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Supplemental Information for: Chemical and Electronic Structures of Cobalt Oxynitride Films Deposited by NH₃ vs. N₂ Plasma: Theory vs. Experiment

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Fig. S1 Schematic of Chamber 1: UHV chamber for magnetron sputtering and XPS analysis



Fig. S2 Schematic of Chamber 2: UHV chamber for magnetron sputtering and AES analysis

TABLE S1	CoO _{1-x} N _x	Films	prepared
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Film preparation method	Chamber	Composition ¹	Estimated Film thickness (Å)	XRD results	Film No.
Ar:N ₂ sputter dep on Si(100)	Chamber 2	$\begin{array}{c} CoO_{0.4}N_{0.6} \\ (CoO_{0.2}N_{0.8}) \end{array}$	600	Preferred 220 orientation on Si(100)	1
NH ₃ sputter dep on Si(100)	Chamber 1	CoO _{0.2} N _{0.8} (~CoO _{0.1} N0.9)	150	Only Si diffraction peaks observed	2
Ar:N ₂ sputter dep on MgO(100)	Chamber 2	NA	600	Only MgO diffraction peaks observed	3
NH ₃ nitridation of Co/Si(100)	Chamber 1	$\begin{array}{c} CoO_{0.2}N_{0.8} \\ (CoO_{0.1}N_{0.9}) \end{array}$	200	Preferred (220) orientation (Weak diffraction peaks possibly due to thinner film)	4
N ₂ sputter dep on Si(100)	Chamber 1	$\begin{array}{c} CoO_{0.4}N_{0.6} \\ (CoO_{0.2}N_{0.8}) \end{array}$	300	Only Si diffraction peaks observed	5

¹Compositions in parenthesis indicate corrections for surface oxide/hydroxide layers due to either takeoff angle resolved measurements or Ar ion sputtering to remove such layers.



Figure S3. AFM data of cobalt oxynitride film formed by NH₃ plasma nitridation of the metallic film. The rms roughness is 1.9 nm.



Figure S4. Detailed comparison of valence band spectra of Co metal (blue trace) and a cobalt oxynitride film formed by NH₃ plasma nitridation of the metallic film. (The spectra are the same as in Figs. 3a and 3b.)