- Method of depositing a monocrystalline film.
- Greek root: *epi* means "above" and *taxis* means "ordered".
- Grown from: *gaseous* or *liquid* precursors.
- Substrate acts as a seed crystal: film follows that !
- Two kinds: **Homoepitaxy** (same composition) and **Heteroepitaxy** (different composition).

Epitaxy

- Homoepitaxy:

  # To grow more purified films than the substrate.
  # To fabricate layers with different doping levels

- Heteroepitaxy:

  # To grow films of materials of which single crystals cannot be grown.
  # To fabricate integrated crystalline layers of different materials

Epitaxy

- Vapor Phase Epitaxy (VPE)

  $SiCl_4(g) + 2H_2(g) \leftrightarrow Si(s) + 4HCl(g)$ (at 1200^0C)

  # VPE growth rate: proportion of the two source gases

- Liquid Phase Epitaxy (LPE)

  Czochralski method (Si, Ge, GaAs)

  # Growing crystals from melt on solid substrates

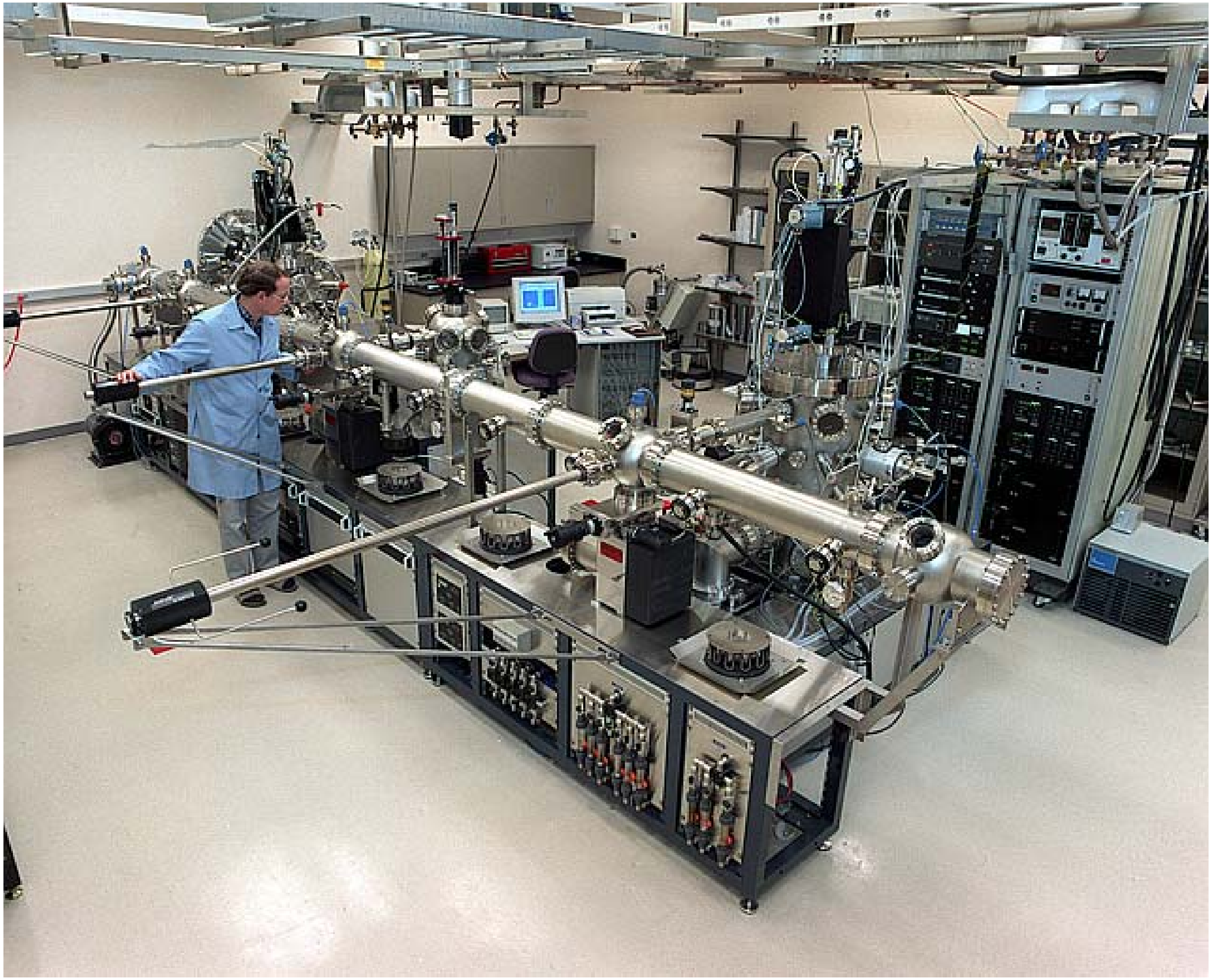
  # Compound semiconductors (ternary and quaternary III-V compounds on GaAs substrates)

- Molecular Beam Epitaxy (MBE)

  # Evaporated beam of particles

  # Very high vacuum (10^{-8} Pa); condense on the substrate

Molecular Beam Epitaxy



Source: William R. Wiley Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA

Molecular Beam Epitaxy: Idea !

