Reaction mechanism of atomic layer deposition of zinc oxide and zinc sulfide using bifunctional organic reactants

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Atomic layer deposition (ALD) can grow thin films with atomic-level thickness control. Together with the diethylzinc (DEZ) precursor, often used reactants for ZnO ALD is H_2O and O_3, and that for ZnS ALD is H_2S. However, H_2O or O_3 may damage subtle substrates; H_2S is highly toxic. Recently, new ALD processes for ZnO and ZnS using 1,5-pentanediol (PD) and 1,5-pentaneditiol (PDT) were reported [1,2], so that the organic moieties of the reactants are removed during deposition. However, using 1,2-ethanediol (ED, ethyleneglycol) or 1,2-ethanedithiol (EDT), the organic moiety remained in the films [3,4]. In this study, the reactions for ZnO and ZnS ALD using PD, PDT, ED, and EDT are reported using density functional theory (DFT) simulations. The OH and SH active sites on surface can be generated by intramolecular beta-H transfer, removing the organic parts from the films; in contrary, such mechanism is unavailable for ED or EDT. Consequently, PD and PDT can be utilized as alternative reactant for ZnO and ZnS ALD.

References

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