Development of Parametric Inventories for Semiconductor Wafer Fabrication

NSF/SRC Engineering Research Center for Environmentally Benign Semiconductor Manufacturing TeleSeminar May 27, 2004

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Why Life Cycle Inventory

- Focus is often on the "impact" portion of Life Cycle Analysis (LCA)
- BUT impact is not valid if inventory is not valid (or nonexistent).
- For most products, inventories can be developed by
 - Reverse engineering of products and/or

- Analyzing relatively simple processes



Energy Requirements for Use and Manufacture of a Microchip



Adopted from Williams, et al (2002) with modifications based on SEMATECH survey

Focus on Wafer Fab

 Exact numbers may not be available, but all available data suggest that wafer fab is most critical phase for energy

Assumptions:

 Energy consumption is reasonable surrogate for mass balances

 Energy is critical for multiple impacts (resource consumption, global warming, etc)

Developing Life Cycle Inventories for Wafer Fabrication

- Wafer fabrication is resource intensive, using large amounts of energy, water, and chemicals
- Inventories are poorly understood or documented
- Reverse engineering of the silicon chip reveals little about how it was manufactured
 - Most of the materials used in the manufacturing process never reside on the wafer or are later removed
- Process flows (the sequence of unit operations and recipes) are complex and change rapidly

Challenges for Resource Inventory Development in Wafer Fab

- Many products, each with short lifetimes (18 to 24 months)
- Product-based approach requires frequent development of many inventories (one per product)
- Difficult to predict how changes in product or process design (including equipment selection) will affect inventory
- Difficult to perform tradeoff analyses

Alternative Approach

- Get 80% of the information with 20% of the data
- Develop process-based, parametric modules where material and energy flows are related to
 - Equipment type (technology)
 - Material selection
 - Product design
- Develop "typical" mass and energy flows for each unit operation, with the opportunity to add detail as needed

Requirements

- Define system boundaries
- Define functional unit
- Define inventory focus
- Define system of data organization and management

System Boundaries

- Gate-to-gate approach suitable for later insertion into full LCA
- To date, have looked only at direct wafer fabrication processes, but hope to include infrastructure as well





consumer product

wafer



Functional Unit Selection

- Consumer product (e.g., computer)
- Packaged component
- 1 cm² of processed silicon ("die equivalent")
 - Fully processed wafer

Functional Unit: Wafer

- Focus is at the level where most of the material and energy flows occur
- Good sensitivity to both process and product variations
- Data is more "generic" or universally applicable when managed at the wafer level than at the die level
- Only 3 different wafer sizes for CMOS.
 Increase in wafer size only slightly increases material and energy flows
 - e.g. 400 kWh per 4 inch wafer with 52 1 cm2 die per wafer and 500 kWh per 8 inch wafer with 261 die per wafer – only a 20% error if use wafer data, but 500% error if use die

Top "20" Chemicals of Interest

Sulfuric Acid (H_2SO_4) Isopropyl Alcohol ((CH₃)₂CHOH) Phosphoric Acid (H₃PO₄) Hydrochloric Acid (HCl) Tetramethyl Ammonium Hydroxide Sodium Hydroxide (NaOH) $((CH_3)_4NH_4)$ Nitric Acid (HNO₃) Hydrofluoric Acid (HF) Hydrogen Peroxide (H₂O₂) N-Methyl Pyrrolidone (C₅H_oNO) Nitrogen Trifluoride (NF₃) Ammonium Fluoride (NH_4F) Ammonium Hydroxide (NH₄OH)

Butylacetate (CH₃COO(CH₂)₃CH₃) Ethyl Lactate $(C_5H_{10}O_{3})$ Hexamethyl Disilazane (C₆H₁₉NSi₂) Silica, Amorphous (SiO₂) **Propylene Glycol Monomethyl Ether** Acetate $(C_6H_{12}O_3/CH_3CH(OCOCH_3)CH_2OCH_3)$ Acetic Acid (CH₃COOH) Water Photo Resists Energy ACT-690c ($H_2N(CH_2)_2OH$) Acetone (CH₃COCH₃)



Resource Consumption in the Wafer Fab



Adopted from Williams, et al (2002) with modifications based on SEMATECH survey

Inventory Focus

- Specialty chemicals are small portion of inventory
 - Costly on a per unit basis (e.g. \$500/liter of resist)
 - Tied to specific processes (photolithography), thus mass balances are straightforward
 - Environmental impacts are relatively easy to define (MSDS)
 - Energy, water, and elemental gases form the bulk of the inventory
 - Important economically and environmentally
 - Much less sensitivity to proprietary data
 - More challenging to accurately measure because ubiquitous (not tied to specific process)



Cost of Energy vs. Photoresist

 Wafer with 20 mask layers, resist at \$500/liter, and 3 ml of resist per layer = \$30 per wafer

 Wafer that requires 500 kWh per wafer at \$0.06 per kWh = \$30 per wafer



Unit Operations as Focal Point for Inventory Development

- Unit operations relatively unchanged for the last 45 years
- Relatively little variation between fabs (due to equipment cost)

 Most variation in resource inventory can be approximated based on equipment type and process recipes



Wafer Clean and Furnace Unit Operations

- Significant use of energy, water, and elemental gases
- Reasonably uniform from facility to facility
- Large body of general knowledge (less proprietary than other operations)
- Relatively easy to differentiate between equipment types (e.g. horizontal vs. vertical furnaces) and processes (e.g. KOH and RCA)