- Objective: To deposit single crystal thin films !
- Inventors: J.R. Arthur and Alfred Y. Chuo (Bell Labs, 1960)
- Very/Ultra high vacuum (10^{-8} Pa)
- Important aspect: slow deposition rate (1 micron/hour)
- Slow deposition rates require proportionally better vacuum.

Molecular Beam Epitaxy: Process

- Ultra-pure elements are heated in separate quasi-knudson effusion cells (e.g., Ga and As) until they begin to slowly sublimate.

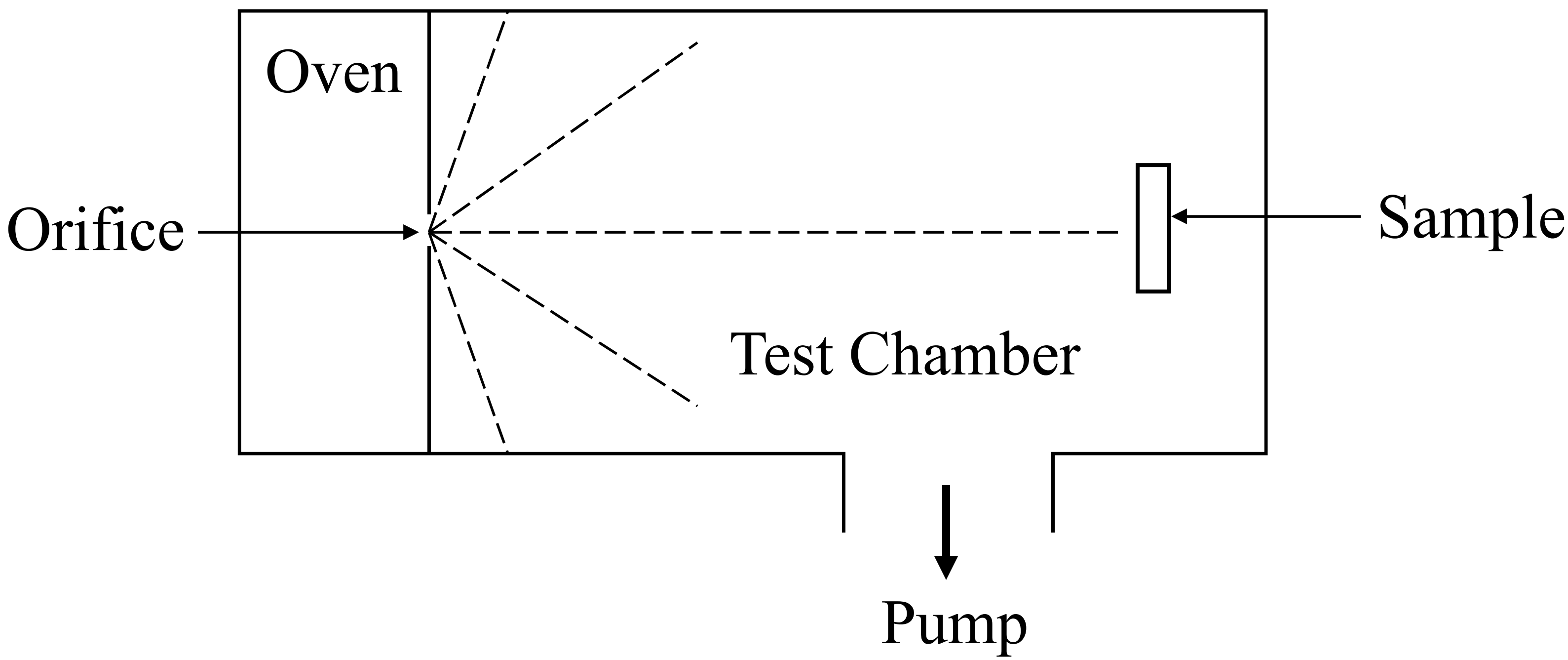
- Gaseous elements then condense on the wafer, where they may react with each other (e.g., GaAs).

