Properties of transition metal pairs at the surface of GaN and GaN:Si,Mg

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The application of powerful nanocharacterization methods has allowed visualizing the nanoscale aggregation of transition metal (TM) cations in various semiconductors, either intrinsic or co-doped by shallow impurities [1]. This opens up new possibilities for nanomagnetism and nanospintronics provided that the formation of buried ferro- and/or antiferromagnetic (FM and AFM, respectively) nanocrystals can be controlled at the nanometer scale, possibly by n- and/or p-type co-doping.

We present results from density functional theory calculations (employing the GGA and GGA+*U* approaches) for wz-GaN doped with either Cr, Mn or Fe, also considering co-doping with either Si or Mg. Our results confirm that transition metal (TM) cations have a strong tendency to aggregate in GaN, *i.e.*, to form TM-rich nanocrystals [2]. For instance, the GGA+*U* pairing energies for Cr, Mn, and Fe in wz-GaN are −750, −670, and −160 meV, respectively (similar values have been also obtained for zb-GaN) [3]. We find, however, that at the (0001) wz-GaN gallium surface only Fe ions tend to aggregate while Cr and Mn ions repel each other [3], which suggests that Fe-rich aggregates can form during the epitaxial growth process. The magnetic interaction between magnetic ions has also different character in the bulk than at the surface: the Mn pair is coupled ferromagnetically in the bulk but antiferromagnetically at the Ga surface. To complete this picture, we demonstrate how co-doping with Si and Mg affects the formation of TM pairs and influences the magnetic coupling between TM ions, again finding significant differences between the case of aggregation in the bulk and at the surface [4].

References:

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