Structure and optical properties of reconstructed Si and Ge surfaces

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When a crystal is cut in a specific direction the surface of the system differs from the bulk as the forces on the bulk atoms are not similar to those on surface atoms. This is called surface reconstruction. When these systems are energetically relaxed, sometimes they form special ordered structures such as one dimensional atomic chains or rows of dimers etc. due to surface reconstruction. Systems with reconstructed surfaces can exhibit completely different electronic and optical properties than bulk. They may also produce structural anisotropy. A combination of optical experimental measurements and computer simulations may be used to identify those special structures on the surfaces by exploiting the anisotropy. Reflectance anisotropy (RA) spectroscopy is one of them. It is a linear optical technique that provides optical information about ordered surfaces and interfaces that are anisotropic in the surface plane. RA spectroscopy is a technique where the reflectance of a surface for normal incidence light is measured for two perpendicular polarizations of the light over the visible range of photon energies. A major advantage of RA spectroscopy is that it can function in a range of environments inaccessible to conventional surface techniques. It is very surface sensitive and does not damage the surface. It has mainly been used as a fingerprint technique, because calculating the optical response from first principles is computationally expensive.

Si surfaces have been more intensively studied than Ge, due to its importance in semiconductor device manufacturing, although both have been studied in detail [1, 2]. This project is investigating a recently developed more efficient *ab initio* approach, which uses hybrid density functional theory (DFT) for calculating the optical response of different reconstructions for Si and Ge for comparison with experiment. In this work the RA spectra are calculated for different Si and Ge systems. Some of the structures, such as Si(111)-(5×2)-Au [3] or Si(110)-(16×2) [4] are not definitely known. So the aim of this project is to predict the right structures for these systems and test the method using known structures (clean Si(111)-(2×1) [5], Ge(001) [6], and Ge(001)-(2×1)-Sb [7]) with the help of RA spectra measurements. RA spectroscopy measures optical transitions between the occupied and vacant states. If the electronic structure of a system is correct only then will the calculated RA spectra agree with the experiment.

All the structures in this work were optimized using the CRYSTAL [8] code, which uses hybrid DFT with gaussian basis sets. The electronic structures were calculated with optimized k point densities. Lastly we calculated the optical properties and RA spectra, with the help of EXCITON [9] code, from those structures. In the experimental part, low energy electron diffraction (LEED) is used to check the surface reconstruction. After checking the surface by LEED, the RA spectrum is measured in the range from infrared to visible light. Some of the calculated RA spectra match with experiment very well at some points of energy and disagree at some energy values. So we have to investigate the reconstructed systems further to get a better agreement between experiment and theory.

References

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