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Integrated Sustainability Analysis of Atomic Layer Deposition for Microelectronics Manufacturing

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Integrated Sustainability Analysis of Atomic Layer Deposition for Microelectronics Manufacturing

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Atomic layer deposition (ALD) is a promising nanotechnology for wide applications in microelectronics manufacturing due to its ability to control layer growth at atomic scale. Sustainability of ALD technology needs to be quantitatively investigated in this early development stage to improve its economic and environmental performance. In this paper, we present an integrated sustainability analysis of ALD technology through material and energy flow analyses. The study is performed on the ALD of Al_2O_3 high- κ dielectric film through trimethylaluminum and water binary reactions. The precursor utilizations, methane emissions, and nanowaste generations from the ALD process are all quantitatively studied. Energy flow analysis demonstrates that the ALD process energy consumption is mainly determined by the ALD cycle time rather than the process temperature. Scale-up performance of the ALD technology is also studied for both emission generations and energy consumptions. Strategies and methods for improving the sustainability performance of the ALD technology are suggested based on the analysis.
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Keywords: atomic layer deposition, sustainable manufacturing, material flow analysis, energy flow analysis, Al_2O_3 dielectric film

1 Introduction

As the miniaturization trend continues in the semiconductor manufacturing industry, atomic layer deposition (ALD) has received increasing attention in recent years due to its ability to obtain atomic layer control of film growth [1–3]. ALD can deposit highly uniform and conformal thin films on extremely complex surfaces [4], and accordingly, has potential applications on a wide variety of electronic products including complementary metal-oxide-semiconductor (CMOS) chips, flat panel display, optical filters, etc. [5].

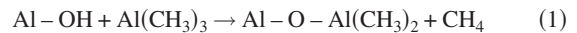
ALD operates by alternating the exposure of a surface to vapors of two or more chemical reactants to deposit an atomic layer film on the surface. The chemical reactions are separated by complete purging in between. In ALD operations, the surface reaction is self-limited, and the film thickness could be accurately controlled in atomic scale. As needed, the deposition process can be repeated to obtain a film layer for a specific thickness.

A wide variety of solid materials could be deposited through ALD, based on the needs of specific applications [6–11]. The typical application of ALD is on deposition of Al_2O_3 high- κ dielectric films to replace conventional SiO_2 dielectric gate in the metal oxide semiconductor field effect transistors (MOSFETs) to support the miniaturization of the microtransistors [12–15].

In atomic layer deposition, the film thickness increment and surface roughness profiles depend on the chemical reaction process on the surface of the silicon wafer. Reaction sufficiency relies on the concentrations of the reactants in the ALD reactor and the process temperature. As demonstrated through ALD experiments, the accuracy of Al_2O_3 film thickness can be successfully controlled at 0.1 ± 0.01 nm [16], while the roughness of the growing surface can be maintained less than 0.3 nm [17].

Typical ALD of Al_2O_3 dielectric film uses trimethylaluminum (TMA), $\text{Al}(\text{CH}_3)_3$, as the metal source, and deionized water, H_2O ,

as the oxidant. Deposition mechanism of Al_2O_3 by ALD is based on the chemical vapor deposition (CVD) reaction: $2\text{Al}(\text{CH}_3)_3 + 3\text{H}_2\text{O} \rightarrow \text{Al}_2\text{O}_3 + 6\text{CH}_4$. In the ALD process, this CVD reaction is split into the following two half reactions:



This ALD process depends on the surface reactions between TMA, water, and hydroxyls to form the Al_2O_3 layers. In the ALD operations, the growth rate is an important indicator of the deposition efficiency. Generally, higher concentrations of precursor materials lead to higher growth rates in ALD of Al_2O_3 from the TMA and water binary reactions [18]. In order to obtain a sufficient surface reaction and a higher growth rate, excessive amount of precursor materials are usually supplied into the ALD system [18]. The excessive material consumed, however, is not only a cost issue but also an environmental concern in the production of Al_2O_3 dielectric gate in the semiconductor manufacturing industry.

The precursor material TMA, Chemical Abstract Service (CAS) No. 75-24-1, is a flammable and toxic chemical. When released into the atmosphere, TMA is pyrophoric and can readily react with hydroxyls and water in the air, and form Al_2O_3 nanoparticles, which could be harmful for both occupational and public health if in relatively high concentrations.