- The term "beam" means the evaporated atoms do not interact with each other or with other vacuum chamber gases until they reach the wafer.

Molecular Beam

- A collection of gas molecules moving in the same direction.

- Simplest way to generate: Effusion cell or Knudsen cell



Knudson cell effusion beam system

Molecular beam

- Oven contains the material to make the beam.
- Oven is connected to a vacuum system through a hole.
- The substrate is located with a line-of-sight to the oven aperture.
- From kinetic theory, the flow through the aperture is simply the molecular impingement rate on the area of the orifice.

Molecular Beam

- Impingement rate is:

$$I = \frac{1}{4}n\bar{v} = \frac{1}{4}\left(\frac{p}{kT}\right)\sqrt{\left(\frac{8kT}{\pi m}\right)}$$

- The total flux through the hole will thus be:

$$Q = IA = \frac{p\pi r^2}{\sqrt{2\pi mkT}}$$

- The spatial distribution of molecules from the orifice of a knudsen cell is normally a cosine distribution:

$$I' = \frac{1}{4}n\bar{v}\left(\frac{\cos\vartheta}{\pi}\right)$$

Molecular Beam

- The intensity drops off as the square of the distance from the orifice.

$$I_{sub} = IA\left(\frac{\cos\vartheta}{\pi}\right)\left(\frac{1}{L^2}\right)$$

$$or,$$

$$I_{sub} = \left[\frac{p}{\sqrt{2\pi mkT}}\right]\left(\frac{r}{L}\right)^2 \cos\vartheta$$

- High velocity, greater probability; the appropriate distribution:

$$\frac{dn_v}{n} = 2\left(\frac{v^3}{\alpha^4}\right)\exp\left(\frac{-v^2}{\alpha^2}\right)dv$$

$$where\ \alpha = \sqrt{2kT/m}$$

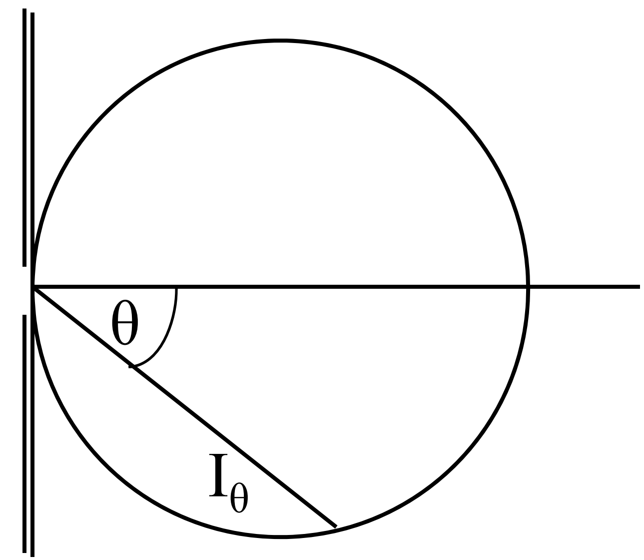
Molecular Beam

- Integrating the equation gives:

$$E_{tr} = 2kT$$

as the mean translational energy of the molecules

Intensity is maximum in the direction normal to the orifice and decreases with increasing θ, which causes problems.



Use collimator, a barrier with a small hole; it intercepts all of the flow except for that traveling towards the sample.

MBE: In-situ process diagnostics

- RHEED (Reflection High Energy Electron Diffraction) is used to monitor the growth of the crystal layers.
- Computer controlled shutters of each furnace allows precise control of the thickness of each layer, down to a single layer of atoms.
- Intricate structures of layers of different materials can be fabricated this way e.g., semiconductor lasers, LEDs.
- Systems requiring substrates to be cooled: Cryopumps and Cryopanels are used using liquid nitrogen.

ATG Instability

- Ataro-Tiller-Grinfeld (ATG) Instability: Often encountered during MBE.

- If there is a lattice mismatch between the substrate and the growing film, elastic energy is accumulated in the growing film.

- At some critical film thickness, the film may break/crack to lower the free energy of the film.

- The critical film thickness depends on the Young's moduli, mismatch size, and surface tensions.

Assignment

- Solve the equation to find the mean translational energy (E_{tr}) of the molecules:

$$\frac{dn_v}{n} = 2\left(\frac{v^3}{\alpha^4}\right)\exp\left(\frac{-v^2}{\alpha^2}\right)dv$$

$$where\ \alpha = \sqrt{2kT/m}$$

- What fraction of the molecules in a molecular beam of N_2 formed by effusion of N_2 gas initially at 300 K from an orifice at a large Knudsen number will have kinetic energies greater than 8kcal/mol?