computer reconstruction algorithms were proposed to recover the 3D structure of atoms surrounding an atomic source of a (spherical) reference wave. A major limitation of all these methods is that, due to the decay of the reference wave with the inverse of the distance from the source, the reconstructed image contains information only about atoms rather close to the source. In the case of surface crystallography, a more useful direct method would be one capable of recovering the entire contents of a large surface unit cell. We will describe in this talk an alternative holographic interpretation of x-ray and electron diffraction patterns from surfaces which accomplishes this task by taking as the reference wave the delocalized one scattered by the entire bulk substrate and show some results from applications to surface x-ray diffraction (SXRD) [1] and low energy electron diffraction (LEED) [2].

[1] Lyman P.F., Shneerson V.L., Fung R., Harder R.J., Lu E.D., Parihar S.S., Saldin D.K., *Phys. Rev. B*, 2005, **74**, 081402(R0). [2] Saldin D.K, Seubert A., Heinz K., *Phys. Rev.Lett.*, 2002, **88**, 115507.
Keywords: holography, surfaces, structure

MS75.29.3
X-Day Diffraction from Semiconductor Nanostructures
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Self-organized nanostructures are of great interest in semiconductor technology due to the enhancement they introduce for device design. Quantum confinement effects and the combination of different materials lead to electronic states that cannot be realized using bulk materials or planar heterostructures. Key properties of nanostructures, such as chemical composition, shape, size, and strain state, depend sensitively on growth conditions.

X-ray diffraction techniques have been successfully used for the characterization of such nanostructures, both after growth as well as in situ during fabrication [1]. The main advantages of x-ray techniques are that they can be applied to capped structures, that they provide statistically well averaged results, and the high sensitivity to lattice strain.

In this presentation, the techniques used for the structural characterization of nanostructures will be discussed, together with recent results in particular on SiGe islands embedded in Si samples. The composition and strain distribution within the nanostructures is derived from reciprocal space maps recorded in coplanar or grazing incidence diffraction (GID) geometry. Anomalous scattering is used to obtain material sensitivity even in the case of GID.

[1] *for a review see:* Stangl J., Holý V., Bauer G., *Rev. Mod. Phys.*, 2004, **76**, 725, *and references therein.*
Keywords: Nanostructure, composition, diffraction

MS75.29.4
Interaction of NO and CO with Surface of Pd Nanoclusters studied by XRD
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The developed recently technique of monitoring in situ a position,width and intensity of XRD profile during chemisorption or a surface reaction [1,2,3] was used to study interaction of NO and CO with Pd nanocrystal surface. The peaks evolution was interpreted via atomistic simulation. Additional insight into the surface morphology is provided by measuring time required for a transition of the Pd nanocrystals into beta hydride phase in hydrogen atmosphere. The adsorption of both gases hinders hydride transition slowing down the rate of hydrogen dissociation.

The study is an attempt to shed light on a possible surface reconstruction of the nanocrystals occurring on chemisorption. Up to date evidence for a similar phenomena could be only collected with surface science techniques on single crystals under very low gaseous pressure.

[1] Kaszkur Z., *J. Appl. Cryst.*, 2000, **33**, 87. [2] Kaszkur Z., *J. Appl. Cryst.*, 2000, **33**, 1262. [3] Kaszkur Z., *Phys. Chem. Chem. Phys.*, 2004, **6**, 193.
Keywords: nanocrystals, palladium, surface reconstruction

MS75.29.5
Three Dimensional Charge Density Measurements at Surfaces
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Charge density measurements in bulk materials using primarily x-ray diffraction but in some cases transmission electron diffraction is a very well established field. In principle, being able to directly measure the charge density at a surface is at least as scientifically interesting if not more so; one could start to directly probe numerous important processes such as bond formation at a surface. Until very recently it has not been possible to achieve this due to experimental problems. The first work reported was with transmission electron diffraction for the MgO (111) √3x√3 R30 surface where significant charge transfer was measured, but only in two dimensions. We will describe here results using surface x-ray diffraction for the Si (001) 2x1-H surface where a charge density analysis has been done in three-dimensions.
Keywords: surfaces, charge density, X-ray diffraction

MS76 NEW ALGORITHMS FOR STRUCTURE PREDICTION
Chairpersons: Peter Erk, Sam Motherwell

MS76.29.1
Assessing Lattice Energy Minimisation for Crystal Structure Prediction
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The goal of reliable crystal structure prediction has been a driving force for the development of methodologies in modelling molecular organic crystals. The first step in crystal structure prediction involves a search for all low energy structures on the potential energy surface. Such searches usually generate far more energetically feasible structures than are known or are likely to be observed and the energy differences between possible structures are typically very small. Therefore, the ordering of energetic stability requires a high quality model for the lattice energy.

Several options for modelling the energies of predicted crystal structures are examined: empirical atom-atom potentials with atomic charges and multipoles; the recently developed semiclassical density sums (SCDS or "Pixel") method [1]; and periodic density functional theory calculations. The models are assessed on a test set of small organic molecules [2] and results of the most recent (third) blind test of crystal structure prediction are also examined. Advantages and shortcomings of the various methods are discussed.

[1] a) Gavezzotti A., *J. Phys. Chem. B*, 2002, **106**, 4145-4154; b) Gavezzotti A., *J. Phys. Chem. B*, 2003, **107**, 2344-2353. [2] a) Day G. M., Chisholm J., Shan N., Motherwell W. D. S., Jones W., *Crystal Growth & Design*, 2004, **4**, 1327-1340; b) Day G. M., Motherwell W. D. S., Jones W., *Crystal Growth & Design*, 2005, *in press.*
Keywords: molecular modelling, crystal structure prediction, energy minimization

MS76.29.2
A Hybrid Method for the Accurate Energy Ranking of Molecular Crystals
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