Besides, the principal byproducts of the ALD process is methane, which is a major greenhouse gas and has a global warming potential 25 times that of carbon dioxide [19]. As dielectric materials are widely used in semiconductor industry, manufacturing of Al_2O_3 dielectric gate through $\text{Al}(\text{CH}_3)_3$ and H_2O binary reactions could have significant impact on global warming. A rough estimate of the global dielectric material demand in the semiconductor industry is in the range of 10^8 kg per year [20,21]. Based on the Al_2O_3 CVD reaction, deposition of 1 kg Al_2O_3 would generate 0.94 kg of CH_4 , which is equivalent to 23.5 kg of CO_2 .

Besides the material use and emission generations, energy consumption of ALD is another concern for both economic and envi-

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ronmental justifications. ALD has to be operated at the vapor phase of the precursor materials and requires ultrahigh vacuum conditions. The energy consumption of ALD for such process operations as heating, pumping, monitoring, controlling, etc., would contribute not only to the cost of the deposited dielectric films but also to the generation of various pollutant emissions from the energy production and supply industry.

For sustainable manufacturing of Al_2O_3 dielectric gate in semiconductor industry, both material and energy consumptions of the ALD process needs to be well understood to support decision-making during the process improvement and system optimization of ALD technology. In this paper, we present an integrated sustainability analysis of the ALD process for Al_2O_3 dielectric gate in microelectronic manufacturing. The integrated sustainability analysis is conducted on both material and energy use of the ALD process. Material and energy flow analyses are performed to quantify the material and energy consumptions, identify the process emissions, and track the process flows within the ALD reaction system. These results could be helpful in improving both the economic and environmental performances of the ALD technology to achieve a sustainable application of the ALD technology in microelectronics manufacturing.

2 Material Flow Analysis

Material flow analysis is performed here to gain deep insights into the ALD system and to obtain a comprehensive understanding of the material flows throughout the ALD processes. The ALD material flows are modeled on the process by using the Cambridge NanoTech Savannah S200 ALD system. The reactor is customized for 10.16 cm (4 in.) standard silicon wafers, with 15.24 cm (6 in.) inner diameter and half inch inner depth. Nitrogen is used as the carrier and purge gas to transport TMA and water precursor vapors to the silicon surface, and purge reaction gases out of the reactor during each half-cycle reaction. The temperature of the reactor and the outlet pipeline are maintained at 200°C and 160°C , respectively. An Edwards RV5 rotary vane pump is connected to the end of the outlet pipeline to vacuum the reactor at the beginning and pump excessive materials out of the reactor during the experiment.

Before the ALD operations, the wafer surface is fully hydroxylated through a sufficient pulsing of H_2O vapor in the ALD reactor, which also leads to the coverage of hydroxyls on the inner surface of the ALD reactor and the outlet pipeline. In the following, TMA and water are alternatively supplied into the reactor through separate inlet pipelines to avoid their reaction prior to the surface deposition.

As the precursor vapors are introduced into the reactor, the Al_2O_3 film would be formed and deposited not only on the surface of the silicon wafer but also on the inner surface of the reactor. Excessive precursors from the reactor, when pumped out, would be deposited on the inner surface of the outlet pipeline, while the remaining materials, if any, would be potential for environmental emissions. From mass balance, the total amount of materials supplied into the ALD system equals to the sum of the amount deposited on the wafer, reactor, and outlet pipeline, and the amount potential for environmental emissions, as shown below

$$\sum M_{\text{input}} = \sum M_{\text{wafer}} + \sum M_{\text{reactor}} + \sum M_{\text{pipeline}} + \sum M_{\text{emission}} \quad (3)$$

ALD is noted as a self-limiting chemical process. Al_2O_3 film deposition rate per cycle is initially proportional to the exposure of precursor materials but saturates to a maximum value after certain reaction sufficiency. Accordingly, the supplied excessive amount of precursor materials are all wasted, which generates both economic and environmental concerns of the ALD applications. In the ALD operation, the supplied amount of precursor materials should be optimally determined to ensure their best utilizations, which would consequently improve both the economic

