Precursor and Co-Reactant Selection: A Figure of Merit

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Developing novel precursors for atomic layer deposition (ALD) processes is a complicated task: the selected chemical compounds must be volatile and thermally stable, yet reactive with a surface, and perhaps even demonstrate selective reactivity among several different surfaces. Additionally, it is helpful if the precursors are liquid (for handling and to improve the kinetics of evaporation) and robust to a change in the chemical environment.

To initially study a compound for potential use as a precursor, one must understand both the volatility and thermal stability. We have recently established a Figure of Merit (FoM) for potential precursor compounds based on volatility and decomposition. Conceptually, this FoM alters the ratio in temperature between a judiciously chosen onset of decomposition and onset of thermolysis and modifies that with respect to the residual mass left behind in a standard thermogravimetric ramp experiment. In this way, the larger the value for the FoM, the better the precursor, with negative values representing compounds that decompose before acceptable volatility is achieved.

$$\sigma = \left(\frac{T_d}{T_v} - 1\right)\left(1 - \frac{\%m_r}{M_c \Big/ M_p \times 100\%}\right)$$

where T_d = temperature of the onset of decomposition, K
T_v = temperature of the onset of volatility, K
$\%m_r$ = the residual mass in thermogravimetry
M_c = the molar mass of the metal in the precursor, D_a
M_p = the molar mass of the precursor, D_a

Figure 1. A proposed Figure of Merit for ALD precursor compounds.

Selection of the onset of volatility and decomposition, as well as the construction of this Figure of Merit will be examined with respect to potential precursors for transition metals (Ni, Co, W, Mo, Au, Ag, Cu) as well as main group metals (Al, Ga, In, Sn, Pb) that are presently being developed in our group.