Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Atomic structure of the interface between Fe and AlGaAs and its impact on spin transport THOMAS ZEGA, AUBREY HANBICKI, STEVEN ERWIN, IGOR ZUTIC[1], GEORGE KIOSEOGLOU, CONNIE LI, BEREND JONKER, RHONDA STROUD, Materials Science and Technology Division, Naval Research Laboratory, Washington, D.C. 20375 — We combined density-functional theory (DFT) with experimental- and simulated- transmission-electron-microscope (TEM) imaging to determine the atomic structure of the interface between Fe and AlGaAs in light-emitting diodes (LEDs) used to investigate the transport of spin-polarized electrons. We show that a 44% increase in the spin-injection efficiency occurs after a low-temperature anneal, which produces an interface consisting of a single atomic plane of alternating Fe and As atoms. Our results provide the structural information required to develop accurate models of charge transport and spin injection at complex interfaces between dissimilar materials.

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Date submitted: 03 Dec 2005 Electronic form version 1.4