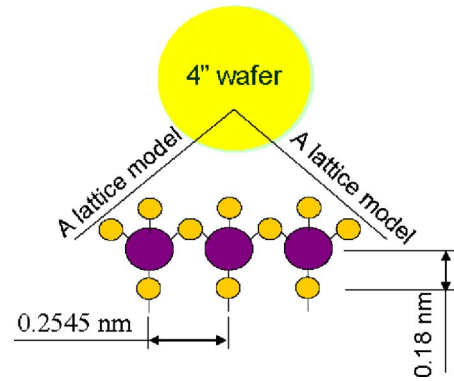


Fig. 1 ALD lattice configurations

and environmental performances of the ALD technology. Unfortunately, such an optimal supply pattern is not established yet; excessive amount of precursors are usually loaded into the ALD system to ensure a sufficient surface reaction and a high film growth rate [18]. Due to the variation in the ALD system dimensions, the common practice to control the supply of precursor materials is to set the pressure of the materials in the ALD system. The effect of process pressure on ALD of Al_2O_3 has been studied at various pressure levels [22]. In this analysis, we investigate the precursor material flows of the ALD system under 600 mTorr, 800 mTorr, and 1000 mTorr pressures, by following [22]. The partial pressure of the TMA precursor is set at 15% of the process pressure by following [13], while the partial pressure of supplied water is decided by considering the correlations between the TMA and H_2O precursors in the ALD binary reactions. According to the Al_2O_3 deposition mechanism, a complete reaction of the precursors in the ALD system needs water molecules to be supplied at an amount one and a half times of the TMA. But in real operations, a larger water dose is preferred due to its ability to enhance the Al_2O_3 layer growth rate [23]. Here we set the amount of water supplied as double of the TMA amount, namely, with partial pressure set at 30% of the process pressure to ensure a high growth rate and a complete reaction of the precursors in the ALD system.

As demonstrated by the ALD reaction, each TMA molecule needs a hydroxyl molecule and 1.5 H_2O molecules to form one Al_2O_3 molecule. The amount of Al_2O_3 which can be deposited depends on the quantity of hydroxyls on the deposition surface. In the ALD system, the reactor and pipelines are made of stainless steel. As the physical adsorption of hydroxyls on the bulk surface is governed by van der Waals force, the surface concentration of hydroxyls on the silicon wafer and the ALD reactor would be different, which would lead to different amounts of Al_2O_3 deposition on the two types of surfaces. For the surface deposition of Al_2O_3 on a silicon wafer, here we employ a lattice model to calculate the surface concentration of Al_2O_3 , as shown in Fig. 1 above. In Al_2O_3 molecular structure, the Al-O bond length is 1.8×10^{-10} m [24]. The Al-O-Al bond angle is 90 deg in the surface distribution [25]. As a result, the Al-Al bond length is $\sqrt{2} \times 1.8 \times 10^{-10} = 2.545 \times 10^{-10}$ m. So for each Al atom deposited on the wafer surface, it occupies a surface area of 6.477×10^{-20} m^2 . As a result, the maximum number of Al atoms which could be deposited within each square centimeter is 1.544×10^{14} atoms. The maximum Al concentration which could be achieved through a full surface deposition is 2.564×10^{-9} mole/ cm^2 on the silicon wafer surface. During surface reactions, one Al atom needs one hydroxyl molecule, and the surface deposition of Al_2O_3 is limited by the surface coverage of hydroxyls. Due to the surface deficiency and incomplete hydroxylation, the hydroxyl concentration has been experimentally identified between 70% and 80% of the maximum surface coverage [17]. Here we take an average of 75% for the surface coverage of Al_2O_3 . As calculated, the Al

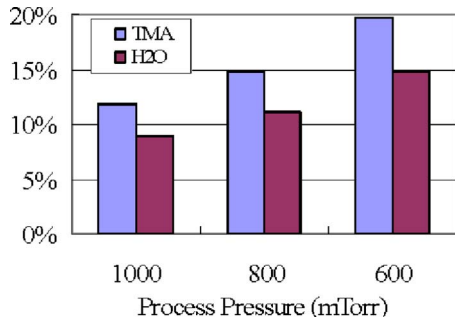


Fig. 2 Material utilization efficiency of TMA and H₂O at three process pressures

atoms deposited on the 10.16 cm (4 in.) silicon wafer is 1.56×10^{-7} moles per ALD cycle, and the Al₂O₃ amount deposited is 7.8×10^{-8} mole per ALD cycle. Following the same principle, the amount of Al₂O₃ deposited on the inner surface of the ALD reactor and the outlet pipeline can also be obtained.

