

Improved *ab initio* calculation of surface second-harmonic generation from Si(111)(1×1):H

S. M. Anderson,^a N. Tancogne-Dejean,^{b,c,d} B. S . Mendoza,^a and V. Vénierd.^{c,d}

^aCentro de Investigaciones en Óptica, León, Guanajuato, México

^bLaboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA/DSM, 91128
Palaiseau, France

^cMax Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149,
D-22761 Hamburg, Germany

^dEuropean Theoretical Spectroscopy Facility (ETSF), Palaiseau, France

We carry out an improved *ab initio* calculation of surface second-harmonic generation from the Si(111)(1×1):H surface. This calculation includes three new features in one unique formulation: (i) the scissors correction, (ii) the contribution of the nonlocal part of the pseudopotentials, and (iii) the inclusion of a cut function to extract the surface response, all within the independent particle approximation [1]. We apply these improvements on the Si(111)(1×1):H surface and compare with various experimental spectra from several different sources. We also revisit the three layer model for the SSHG yield and demonstrate that it provides more accurate results over several, more common, two layer models. We demonstrate the importance of using properly relaxed coordinates for the theoretical calculations. We conclude that this new approach to the calculation of the second-harmonic spectra is versatile and accurate within this level of approximation [2]. This well-characterized surface offers an excellent platform for comparison with theory, and allows us to offer this study as an efficient benchmark for this type of calculation.

Keywords: 78.68.+m; 42.65.An; 71.15.Mb; 42.65.Ky; 78.66.-w

References

- [1] S. M. Anderson, N. Tancogne-Dejean, B. S . Mendoza, and V. Vénierd, Phys. Rev. B **91**, 075302 (2105).
- [2] S. M. Anderson, N. Tancogne-Dejean, B. S . Mendoza, and V. Vénierd, Phys. Rev. B in press.