Thin films size effect on anisotropy optical properties of gold and silver

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1. Introduction

The electromagnetic properties of the nanoscale optical devices can be determined by the geometry of the structure and the chosen material. Recently, the experimental bulk material properties of noble metals are widely used to invistiate and to design the plasmonic devices. However, it is known that the material properties are different from the bulk to nanometer-scale material. The *ab initio* method can be applied to calculate the material propertiess. Jun *et al.* [1] reported that the optical properties of nanoparticles can be calculated by density functional theory (DFT). In this study, the permittivity of Au(100) and Ag(100) thin films were calculated. In particular, the size dependent thin films and their anisotropic properties were revealed.

2. Results and Discussions

The predicted permittivity (imaginary part) of gold and silver thin films by *ab initio method* are shown in Fig. 1. It is worthy to note that only the interband transition is included in our calculation.

The in-plane permittivity of thin films exhibits the same peak as bulk around 2eV (gold) and 3.5eV (silver), because the infinitely large structure is similar in bulk and in-plane direction. The value increases with the additional layers, which illustrate more energy loss in thin films. In particular, the interband contributions demonstrate a peak around 0.5eV. This may be resulted from the shifting of the underlying band.

A large difference is found between in-plane and out-of-plane permittivities in both gold and silver thin films. The anisotropy of the permittivity is dominated by interband transition due to the confined dimension along the out-of-plane direction. The trend is similar as the data reported by Slimane *et al.* [2]

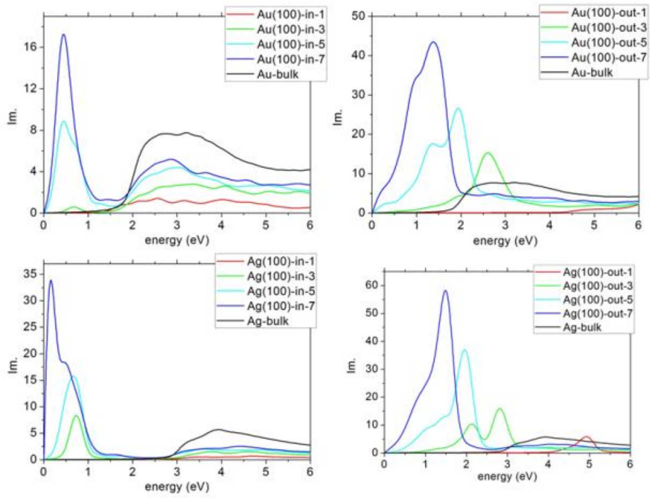

Fig. 1. Imaginary part of the permittivity of (a) in-plane in Au(100); (b) out-of-plane in Au(100); (c) in-plane in Ag(100); (d) out-of-plane in Ag(100) with one to seven layers.

3. Conclusions

The anisotropic permittivities of gold, silver thin films are shown and they are contributed by the shifting band in confined dimension. The calculated material properties may be used in future design of nanoscale optical devices.

Acknowledgement

This work is supported by the Ministry of Science and Technology of Taiwan (104-2221-E-002-079-MY3) and NTU project (NTU-ERP-105R891404). We are grateful to the National Center for High-Performance Computing, Taiwan, for providing us with computing time and facilities.

References

[1] Jun Yun *et al.*, Physical Review B 84(23), 235430, 2011

[2] Slimane Laref *et al.*, Optics Express, 21(10), 11827, 2013