In the ALD of Al₂O₃, only the material deposited on the wafer surface is desired and produces economic value. The material utilization efficiency of the precursor materials η , defined as the ratio between the amount of precursor deposited on the wafer and the total amount of input material, is a meaningful metric for assessing the material usage of precursor materials in the ALD system

$$\eta = \frac{\sum M_{\text{wafer}}}{\sum M_{\text{input}}} \quad (4)$$

The input amounts of precursors could be calculated through ideal gas law for each ALD cycle when the pressure, temperature, and volume are known for the ALD operations. As the partial pressure of TMA and H₂O are set at 15% and 30% of the process pressure, the TMA amounts loaded per ALD cycle are 1.31×10^{-6} , 1.05×10^{-6} , and 7.88×10^{-7} moles at 1000 mTorr, 800 mTorr, and 600 mTorr, respectively; the H₂O amounts loaded per ALD cycle are twice of the TMA amount. As a result, the material utilization efficiencies of the TMA and H₂O precursors, as calculated through Eq. (4) for the three process pressure conditions of ALD operations, are shown in Fig. 2 above.

In this ALD operation, both precursors have low material utilization efficiencies at the three pressure levels. TMA is between 12% and 20%, and H₂O is between 8% and 15%. As identified in the current ALD system, the material utilization efficiency is limited mainly by the surface area ratio between the silicon wafer and the ALD reactor. The reactor used in this ALD system is in a cylindrical shape and has a surface area five times that of the silicon wafer. Increasing the surface area ratio between the silicon wafer and the reactor can improve the material usage efficiencies, while an optimal supply pattern of precursor materials based on the ALD system dimensions and process parameters is also needed.

Besides the deposition on the silicon surface, Al₂O₃ films are also deposited on the inner surface of the ALD reactor and on the inner surface of the outlet pipeline. The surface coverage of hydroxyls on a stainless steel surface is approximately 1.30×10^{-9} mole/cm² at 200°C and 1.35×10^{-9} mole/cm² at 160°C [26]. Since each hydroxyl molecule can deposit one Al atom, the same moles of TMA precursor would be deposited on the inner surface of the reactor and outlet pipeline through the ALD binary reaction. The remaining precursors from the surface reactions of the ALD system would be potential for environmental emissions and need to be properly handled at the end of the pipeline.

Since the surface coverage of hydroxyls is fixed on a stainless steel surface under specific temperature condition, the maximum amounts of precursors which can be deposited on the inner surface

Table 1 Percentage of precursor material consumption in the ALD system

	Process pressure (mTorr)	Wafer deposition (%)	Reactor deposition (%)	Pipeline deposition (%)	Potential emission (%)
Al(CH ₃) ₃	1000	12	35	50	3
	800	15	43	42	0
	600	20	57	23	0
H ₂ O	1000	9	26	38	27
	800	11	32	47	10
	600	15	43	42	0

of the reactor and outlet pipeline are also fixed. If the supplied TMA amount exceeds the maximum capacity of the reactor and outlet pipeline, the remaining precursors could be potential for environmental emissions. As shown in Table 1 above, 3% of the loaded TMA at 1000 mTorr are potential for environmental emissions, while TMA loaded at the other two pressure conditions could be completely consumed in the ALD system.

As water is readily available and environmentally benign, a high dose of water is recommended in the ALD reaction, not only to enhance the growth rate of Al₂O₃ film but also to react with the excessive toxic TMA in the ALD system to prevent its emission into the air. A sufficiently long outlet pipeline could be used to fully consume the excessive TMA in such a case. In order to achieve a sufficient ALD surface reaction and to eliminate the TMA from potential emission, the following material supply guideline is recommended to use in loading the TMA precursor materials:

$$\sum M_{\text{wafer}} + \sum M_{\text{reactor}} < \sum M_{\text{input}} < \sum M_{\text{wafer}} + \sum M_{\text{reactor}} + \sum M_{\text{pipeline}} \quad (5)$$

For understanding the environmental performance of the ALD technology, the amounts of TMA and water wasted from the ALD process are shown in Figs. 3 and 4 below. The wasted amounts are calculated for depositing a single Al₂O₃ film on a 10.16 cm (4 in.) silicon wafer with a typical thickness between 20 Å and 200 Å.

