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Cation dopant distributions in Mn-doped ZnO nanostructures and thin films: experiment and Monte Carlo simulations T.C. DROUBAY, Pacific Northwest National Lab, D.J. KEAVNEY, S.M. HEALD, Argonne National Lab, T.C. KASPAR, B.P. KASPAR, C.M. WANG, Pacific Northwest National Lab, C.A. JOHNSON, K.M. WHITAKER, D.R. GAMELIN, Chemistry, Univ. of Washington, S.A. CHAMBERS, Pacific Northwest National Lab — Anion or cation doping at relatively high concentrations of several atomic percent is frequently suggested to realize synthetic materials with qualitatively new functionality. While the statistical probability of obtaining singles, dimers, and trimers has been determined for bulk lattices, these distributions are significantly altered in nanostructures and thin films due to the presence of under-coordinated surface sites. The dopant distributions in nanostructures and thin films of doped wurtzite ZnO have been determined from Monte Carlo simulations. Using empirical expressions derived from the MC simulations that accurately predict dopant bonding configurations as a function of surface-to-volume ratio and concentration, experimental results for epitaxial films of Mn-doped ZnO will be discussed. X-ray absorption and x-ray magnetic circular dichroism revealed that Mn(II) substituted for Zn in the Mn:ZnO films, which were deposited by PLD using targets created from Mn:ZnO nanoparticles. However, while substitutional, the Mn distribution is not stochastic but rather tends to segregate, yielding higher local concentrations than anticipated.

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