Electronic Structure and Magneto-Optical Anisotropy of FeCu Superlattice: First-Principles Study

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The magneto-optical anisotropy (MOA) properties of FeCu superlattice is presented based on first-principles study. Calculations were carried out by using a full-potential linearized augmented plane wave (FLAPW) method with the generalized gradient approximation and the optical conductivity tensors were estimated by the Kubo formula, where the anisotropy of the off-diagonal component of the optical conductivity tensors for both polar and transverse magnetization geometries are determined in photon energy range of 0 – 8 eV. The results predict that the main effect of MOA comes from the change of the orbital character of the wave functions due to the change of the magnetization direction, and it is found that by analyzing the orbital character of partial density of states, there is a dependence of the Fe $d_{x^2-y^2}$ and d_{xy} states on the magnetization direction at –1.2 eV. In addition, the correlation between the energy dependence of MOA spectra and the band structure of the superlattice is clarified, for example, the peaks in the MOA spectrum at 0.7 eV, 1.8 eV, and 3.3 eV are dominated by the transition at the Brillouin zone edge along the $\Gamma-X$, $Z-\Gamma$, and $X-M$, respectively. Further discussions will be presented.

Keywords: magneto-optical anisotropy, superlattice, optical conductivity