Epitaxy

- growth of thin crystalline layers upon a crystalline substrate
 - heteroepitaxy
 - dissimilar film and substrate
 - autoepitaxy
 - same film and substrate composition
- techniques

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- Vapor-Phase Epitaxy (VPE)
 - CVD: Metal-organic VPE (MOCVD, OMVPE, ...)
 - PVD: Molecular Beam Epitaxy (MBE)
- Liquid-Phase Epitaxy (LPE)
 - mainly for compound semiconductors
- Solid-Phase Epitaxy
 - recystallization of amorphized or polycrystalline layers
- applications
 - bipolar, BiCMOS IC's
 - 2-5 µm in high speed digital
 - 10-20 µm in linear circuits
 - special devices
 - SOI, SOS
 - HEMT, MODFET, HBT

Vapor Phase Epitaxy

- transport of reactants to the substrate from gas stream primarily laminar(uniform velocity) away from the substrate, parallel to substrate face
 - friction at surfaces forces gas flow velocity to be zero at substrate face
 - stagnant boundary layer at interface through which reactants must diffuse
 - causes concentration, temperature gradients between gas & substrate



from Sze, 2nd ed., p. 68.

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VPE System Design

• general requirements:

- cleanliness essential
 - particle
 - gas purity (H₂ typically 99.9999%)
- precise control of gas flows necessary
- provision for in situ etch
- substrate mounting and slice carrier designed to minimize turbulence
 - chamfer wafer edges
 - recess wafer slots
- boundary layer control via tilted carrier to increase gas velocity as x increases
- heating of susceptor via (cold wall)
 - induction
 - radiant lamps
- use of LPCVD:
 - increases boundary layer thickness for given gas velocity
 - produces good uniformity

Silicon VPE chemistry

- hydrogen reduction of chlorosilanes:
 - silicon tetrachloride, SiCl₄
 - dichlorosilane, SiH₂Cl₂
 - trichlorosilane, SiHCl₃
- reaction paths: T ≥ 800°C
 - predominant species formed are HCI and SiCl₂; at temperatures between 1150-1250°C

 $\underbrace{SiCl_2}_{adsorb} + \underbrace{SiCl_2}_{adsorb} \Leftrightarrow \underbrace{Si}_{solid} + \underbrace{SiCl_4}_{desorbs}$

- SiCl₄ reacts again in gas phase to produce HCl, SiCl₂
- overall reaction:
 SiCl₄ + 2H₂ ≒ Si + 4HCI
- all these are reversible reactions
 - etching occurs if have SiCl₄ rich gas stream





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Silicon VPE growth

- homogeneous nucleation
 - reactants combine to form isolated nuclei in gas phase, then attach to substrate surface
 - can cause poor crystal quality growth
- heterogeneous nucleation
 - reactants coalesce only on the surface where deposition occurs
 - note growth is lateral, not really vertical:
 - adsorbed species move rapidly by surface diffusion until they find a "kink," frequently a screw-type dislocation



Deposition rate limiters

- reaction rate limited
 - growth rate limited by chemical kinetics
 - conventional exp(-E/kT) behavior
 - also depends on reactant partial pressures
- mass transfer limited
 - reaction rate very "fast" compared to diffusion across stagnant boundary layer
 - growth rate weakly dependent on temperature
- operate in the mass-transfer regime to prevent extreme sensitivity to temperature variations across and between wafers



adapted from Sze, 2nd ed., p. 62.

Comparison of silicon VPE sources

- silicon tetrachloride:
 - highest temperature required to produce SiCl₂
 - most stable chlorosilane
 - least deposited silicon per gas input
- trichlorosilane:
 - approx. 50°C lower growth temperature
- dichlorosilane:
 - lowest temperature of chlorosilane processes
 - most efficient deposition per gas input
- silane:

have to be careful to avoid poly growth

reactant	growth rate (μm / min)	temp. (°C)	allowed oxidizer (ppm)
SiCl ₄	~0.4 – 1.5	1150 – 1250	5 - 10
SiHCl₃	~0.4 - 2	1100 – 1200	5 - 10
SiH ₂ Cl ₂	~0.4 - 3	1050 – 1150	< 5
SiH ₄	~0.2 - 0.3	950 – 1050	< 2

