Abstract Submitted
for the APR11 Meeting of
The American Physical Society

First Principles Study of Optical Losses in Transition Metals and Alloys
A.V. GAVRILENKO, C. GONDER, D. BAKER, C.S. MCKINNEY, V.I. GAVRILENKO, Norfolk State University — Detailed understanding of the physics of optical losses in transition metals is a hot area of modern fundamental science with variety of applications in nano-physics, nano-photonics and nano-plasmonics. The first principles density functional theory is applied to study effects of molecular adsorption on silver (111) oriented nano-films and the alloying effects of Ag$_{1-x}$Cd$_x$, and Ag$_{1-x}$In$_x$-based nanostructures on their optical losses. Optical functions are calculated within the Random Phase Approximation approach. Optical absorption spectra corresponding to the plasmon and band-to-band transitions of alloys show opposite trends in spectral shifts caused by a variation of the content, $x$. With increase of $x$, the electronic energies of band-to-band transitions associated with optical excitations of $d$-electrons indicate well pronounced red shifts. The predicted variations of optical absorption spectra of transition metals alloys agree with experimental data measured on Ag-In and Ag-Cd alloys.

V.I. Gavrilenko

Date submitted: 02 Mar 2011

Electronic form version 1.4