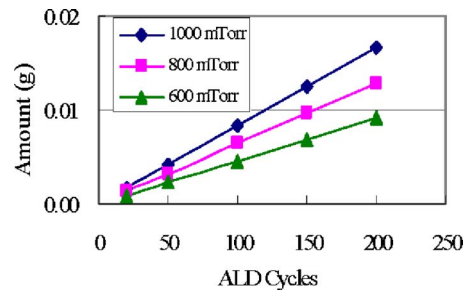


Fig. 3 Wasted TMA amount at three pressure levels

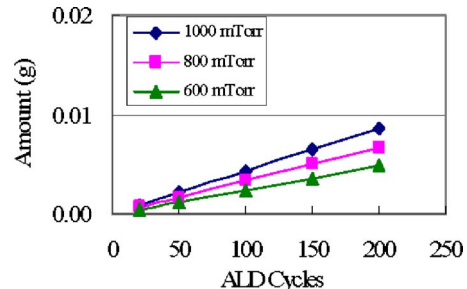


Fig. 4 Wasted H₂O amount at three pressure levels

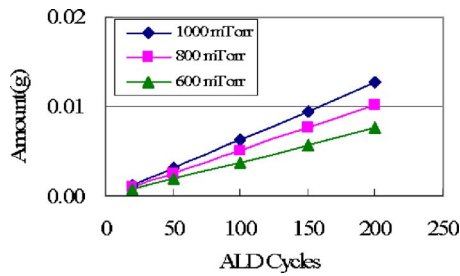


Fig. 5 CH₄ emissions at three pressure levels

Although the wasted amount seems negligible in each case, the total wasted amount from the whole semiconductor industry would be huge, approximately in the level of 10^9 kg per year for TMA and 10^{12} liters per year for deionized water, based on the 10^8 kg Al₂O₃ global annual demand [20,21]. Treatment of these wastes would be a huge burden for both the semiconductor industry and the environment. Increasing the material utilization efficiency through proper ALD system design and optimal precursor supply would be viable solutions to improve both the economic and environmental performance of ALD technology.

The principal emission from this ALD process is CH₄. For the amount of CH₄ being generated, one third is produced from the reaction between TMA and hydroxyls, and the other two thirds from the reaction between H₂O and the absorbed TMA. The amounts of CH₄ emission, based on the TMA input, are shown in Fig. 5 above for the ALD application between 20 cycles and 200 cycles. A rough estimate of the methane emission from global application of the ALD process for Al₂O₃ dielectric gate would be in the amount of 10^8 – 10^9 kg per year, based on the 10^8 kg Al₂O₃ global annual demand [20,21]. Nitrogen, as the carrier and purge gas, is heavily used in the ALD process. The amount of N₂ consumed in a typical ALD of a single Al₂O₃ film on a 10.16 cm (4 in.) silicon wafer is also shown in Fig. 6 below.

Besides the methane emissions, which induce global warming problems, the wasted precursors could form Al₂O₃ nanomaterial wastes both inside and outside of the ALD system. Currently we are lacking methods and techniques to evaluate the human health impact of these nanomaterial wastes but their effects could be very significant as such nanomaterial wastes can easily expose to human beings through various exposure pathways such as inhalation, ingestion, and dermal uptake. The amount of Al₂O₃ nanowastes formed from a single ALD process under the three process pressure conditions are shown in Fig. 7 below [27].

Global generation of nanowastes from the ALD process in the semiconductor industry for Al₂O₃ dielectric gate, as roughly estimated, will be in the level of 10^9 kg/yr [27]. Further research is needed on human health impact assessment and environmental management of these nanowastes, in order to address their sustainability issues in the future.

From the material flow analysis, the precursor waste and emission generations could be significant problems for wide application of the ALD process for Al₂O₃ dielectric gate in the global

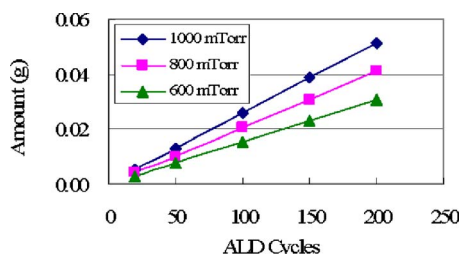


Fig. 6 Nitrogen consumption at three pressure levels

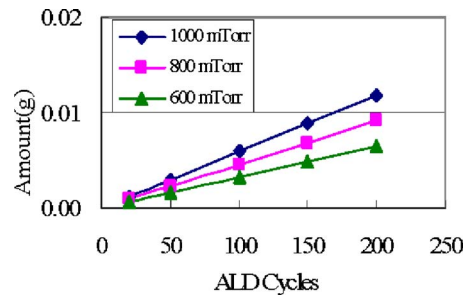


Fig. 7 Al₂O₃ nanowastes generated from the ALD process

semiconductor manufacturing industry. The material utilization efficiency of precursor materials needs to be increased to improve both the economic and environmental performances of the ALD technology. To address this issue, further investigations are needed on both the optimization of the ALD process and feasibility study of using stacked wafer arrangement in the ALD reactor to increase the surface area ratio between the silicon wafer and ALD reactor. Appropriate techniques for methane sequestration and nanowaste management are also needed to reduce the impact of the ALD process on the environment and public health.