Material and Energy Consumption

Use mixture of

- Process (equipment) recipes
- Direct monitoring of equipment
- Mass and energy balances at unit operation
- Treat as a "cost of ownership" problem; look at consumption for
 - Production
 - Test wafers
 - Idle time
 - Maintenance



Energy Consumption

Furnaces

- Equipment monitoring data
- Direct measurement (generally not practical)
- Wet Cleans

$$P_{heating} = \frac{V \times \rho \times c_p \times \Delta T}{n}$$

- Use physical and chemical data from MSDS where available
- Assume efficiency factor of 80% (i.e., 20% lost to atmosphere)

Example of Module at Function Level: Thermal Oxide

Energy and Oxygen Consumption as Functions of Film Thickness

Energy Consumption

Oxygen Consumption





Example of Module at Equipment Level

Wafer Clean Operation

Different equipment types
Same function (standard clean)
Same chemistries

Analysis includes idle time and test runs as well as actual processing

Wet Bench vs. Spray Clean – SPM/HF/RCA

Material	Wet Bench cc per wafer	Spray Cleaning cc per wafer	
49% HF	6.0	2.6	
H ₂ SO _{4,}	110.3	71.2	
HCI	23.0	20.2	
H ₂ 0 ₂	56.5	94.8	
NH₄OH	16.1	21.7	
DI	21,391	37,754	
IPA	324.8	0	
N ₂	No data	1,017,554	

Scenario 1

- A facility uses 10 SPM/HF/RCA cleans per wafer (averaged for all products) and wants to switch from wet bench to spray cleaning process
- Question What is the effect on DI water consumption?
- Answer increase of 16 liters per wafer



Examples of Modules at the Unit Operation Level :

 Consider both equipment selection and throughput

 Vertical furnace (batch process) vs. Rapid Thermal Process (RTP) (single wafer)

 Results may vary by facility or even within a facility

Vertical Furnace vs. RTP

Direct measurements

- RTP
 - 48 kW production
 - 45 kW idle
- Vertical
 - 21 kW production
 - 16 kW idle
- Assumptions
 - Equipment is operating 131 hours per week (80% of 168)
 - Vertical furnace is fully loaded



Energy Consumption as Function of Time

Time_{equip demand} =

Units_{equip} = Roundup [(Time_{equip demand}) / Time_{prod}]

Time_{idle}= (Units_{equip} x Time_{prod}) – Time_{equip demand}

Effects of Equipment on Furnace Unit Operation



Effects of Process Design on Furnace Unit Operation

- Same equipment type (vertical furnace)
- Same function (growing SiO₂ on bare silicon dry oxidation)
- Three different temperatures, eight different thickness

Given any temperature between 700 and 1025°C and thickness between 25 and 1000 Å, can we predict the amount of oxygen consumed?

Oxygen Consumption vs. Thickness for 3 Different Temperatures



Oxygen / Thickness vs. Temperature



Oxygen Consumption vs. Temperature for a 200 Å Oxide



Scenario 2

- Process engineer wants to drop temperature from 1025°C to 950°C on a 200 Å oxide layer in order to improve process control
- Question How does decreasing the temperature affect oxygen consumption?
- Answer
 - At 1025°C, 804 sccs of O2 are consumed
 - At 950°C, 1764 sccs of O2 are consumed (more than double)



 Characterize a "typical" process within a given unit operation
 Vary for specific products or process flows as needed based on known relationships between consumption and/or emissions and key design parameters



Aggregation of Unit Operation Data

		Number of functions				Power	
	Unit			Wafers	Wafers	(kW)	
	Operation	8 layer	6 layer	per run	per hour	Proc	Idle
	Implant	16	16	25	20	27	15
	CVD	13	11	10	15	16	14
1	Wafer	35	31	50	150	8	7.5
	Furnace	21	17	150	35	21	16
	Furnace	7	7	1	10	48	45
	Photo	27	23	1	60	115	48
	Photo	27	23	1	60	90	37
	Etch	24	20	1	35	135	30
	Etch (ash)	27	23	1	20	1	0.8
	Metalliz'n	11	9	1	25	150	83
	CMP	18	14	1	25	29	8



Energy Requirements for 8 vs. 6-Layer Metal MPU



Applications

 Method can be used to quantitatively predict changes in inventory based on product or process design change

- Especially useful for processes that
 - are used repeatedly
 - use significant amounts of bulk chemicals, gases, or water
 - where direct measurement is clumsy or impossible

Impact on Industry

- Industry consortium (SEMATECH) was host to the development of these methodologies and datasets
- Results well received by 12 member companies (major semiconductor companies)
- SEMATECH plans to continue in this area
- Applied Materials, Motorola, AMD, ST Microelectronics interested

Summary

 Inventories that are relatively independent of product type and specific process recipes

- Allows trade-off analyses to be made

 Facilitates predictions about environmental consequences as a function of product or process design changes

 Contain less sensitive or proprietary manufacturing information thus increase potential for sharing of data along the supply chain

Future Work

- Focus on energy-
 - More critical as move to deep UV
 - Assume that it is a reasonable surrogate for material consumption
 - Data is less sensitive and easier to share
 - Critical for economic health of industry

 Look at equipment factory integration (thermal management) as well as energy requirements for process operations

Work with equipment suppliers