The unique properties of atomic layer deposition (ALD) films have captured considerable interest from IC manufacturers facing challenging manufacturing needs. ALD films grow uniquely continuous on any substrate topology with complete conformality and excellent uniformity. The layer-by-layer growth mechanism allows for atomic-level control of film thickness and properties, and the pinhole-free films exhibit low-stress.

Saddled, however, with tradeoffs between throughput and maintainability, ALD’s relatively slow deposition rate and short maintenance cycles have so-far constituted a high cost-of-ownership obstacle to full-scale commercialization of the technology. High productivity ALD requires separate optimization of throughput and material utilization. Improving efficiency of both chemical delivery and chemical utilization without sacrificing throughput is the enabling solution.

**ALD process tradeoff**

ALD is a cyclic process carried out by dividing a conventional chemical vapor deposition (CVD) process into an iterated sequence of self-terminating process steps. An ALD cycle contains several (at least two) dose steps in which reactive chemicals are separately delivered into the process chamber. Each dose step is typically followed by an inert gas purge step that eliminates the reactive chemicals from the process space prior to introducing the next precursor.

Standard implementation of ALD is practiced with constant pressure and gas flow throughout the entire process. These process parameters dictate throughput and performance by determining the characteristic gas residence time, \( \tau \), within the flow system: 
\[
\tau = \frac{VP}{Q},
\]
where \( V \) is the process chamber volume; \( P \) and \( Q \) represent the pressure and the flow rate of the gas, respectively.

In the typical constant gas flow practice, the flow rate is determined as a compromise between the need to flush the chemicals out of the process chamber efficiently during the purge step and the desire to obtain sufficient material utilization during the dose step. Typical flow is set within the range of 100-500sccm. Most chemical sources, especially those for low-volatility precursors, cannot support this high level of flow. Chemicals are therefore seeded into a flow of carrier gas with concentrations that commonly fall below 1% for low-volatility precursors. The resulting gas residence time (for 200-300mm wafer-size chambers) falls within the mid-range of 10-40msec. As the chemical utilization at a given exposure (dose) scales approximately with the gas residence time, the standard chemical utilization is quite low – dropping to several percent, at best.
Figure 1. Residence time modulation achieves shorter purge time and higher material utilization as compared to ALD with fixed residence time.

The first impact of a diluted chemical dose is a compromised throughput because of an extended dose time. Because the dose time required to complete the reaction to saturation is inversely proportional to both chemical utilization and the chemical partial pressure (dose time \( \propto \) exposure / partial pressure \( \times \) utilization), the dose step is performed at intervals substantially longer than the gas residence time.

Additionally, the large quantity of unused reactive chemicals constitutes a severe maintenance load on the deposition system. While an optimized ALD process suppresses intermixing of the precursor chemicals in the process space above and around the wafer, CVD growth inevitably occurs downstream from the process space. The growth of inferior CVD films scales with the maintenance load of unused chemicals and establishes proportionally shorter maintenance cycles.

While the 10-40msec residence time range is too short to constitute sufficient material utilization during dosing, it also compromises the purge step as the purge efficiency declines exponentially with residence time.

Ideally, optimized ALD performance needs to avoid the tradeoff between dose and purge. The dose step should be optimized with a long residence time to increase material utilization, which can be achieved with low flow and high chemical pressure. Conversely, the purge step should be optimized with a short residence time in order to improve the purge efficiency. High flow and low chemical pressure should therefore be maintained at the purge step.

**De-coupling dose and purge**

Fast modulation of residence time between the dose and purge steps can be accomplished with a new gas routing architecture that uses off-the-shelf components.
During the dose time, the chemical flow is reduced while the pressure is maintained at standard ALD levels (hundreds of milliTorrs). The flow restriction is obtained by synchronizing the chemical flow into the process chamber with a high flow of inert gas into the downstream area below the process space. If the pressure gradient between the process space (above and around the wafer) and the downstream space (below the wafer) is kept to a minimum, the gas draw out of the process space can be choked down substantially to a flow as low as 10sccm or less. On the other hand, the flow during the purge step is allowed to increase to a high level, while the inert gas flow into the downstream space is concurrently turned off to eliminate the draw restriction.

Using this technique, the gas residence time can be modulated by ~3 orders of magnitude (Fig.1). Purge times on the order of 1sec and chemical utilization of a few percent are obtained with typical ALD processes. In contrast, a purge time as short as 100msec and a chemical utilization >30% were achieved by decoupling dose and purge process conditions.

**High productivity ALD**

Introducing fast modulation of the gas residence time results in the separate optimization of throughput and maintainability – both key for achieving high productivity. Cycle time as low as 450msec was achieved with an ALD film of Al$_2$O$_3$ from commonly used trimethylaluminum (TMA) and water precursors. The process parameters used were the following: TMA dose=50msec, TMA purge=100msec, water dose=150msec, and water purge=150msec. This ALD cycle time is equivalent to a deposition rate >11nm/min, which is compatible with standard throughput requirements for production.

Since the flow during the dose step is allowed to go down to a few sccms, there is no longer a need to seed the chemicals into a carrier gas. This means that the chemical dose is delivered at 100% concentration. Furthermore, a dose increase does not necessitate an increased dose time. Al$_2$O$_3$ ALD was used on patterned wafers, achieving 100% conformality with the same cycle time of 450msec, despite a 20× dose increase.

The ability to dose at a low flow and 100% chemical concentration is crucial for ALD applications requiring low-volatility precursors, such as high-$k$ hafnium-based oxides, diffusion barriers and copper
films. Dose time independence of chemical delivery conditions was verified down to a source pressure of 0.5Torr, which implies feasibility of a sub-100msec dose time with low-volatility precursors. Current ALD deposition rates for such film processes are extremely slow.

By dosing at full chemical concentration and high material utilization, maintainability is substantially improved. Films as thick as 0.5μm have been deposited so far without process or equipment fatigue. Maintainability exceeding 45,000 wafers with 50Å films has also been demonstrated (Fig. 2).

High productivity ALD can be achieved by breaking away from the deadlocking tradeoff between dose and purge, as well as throughput and material utilization. The solution is to allow the gas residence time to modulate between the dose and purge steps. High-throughput and maintainability exceeding CVD and other established deposition techniques show that ALD can be production-compatible and cost-effective.

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