3 Energy Flow Analysis

Besides material consumptions and waste generations, energy consumption of ALD process is also significant and needs to be systematically investigated to provide decision support in improving the sustainability of the ALD technology. During operation, the whole ALD system needs to be heated to maintain the vapor phase of each precursor reactant, and meanwhile, to supply the activation energy to the chemical reaction. The energy consumed by ALD not only contributes to its economic cost but also produces indirect emissions from the power generation and supply industry. In this section, we conduct a detailed energy flow analysis for the ALD of Al₂O₃ dielectric gate on a 10.16 cm (4 in.) silicon wafer. The energy consumptions are investigated for each process and component of the ALD system, with an aim to provide useful information for improving both the economic and environmental performances of the ALD technology.

ALD process temperature is a critical parameter in evaluating the energy consumption of the ALD system. In ALD operations, sufficient energy must be supplied into the ALD system to overcome the energetic barrier of the surface chemistry and maintain the reaction conditions. Through the density functional theory (DFT), the activation energies for trimethylaluminum and water were estimated to be 0.52 eV and 0.70 eV, respectively [1]. Current ALD of Al₂O₃ films has been studied at temperatures ranging from 33°C to 500°C [23,28–30]. It has been found lower process temperature would result in lower growth rate due to incomplete surface reactions, while an extended purging time must be used at lower temperatures to produce the same quality of Al₂O₃ films [30]. While high temperature can facilitate the surface reactions, too high a temperature can cause the evaporation of hydroxyls and reduce the number of active sites on the surface, which would lead to a low growth rate eventually. Experimental studies have confirmed that the Al₂O₃ film thickness increment per cycle decreases with decreasing temperature at temperatures below 77°C and decreases with increasing temperature above 227°C [17]. Besides the evaporation issue, TMA is also decomposing at a temperature above 300°C, which could lead to an uncontrolled growth of the Al₂O₃ film [31]. From the experiment, the highest growth rate of the Al₂O₃ films was found around 200°C [23]. In our experiment, the process temperature is set at 200°C to ensure a high deposition efficiency of Al₂O₃ films. The inlet pipelines are heated to 70°C, while the outlet pipelines are heated to 160°C to facilitate the pulsing and purging of the precursor materials.

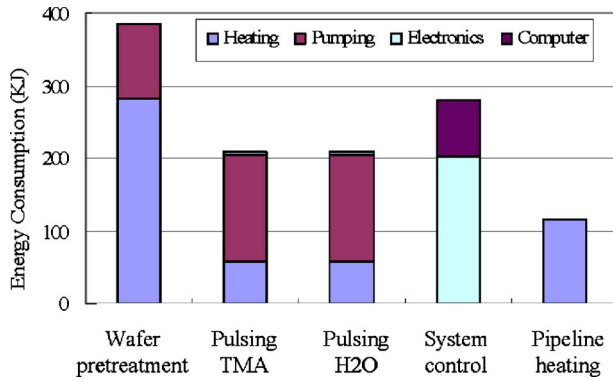


Fig. 8 ALD process energy consumption

For the energy analysis, here we take an equipment centric approach to obtain the energy consumption of each ALD component for heating, pumping, actuating, monitoring, etc. The total energy consumption of the ALD system is calculated as the sum of the energy consumed by each component

$$Q = \sum_{i=1}^n P_i \times t_i \quad (6)$$

where P_i is the power demand of device i and t_i is the operating time of device i .

From Eq. (6), the energy consumption of the ALD system depends on both the system component and the operating time, while the ALD operating time is dictated by the ALD cycle time, which includes the ALD operations in the following four stages: TMA pulsing, TMA purging, H₂O pulsing, and H₂O purging. In the current practice, most of the Al₂O₃ films were deposited by using a 12 s cycle time, with 1 s each on TMA and H₂O pulsing, and 5 s each on TMA and H₂O purging [28,30,32]. Reducing the cycle time can effectively improve not only the deposition efficiency but also the energy consumption of the ALD. Experimental studies have demonstrated that TMA pulse would saturate when the pulse time is longer than 65 ms and H₂O pulse would saturate after 200 ms [5]. Between the two precursor pulsings, a purging must be sufficiently conducted to remove excessive materials from the reactor. Otherwise, a CVD type of component might be produced in the surface reactions. Experimental investigations have confirmed that a short cycle time of 4 s can be used for successful deposition of Al₂O₃ dielectric films, with 0.5 s each on TMA and H₂O pulsing, and 1.5 s each on TMA and H₂O purging [18]. A 4 s cycle time would get the ALD process a throughput around 13–14 wafers per hour for typical 50 Å film applications [5]. As this cycle time could meet the throughput requirement of

the semiconductor industry, we set the cycle time at 4 s in our analysis. In the semiconductor industry, most ALD film applications are in a range between 20 Å and 200 Å [5]. At an average of 0.1 nm layer growth per cycle, we investigate the material and energy flows of the ALD process between 20 cycles and 200 cycles.

