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First-principles Study of the Structural and Magnetic Properties of Cobalt Indium Nitride PAVEL LUKASHEV, WALTER R. L. LAMBRECHT, Department of Physics, Case Western Reserve University, Cleveland, OH 44106-7079 — In previous work we have shown that at atmospheric pressure CoN has the zincblende (ZB) equilibrium crystal structure, in agreement with experimental results of Suzuki et al. [1] The ZB lattice structure would allow for a nice match to semiconductors such as GaN and SiC if the lattice constant of CoN can be slightly increased by doping with suitable atoms with larger atomic radii. In this work we study structural and magnetic properties of $Co_{1-x}In_xN$ alloys. The theoretical framework of our calculations is the density functional method in the local spin density approximation (LSDA). Our calculations are carried out using the full-potential linear muffin-tin orbital band-structure method (FP-LMTO). We find that the lattice constant follows Vegard's law. Furtermore this expansion of the lattice constant leads to more localized behavior for the Co d states and hence the formation of magnetic moments. The magnetic moments and spin-polarization of the density of states at the Fermi level are studied as function of concentration and lattice constant. Finally, a comparison is made with corresponding $Fe_{1-x}In_xN$ alloys.

1. Suzuki K, Kaneko T, Yoshida H, Morita H, Fujimori H J. Alloys Compd. **224**, 232 (1995)

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