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**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.

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