Magnetic moments of Mn in amorphous Si and Ge: theory and experiment

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Abstract Body: Transition metal (TM) doponts are well known to have distinct local magnetic moment in semiconductor matrices due to their partially filled d shells. However, the existence of a local moment of a TM in group IV semiconductor matrices is more complicated than usually speculated. We have observed a striking difference between Mn moment when introduced into Si compared to Ge. Mn moments are large (>3 muB) in amorphous Ge and are totally quenched in amorphous Si. We have studied the magnetic, structural, X-ray absorption spectroscopy (XAS) and transport properties for a wide range of Mn doping concentrations (0.005~0.20) in each matrix. Conductivity data show that the Mn is an effective dopant. HIgh resolution transmission electron microscopy shows a homogeneous amorphous alloy. XAS and atomic density differences are seen which are consistent with the magnetization results. We demonstrate through experimental studies and density function theory calculations that the local d moment for Mn is very sensitive to the bonding distance and coordination numbers, indicating the important role of the local environment at the Mn sites.

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