Ab-initio Calculated Optical and Magneto-Optical Properties of M/Fe (M=Cu, Ag, Au) Superlattices

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Surface Plasmon Resonance (SPR) has been applied in various fields as sensors. One of the crucial issues on the applicability of SPR is the sensitivity of SPR, which should be optimized by properly designing the structures and properties of the sensing layer. Ferromagnetic materials that have large magneto-optical (MO) properties are good candidates for sensing layer as the resulting magneto-optical activity may lead to sensitivity enhancement [1-4]. Among the crucial ingredients for a high MO response are a large Kerr rotation and zero ellipticity. In the present work, by using first principle-density functional theory calculations [5], we study the optical and magneto-optical properties in Cu/Fe, Ag/Fe and Au/Fe superlattice. We particularly focus on the quality factor and Kerr rotation angle which are directly related to the SPR applications. At low energy levels (<2 eV), quality factor in the noble-metal/Fe system increases compared to Fe-bulk and has a peak at the energy of around 1 eV. At 632 nm, the quality factor in the noble-metal/Fe system increases 3 times. Furthermore, the increase in the Kerr rotation only occurs in the Au/Fe system with peaks at energy levels of 4.6 eV and 8.2 eV. The increase of Kerr rotation is due to the decreased the diagonal component of optical conductivity (σ_{xx}) and larger the off-diagonal component of optical conductivity (σ_{xy}) [6]. We also studied the spin and orbital magnetic moments and their correlations with (σ_{xy}). The highest increase in the spin-orbit correlation S^zL^z is found in Au/Fe system. Further discussions will be presented.

Keywords: density functional theory, optical conductivity, Kerr rotation

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