

References

1. Lemaire, P. C.; Parsons, G. N. B Thermal Selective Vapor Etching of TiO₂: Chemical Vapor Etching via WF₆ and Self-Limiting Atomic Layer Etching Using WF₆ and BCl₃. *Chem. Mater.* **2017**, *29* (16), 6653–6665.
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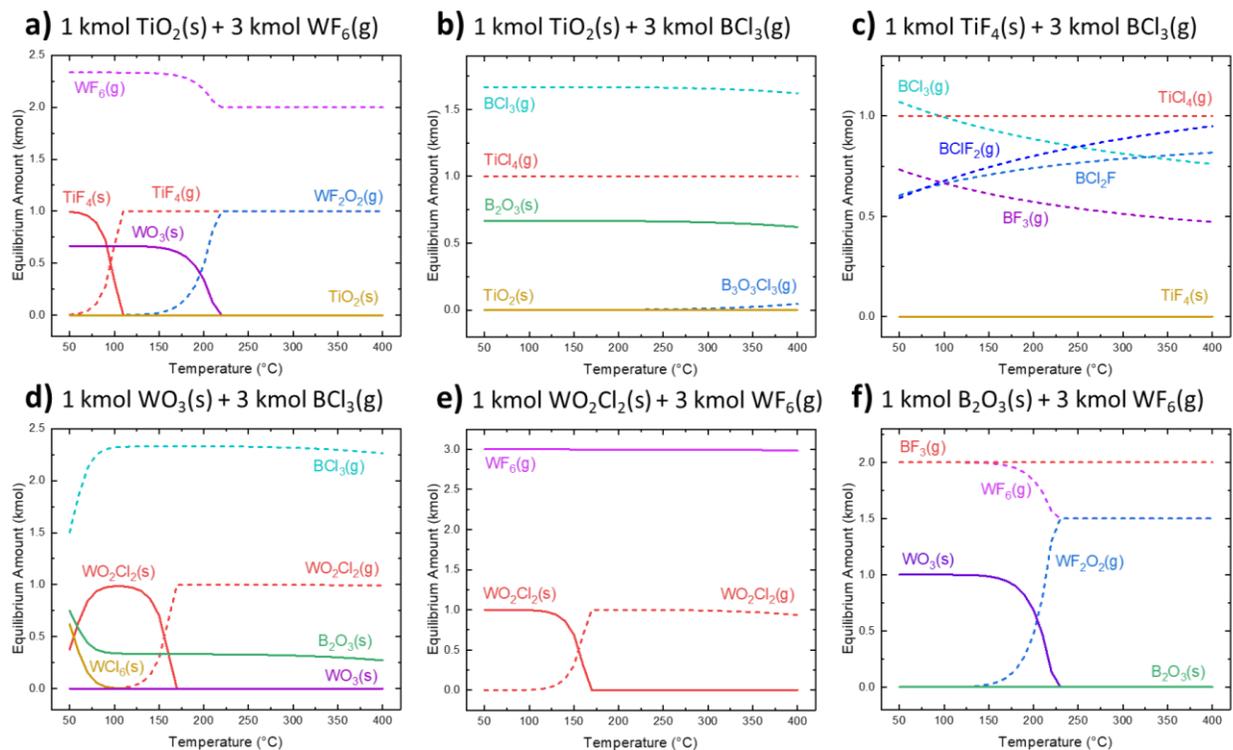


Figure 1. Thermodynamic analysis results from HSC Chemistry depicting the expected equilibrium species concentrations in a closed system during ALE precursor dosing from 50°C to 400°C at 750 mTorr. (a) Exposure of TiO₂ to excess WF₆ in Ar. (b) Exposure of TiO₂ to excess BCl₃ in Ar. (c) Exposure of TiF₄ to excess BCl₃ in Ar. (d) Exposure of WO₃ to excess BCl₃ in Ar. (e) Exposure of WO₂Cl₂ to excess WF₆ in Ar. (f) Exposure of B₂O₃ to excess WF₆ in Ar. Solid lines represent solid products and dashed lines represent volatile products.

Material	Precursor 1	Precursor 2	No Etching	ALE	CVE
TiO ₂	WF ₆	BCl ₃	50°C – 155°C	155°C – 195°C	195°C – 400°C
TiN	WF ₆	BCl ₃	50°C – 400°C	–	–
TiO ₂	MoF ₆	BCl ₃	–	50 – 95°C	95°C – 400°C
TiN	MoF ₆	BCl ₃	50°C – 180°C	180°C – 400°C	–

Table 1. Temperature ranges from HSC Chemistry thermodynamic analysis where no etching, ALE, and CVE is predicted to occur for the following material and precursor systems: TiO₂ with WF₆/BCl₃, TiN with WF₆/BCl₃, TiO₂ with MoF₆/BCl₃, and TiN with MoF₆/BCl₃.