Typical process

- hydrogen backfill and flush
- reactor heating,
 - temperature equilibration
 - H₂ atmosphere, elevated temperature causes reduction (removal) of surface oxides
- in situ etch
 - HCI etch @ 1150-1200°C for 5 min. to remove thin surface layer of silicon
- H₂ flush of HCI, set temperature for growth
- establish source gas, dopant gas flows

Doping and autodoping

- intentional dopants added to gas stream:
 - boron, B_2H_6
 - phosphorus, PH₃
 - arsenic, AsH₃
- in addition to intentional impurities have impurity introduction and redistribution:
 - sources
 - conventional diffusion in crystal
 - gas stream doping of epi due to evaporation of Si, dopants, reactor materials
- minimum background impurity concentration due to reactor, etc. contaminants ≈ 10¹⁴/cm³



Autodoping

- in addition to reactor contaminants also have evaporation and diffusion of dopants from the wafers themselves.
- combined diffusion and evaporation-induced doping dominate the first ~2µm of epi growth



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Problems in bipolar design with epi

typical, idealized configuration for n-p-n transistor:



- problems:
 - lateral autodoping
 - dopant from n+ regions evaporates into stagnant layer, diffuses laterally, dopes adjacent areas
 - pattern shift
 - growth process shifts position of steps on substrate

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Lateral Autodoping

- worse for higher temperatures, lower growth rates
- decreases with decreasing pressure
 - increases vertical diffusion rates
 - lateral autodoping less important in **LPCVD**



Pattern Shift in Epi Growth

- in bipolar process: .
 - 50-100 nm steps in silicon surface from initial oxide mask and from oxidation during drive of n⁺ buried layer
 - must maintain steps for subsequent alignment
- during epi growth:
 - growth is lateral on microscopic scale
 - growth rate depends on crystal surface orientation
 - causes shift and distortion of buried layer pattern
- pattern shift: ٠
 - increases with increasing growth rate and decreasing growth temperature
 - is minimized for:
 - <111> Si by misorienting surface by 2-5°
 - worst case design rule:
 - shift = layer thickness





pattern shift



Heteroepitaxy

- growth of dissimilar film/substrate combination
- what do you need?
 - chemical compatibility
 - thermal compatibility
 - "crystal" compatibility
 - similar lattice structure
 - similar lattice constants
- examples

- silicon-on-sapphire
 - violates lattice match
- Al_xGa_{1-x}As system

Silicon on Sapphire

- heteroepitaxial process, usually pyrolisis of silane at 1000°-1050°C, ≈ 1 µm thick
- sapphire chosen for high temperature, chemical stability
 - lattice mismatched at interface
 - aluminum silicate formed at interface
 - aluminum autodoping from substrate
 - thermal expansion coefficient mismatch
- high defect density:

- stacking faults, misfit dislocations
- density \approx inverse with distance to interface
- Very short minority-carrier lifetimes
 - cannot be used for bipolar IC's
- used only in MOS devices for
 - radiation hardness
 - latch-up immunity

Molecular Beam Epitaxy

- non-CVD vapor phase epitaxy via evaporation of material in ultrahigh vacuum environment. By utilizing very low growth rates (≈ 1µm/hour) can tailor doping profiles and composition on a monolayer scale.
 - growth temperatures 400° 800°C
 - background vacuum pressures ≈ 10⁻¹¹ Torr
 - monolayer formation time > 2 days
 - silicon, SiGe, GaAs, AlGaAs, II-VI materials all grown
- machine design:
 - source materials evaporated from effusion cells
 - (Si MBE uses e-beam evaporators for Si source)
 - temperature control critical, up to 1600°C
 - beams interrupted with mechanical shutters to control composition and doping
 - all growth chamber surfaces cooled to LN2 temp to prevent impurity incorporation in films

Silicon Molecular Beam Epitaxy

- process requires:
 - ultra high vacuum system for deposition
 - very clean initial wafer surface
- flash decompose protective thin oxide in UHV @ 750-850°C
- growth temperature 450-850°C
- epitaxial materials grown:
 - silicon with very abrupt doping profiles
 - metal silicides: NiSi₂, Co₂Si, etc.
 - Ge_xSi_{1-x}/Si
- applications:
 - buried silicides to replace buried layers in bipolar
 - metal base transistor, permeable base transistor
 - HEMTs, HBTs, superlattice devices

Summary Slide

- Epitaxy
- Silicon VPE growth
- Doping and autodoping
- Pattern Shift in Epi Growth
- Heteroepitaxy
- Epitaxial Growth of GaAs
- next topic: <u>metallization</u>