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Software

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SHGYield

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Summary

`SHGYield.py` is a python program for calculating the surface second-harmonic generation (SSHG) yield (in reflectance) for semiconductor surfaces.

SSHG is an effective, nondestructive, and noninvasive probe for studying surface and interface properties, and even for characterizing buried interfaces and nanostructures. The high surface sensitivity of SSHG spectroscopy is due to the fact that within the dipole approximation, the bulk SHG response in centrosymmetric materials is identically zero. The SHG process can occur only at the surface where the inversion symmetry is broken.

This program has several potential applications and uses:

- determining and analyzing the physical origin of SSHG spectra
- predicting and characterizing the radiated SSHG for interesting new materials
- characterizing thin films based on measured SH spectra
- allowing the experimenter to calculate and analyze the SSHG yield to optimize experiments

For example, the figure below is an overview of the angular dependence of the reflected SHG Yield from the Si(111)(1x1)H surface. Experimentalists will find this very useful, as they can plan the experiment accordingly in order to optimize the output signal strength and polarization.

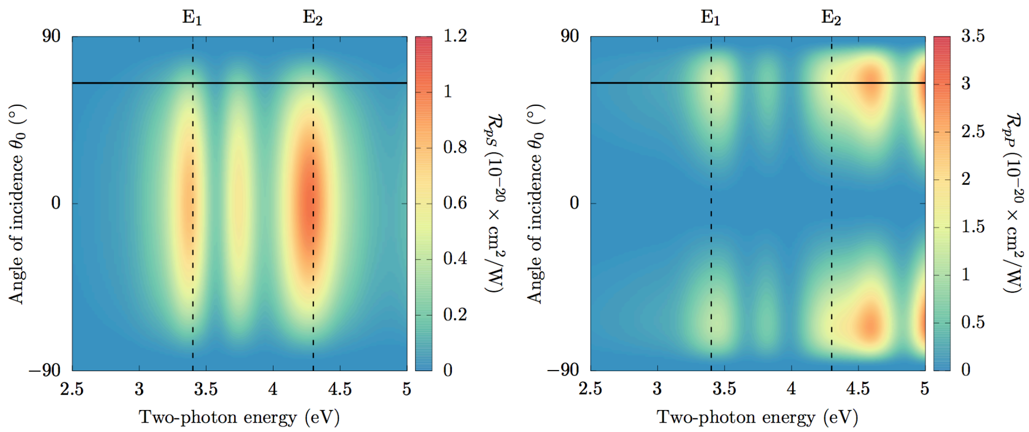

Figure 1: An overview of the angular dependence of the SHG Yield for the Si(111)(1x1)H surface

References

The complete theory is derived step-by-step in Ref. (Anderson and Mendoza 2016b). This software has been developed and used in the following publications:

Anderson, S. M. 2016. "Theoretical Optical Second-Harmonic Calculations for Surfaces." PhD thesis, Loma del Bosque 115, Colonia Lomas del Campestre León, Guanajuato 37150, Mexico: Centro de Investigaciones en Óptica, A. C. doi:10.13140/RG.2.2.35619.66082.

Anderson, S. M., and B. S. Mendoza. 2016a. "Derivation of the Three-Layer Model for Surface Second-Harmonic Generation."

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———. 2017. "Depth-Dependent Three-Layer Model for the Surface Second-Harmonic Generation Yield." *Frontiers in Materials* 4: 12. doi:10.3389/fmats.2017.00012.

Anderson, S. M., N. Tancogne-Dejean, B. S. Mendoza, and V. Véniard. 2015. "Theory of Surface Second-Harmonic Generation for Semiconductors Including Effects of Nonlocal Operators." *Physical Review B* 91 (7). American Physical Society (APS): 075302. doi:10.1103/PhysRevB.91.075302.

Anderson, S. M., N. Tancogne-Dejean, B. S. Mendoza, and V. Véniard. 2016. "Improved *Ab Initio* Calculation of Surface Second-Harmonic Generation from Si(111)(1×1)H." *Physical Review B* 93 (23). American Physical Society (APS): 235304. doi:10.1103/PhysRevB.93.235304.