For the energy analysis, the power demand of each ALD component is measured by a power meter. In this analysis, the ALD operations are divided into five categories: wafer and reactor pre-treatment, pulsing/purging Al(CH₃)₃, pulsing/purging H₂O, pipeline heating, and system control. For the deposition of a 20 nm Al₂O₃ film on a 10.16 cm (4 in.) silicon wafer, the ALD processes consume a total of 1.2 MJ energy, with 62% consumed by process operations, 15% consumed by pipeline heating, and 23% used for system control and data acquisition. A detailed energy flow of the ALD process is demonstrated in Fig. 8 above.

The energy flow analysis demonstrates that heating of the outlet pipeline consumes about twice the energy as the inlet pipeline, while the energy consumed in pulsing TMA and H₂O are at the same level. Wafer pretreatment, due to the length of time for system heating and wafer hydroxylation, is the largest process energy consumer among these four ALD operating activities. The detailed energy consumption of each ALD subprocess for depositing a 20 nm Al₂O₃ film on the 10.16 cm (4 in.) silicon wafer are shown in Fig. 9 below.

As indicated, the energy consumed in the ALD process is mainly for system heating, process pumping, and experimental control. Regarding the 1.2 MJ energy consumed, heating of ALD system for wafer pretreatment, pulsing TMA/H₂O, and pipeline heating totally consumes 513 kJ, which takes a share of 42.7% of the total energy consumption; pumping during wafer pretreatment and pulsing TMA/H₂O totally used 394 kJ energy, which is 32.8% of total energy consumption; the electronics including the computer used for the system control and data collection consume 293 kJ, which accounts for 24.5% of total energy. At a 4 s cycle time, this ALD module has a throughput of 4 wafers per hour for 20 nm film applications (considering 60 s of overhead time for wafer loading, system adjustment, etc.). During the single wafer deposition, a total of 0.49 MJ is consumed in the ALD system preparation, 0.03 MJ energy is consumed in the wafer pretreatment, and about 0.68 MJ is consumed in the ALD cycling. Considering batch production using such single wafer deposition process, the averaged energy consumption is approximately 0.75 MJ/wafer by considering the processing capacity of such an ALD module during a typical 8 h period.

For assessing the energy consumption of the ALD process, the process temperature and cycle time are two critical parameters as they combined dictate the process energy consumption of a specific ALD system. In the ALD operations, the process temperature and cycle time are found to be inversely correlated due to the need

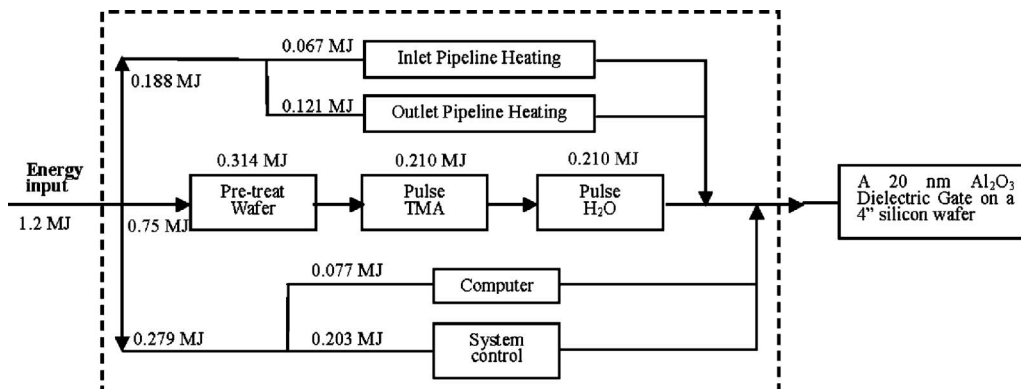


Fig. 9 Energy Flow diagram of 200 cycle ALD processes at 200 °C

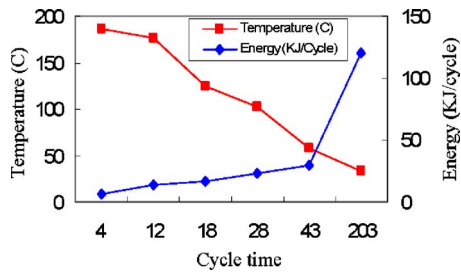


Fig. 10 ALD energy dependence on the process parameters

of the ALD process for avoiding nucleation of molecules in the binary reactions [30], as shown in Fig. 10 below.

