Abstract Submitted
for the TSF05 Meeting of
The American Physical Society

Surface States and Annihilation Characteristics of Positrons Trapped at Reconstructed Surfaces of Silicon[1] NAIL G. FAZLEEV, Physics Department, University of Texas at Arlington — Slow positron beam spectroscopies are currently being developed into sensitive tools for the characterization of surface and near surface phenomena in semiconductors and nanomaterials. Theoretical studies of positrons at surfaces are of intrinsic interest as they represent a system consisting of distinguishable quantum particles in a quasi 2-dimensional potential. Such studies are also necessary to derive the full power of the new surface positron spectroscopies. In this talk, I will report on recent developments in the theory of positron surface interactions and their application to positron surface states and annihilation characteristics of surface trapped positrons at the semiconductor surfaces. Calculations of positron states and annihilation characteristics are performed for the non-reconstructed and reconstructed Si(100)-(2x1), Si(100)-p(2x2), and Si(111)-(7x7) surfaces. The orientation-dependent variations of the atomic density and electron density are found to affect the localization of the positron surface state wave function at reconstructed surfaces. Estimates of the positron binding energy and the positron annihilation characteristics reveal their sensitivity to the specific atomic structure of the topmost layers of semiconductors.

[1]This work was supported in part by the National Science Foundation, the Robert A. Welch Foundation, and the UTA Research Enhancement Program.

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Date submitted: 15 Sep 2005 Electronic form version 1.4