Optical properties of a monoclinic insulator $Cu(H_2O)_2(en)SO_4$, en=$C_2H_8N_2$

Rudolf Sykora[1], Kamil Postava[1], Dominik Legut[1], and Robert Tarasenko[2]

[1]*VSB - Technical University of Ostrava, Nanotechnology Centre, 17. listopadu 15/2172, 708 33 Ostrava-Poruba, Czech Republic*

[2]*Centre of Low Temperature Physics of SAS and P. J. Safarik University, Institute of Physics, Faculty of Science, P. J. Safarik University, Kosice, Slovakia*

$Cu(H_2O)_2(en)SO_4$ was recently identified as a quasi-one-dimensional $S = 1/2$ antiferromagnetic insulator with a theoretically predicted gap of about 2 eV [1]. We used the electronic structure of [1] to predict material's optical properties and, namely, study one aspect related to the structure's monoclinic symmetry (the angle β is 105.5°). The monoclinicity implies that (i) the material is optically biaxial, and (ii) the axes of the dielectric frame, defined as the frame where the real part of the (generally complex) dielectric tensor is diagonal, are not fixed by crystallographic symmetry (and actually depend on frequency). By means of Mueller ellipsometry we measured the system's optical properties, from which the orientation of the dielectric frame was inferred and compared to a prediction of DFT-based (GGA+U, with U=5.5 eV [1]) *ab-initio* calculations. The theoretical orientation was obtained by diagonalizing the dielectric tensor as calculated in the linear-response regime by the VASP code. For comparison we mainly concentrate on the static limit, $\omega \to 0$.

[1] R. Sykora, D. Legut, J. Appl. Phys. **115**, 17B305 (2014).