The ALD process energy consumption, as an upstream environmental impact metric widely adopted in sustainable manufacturing analysis, is found mainly determined by the cycle time of the ALD operations rather than the process temperature. The process energy consumption, in terms of energy consumed per ALD cycle, is also shown in Fig. 10 below for the ALD operations at various cycle times at 200°C process temperature condition.

The common cycle times in the ALD of Al₂O₃ high-κ dielectric gate in semiconductor transistor manufacturing are set at 18 s, 12 s, and 4 s [5,18,28]. Here we have analyzed the total energy consumption of the ALD process for 200 cycles at 200°C at these three cycle times. The results are shown in Fig. 11 below. The results demonstrate that the process energy consumption in a total could be reduced by 18.2% when the ALD cycle time is reduced from 18 s to 12 s, and the process energy could be further reduced by 55.6% when the ALD cycle time is reduced from 12 s to 4 s.

4 Concluding Remarks

Atomic layer deposition is a promising nanotechnology for manufacturing Al₂O₃ dielectric films on microelectronics devices in the semiconductor industry. The material and energy consumptions of the ALD are closely related to its economic and environmental performances, and need to be quantitatively investigated to support its process improvement for a sustainable manufacturing. In this paper, we present an integrated sustainability analysis of the ALD process for depositing Al₂O₃ high-κ dielectric gate based on state-of-the-art laboratory processes, aiming to improve the sustainability performance of the ALD technology at this early development stage. The investigations are made by applying material and energy flow analyses of the ALD process, for deposition of a single Al₂O₃ dielectric film up to 20 nm thickness on a 10.16 cm (4 in.) silicon wafer through trimethylaluminum and water binary reactions.

Material flow analysis is conducted on the ALD process at three precursor supply patterns. Material utilization efficiencies of both precursor materials are obtained for each supply pattern, and material flows of the precursors in the whole ALD system are quantitatively investigated. As assessed, the material utilization efficiencies of both precursors are below 20% in these ALD operations. The utilization of precursors in the current ALD sys-

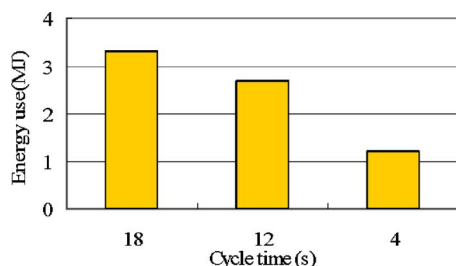


Fig. 11 ALD energy consumption at 200°C for 200 cycles

tem is mainly limited by the small surface area ratio between the silicon wafer and the ALD reactor. In the ALD process, methane is the principal emission. The generation mechanism of methane in the ALD process is identified, and the emission from a single Al₂O₃ film deposition process is quantitatively presented.

From the material flow analysis, the precursor waste could be a significant problem for wide application of the ALD process in global semiconductor manufacturing industry if following the current practice. Increasing the material utilization efficiency of precursor materials could be realized through establishing an optimal precursor supply pattern or through increasing the surface area ratio between the silicon wafer surface and the ALD reactor inner surface. To address this issue, further investigations are needed on both process optimization of the ALD process and a feasibility study of using a stacked wafer arrangement in the ALD reactor.

Energy consumption of the ALD process is assessed by using an equipment centric approach. Energy flows in this ALD system are quantitatively studied. The total energy consumed in the ALD of a 20 nm Al₂O₃ film is approximately 1.2 MJ, with 42.7% used for system heating, 32.8% used for pumping, and 24.5% used by electronics for process monitoring and system control. The ALD process energy consumption, as identified, is mainly determined by the cycle time of the ALD operation, instead of the process temperature. The analytical results demonstrate that the process energy consumption could be significantly reduced by 64% when the cycle time is reduced from 18 s to 4 s. When considering the processing capacity of the ALD module in batch production, the energy consumption of the ALD is approximately in the level of 0.7 MJ/wafer for 20 nm film applications.

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