

structures

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Coherent Diffraction Imaging is a technique for the three-dimensional reconstruction of single objects using coherent X-ray nano-beams. This technique, when used on Bragg reflections [1-5], can be used to recover both the shape and strain inside the objects.

In semi-conductor nanowires (NWs), the knowledge of the exact strain state is essential for the tuning of the physical properties (conduction, photo-emission). While ensemble-averaged studies can provide quantitative information about the shape and strain state [6], this is only possible in the case of a very low dispersion of the structural properties. This presentation will be focused on the study of small (diameter<200nm) homogeneous and heterogeneous NWs and strained Silicon-On-Insulator lines, which have been studied using Coherent Bragg Imaging (CBI) [7,8].

In the case of heterogeneous nanowires, we will show that it is possible to use the small size of existing nano-beams (e.g. 300x500 nm² using a Fresnel Zone Plate on beamline ID01 of the ESRF) to perform CBI measurements on different parts of heterogeneous nanowires, and therefore analyze the strain state near the interface.

We will also discuss the current challenges presented by the method: (i) the requirement to determine the amplitude and phase of the incident focused X-ray beam, (ii) the difficulties of keeping a single object inside a nano-beam while rotating it over ~1° to record the 3D scattering pattern, and (iii) the effects of radiation damage due to the high flux (>10⁴ ph/s/nm²) on the sample.

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Bulk dislocation core dissociation probed by coherent X Rays in silicon

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We present a new approach to probe bulk dislocations by using coherent x-ray diffraction. Coherent X rays are particularly suited for bulk dislocation studies because lattice phase shifts induce typical diffraction patterns which strongly depend on the fine structure of dislocation cores. The strength of the method is demonstrated by performing coherent diffraction of a single dislocation loop in silicon. The measured dissociation is proved to be unusually large compared to known dissociations. This work opens a route for the study of

dislocation cores in a static and dynamical regime, and under various external constraints.

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Predicting the behaviour of lone-pair electrons

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If one defines the bonding strength of an ion as the valence of a typical bond, the valence matching rule states that stable bonds will be formed only between ions having bonding strengths that do not differ by more than a factor of two. This rule limits the range of compounds that can form and indicates that weak cations bond only to weak anions and strong cations only to strong anions. This rule is obeyed in all compounds whose atoms can be assigned a formal cation or anion charge (valence) regardless of whether the bonding is ionic or covalent, with only two exceptions: the presence of steric stress or electronic anisotropies. Ions with lone pairs, namely cations in lower oxidation states and anions, also obey this rule in compounds in which the lone pairs are described as 'inactive'. However, the presence of lone pairs in the valence shell provides a flexibility not available to normal ions. An ion with lone pairs can bond to a counterion with a bonding strength greater than twice its own bonding strength if the lone-pair electrons in the region of the bond are converted to bonding electrons. This allows the ion to form a stronger bond to match the larger bonding strength of the counterion. To conserve the number of lone pairs, bonding electrons on the opposite side of the ion are converted to lone pairs, leading to the characteristic asymmetry associated with stereoactive lone pairs. This model leads to a number of conclusions. It is possible to predict when and how lone pairs result in asymmetric coordination, it reveals that 'dative' bonds do not involve lone pairs but usually result from hydrogen bonding, and it predicts that monovalent anions bonded to electron-rich cations (those with bonding strengths greater than 1.0 vu (valence units)) will necessarily form finite molecules containing bonds of exactly 1.00 vu, i.e., electron-pair bonds. Although such bonds are generally considered to be prototypical covalent bonds, they are predicted as a special case of the ionic model.

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Revealing electron conjugation through an observable

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The Source Function (SF) [1,2] enables one to view chemical bonding and other chemical paradigms under a new perspective and using only information from the electron density observable, ρ , and its derivatives. Being completely independent from the tools used to get ρ , the SF represents a very useful descriptor, able in some cases to bridge the gap between the rich information one gains from an *ab-initio*