Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Hartree-Fock Cluster Investigation of Locations for Erbium in Silicon[1] JUNHO JEONG, R.H. SCHEICHER[2], N. SAHOO, M.B. HUANG, T.P. DAS[3], Dept. of Physics, SUNY at Albany, NY, LEE CHOW, Dept. of Physics, Univ. of Central Florida, Orlando, S. BYAHUT, D.R. MISHRA, M.M. ARYAL, N.B. MAHARJAN, D.D. PAUDYAL, Central Dept. of Physics, Tribhuvan University, Kathmandu, Nepal — Using the Hartree-Fock Cluster Procedure, we have investigated three locations hexagonal and tetrahedral interstitial (H_i and T_i) and substitutional (S) for Er^{3+} in Silicon including relaxation effects of the Si neighbors of Er^{3+}. Our results for the binding energies show that S is the most stable site for Er^{3+}, in contrast with the results from the most recent channeling measurements,[4] which can best be explained assuming that Er^{3+} is at T_i site. Possible reasons for the difference will be suggested. Magnetic hyperfine fields obtained for the Er nucleus at various sites will be discussed.

[1]Supported by NSF US-Nepal Program, UGC Nepal and Senior Fulbright Post-Doctoral Fellowship (S.B.)
[2]Current Address: Dept. of Physics, Uppsala University, Sweden
[3]Also: Dept. of Physics, University of Central Florida, Orlando, Florida
[4]M. B. Huang et al., Appl. Phys. Lett. 81, 2734 (2002)

Ralph Scheicher
Uppsala University

Date submitted: 22 Dec 2004 Electronic form version 1.4