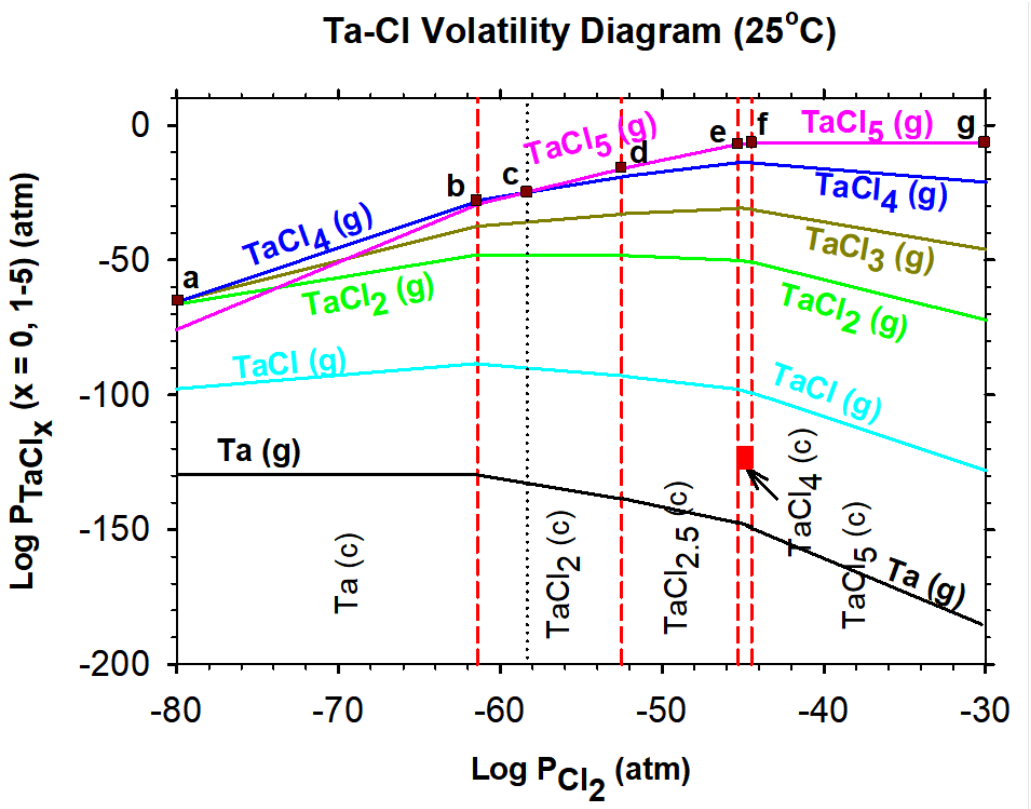

Figure 1. Volatility diagrams of the Ta-Cl system at 25°C (above) and other temperatures (-25 to 100°C) provide the equilibrium partial pressures of various Ta-Cl gaseous species over stable Ta-Cl compounds that may form when a Ta substrate is exposed to different Cl_2 partial pressures at various temperatures. A suitable temperature and Cl_2 partial pressure for the formation of the desired Ta-Cl compound (passivation product) can then be selected so that its vapor pressure is very low ($<10^{-10}$ atm) in order to have a negligible etch rate during Step 1 (passivation step) of a typical ALE process.

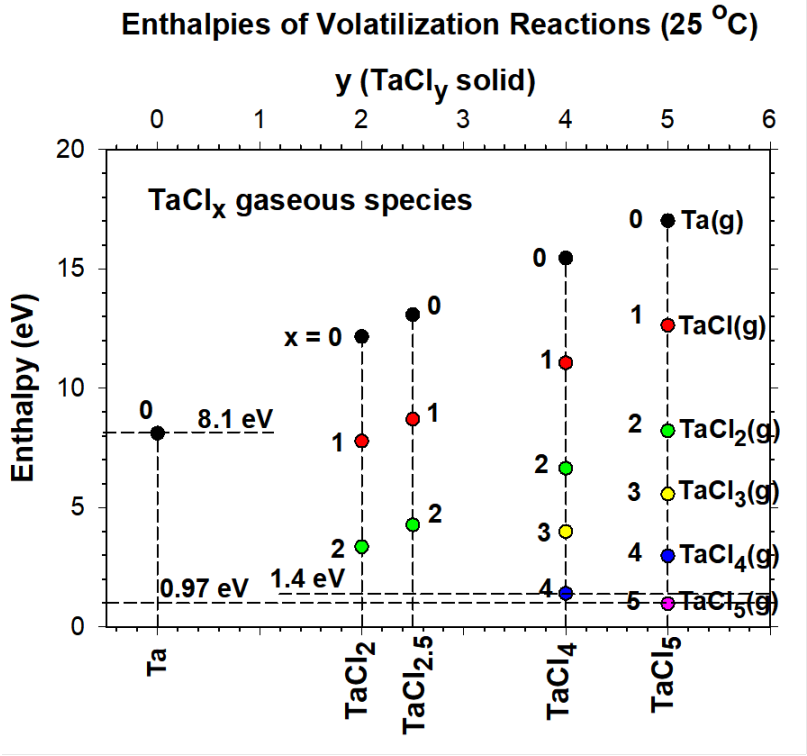

Figure 2. Enthalpies for various $TaCl_y$ (solid)/$TaCl_x$ (gas) volatilization or sputtering reactions that are approximately equal to the surface binding energies of the solid compounds, which are relevant during Step 2 (ion sputtering step) of a directional ALE process, can be computed thermodynamically. It is seen that the $TaCl_5$ compound is the best choice for the passivation product in Step 1 of ALE since the enthalpy difference between the Ta/Ta(g) and $TaCl_5$/$TaCl_5$(g) reactions is the largest (≈ +7 eV).