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Gd in GaN: the role of magnetic vacancy clusters[1]

ALEXANDER THIESS, PETER H. DEDERICHS, STEFAN BLÜGEL, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany, WALTER R.L. LAMBRECHT, Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106-7079, USA — Five years after the experimental discovery of colossal magnetic moments and ferromagnetic ordering above room temperature in gadolinium doped gallium nitride the identification of its microscopic origin is still not accomplished. Here, we are proposing a new model explaining the origin: the clustering of magnetic gallium vacancies. First, we show that such clustered gallium vacancies indeed can preferentially occur by utilizing a simplified growth model, for which we provide the input by large-scale first-principles Green function calculations. The same calculations reveal that the dangling bond nitrogen states around gallium vacancies become significantly spin-polarized. Moreover, we are able to extract a rich set of information on the magnetic exchange interactions between those spin-polarized atoms. These exchange interactions are the basis for our study on the thermal behavior of magnetic vacancy clusters by means of Monte-Carlo simulations. We present the resulting magnetic properties of our simulations and highlight important similarities to the experiment that all point at gallium vacancy clusters as the origin of the experimentally observed magnetic properties in GaN:Gd.

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