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On subgroups of hyperbolic crystallographic groups

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The characterization of the subgroup structure of crystallographic groups is one of the problems in mathematical crystallography which is of general interest. Subgroups of crystallographic groups are essential for a number of important studies in chemical research such as providing a concise tool for classifying crystal structures. Moreover, group-subgroup relations are useful, for example, in understanding the domain structures of twinned crystals and in the study of phase transitions.

The subgroups of crystallographic groups in the Euclidean and spherical cases have been studied extensively in previous works. On the other hand, investigating the subgroups of hyperbolic crystallographic groups is still a viable topic to explore. The motivation of this work is to discuss a method of arriving at the subgroups of crystallographic groups particularly those that exist in hyperbolic 3-space. We will discuss low index subgroups and properties pertaining to normal subgroups, conjugacy classes and torsion free subgroups. Some applications of these groups will also be explained.

Examples of these groups are called Tetrahedral groups, which are groups of symmetries of tilings in space by tetrahedra, belong to the important family of discrete groups known as crystallographic reflection groups. Tetrahedral groups arise in connection with various extremal problems in hyperbolic 3-manifolds and orbifolds. Among its two dimensional subgroups are the triangle groups, which are currently finding applications in the construction of chemical networks by projecting hyperbolic tilings into triply periodic minimal surfaces. More recently, in [1], the subgroup lattice of the triangle group *642 was used to give an enumeration of crystal nets, interest of which arises from their relevance to condensed materials. Hyperbolic triangle groups also play a role in dealing with structures of the fullerene family [2].

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Interfaces of lanthanum and strontium manganite superlattices

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The manganites have been investigated for applications in magnetic devices. In the simple perovskite form, $LaMnO_3$ and $SrMnO_3$ are individually antiferromagnetic insulators. An alloy of these materials, $La_{(1-x)}Sr_xMnO_3$, undergoes an antiferromagnetic-ferromagnetic transition at concentrations of $0.15<x<0.5$ [1]. Superlattices of $LaMnO_3$ (LMO) and $SrMnO_3$ (SMO) can be grown by molecular beam epitaxy (MBE) with layer by layer control. While keeping the stoichiometry constant but changing the film thickness, the electrical and magnetic transport of these superlattices can vary by orders of magnitude [2]. This behavior is related to the localization of electrons, presence of interfacial states [3], film abruptness [4], and the strain in the films.

We can also remove selected MnO_2 layers of the superlattice to form a Ruddleson-Popper structure. By distorting the oxygen octahedra around Mn cations, the magnetic properties can be engineered differently from the perovskites. In superlattices it has been shown that the magnetization under an applied magnetic field is asymmetric parallel and normal to the film growth direction [5].

In superlattices, the density of interfaces is comparable to film thickness. To understand the origin of the magnetization, an investigation of the nanostructure and interfaces is essential. Scanning transmission electron microscopy (STEM) has the capability to collect images, diffraction patterns, and spectroscopy on individual films. With aberration corrected optics, a probe size of 1 Angstrom, or smaller is achieved in STEM mode, which can image oxides at atomic resolution and obtain chemical and electronic structural information on the atomic scale with electron energy loss spectroscopy (EELS).

We have investigated the interfaces of manganites in both the perovskite and Ruddleson Popper phases with aberration corrected electron microscopy. For the perovskites, the films are grown with high quality and exhibit near perfect epitaxy. A magnetic transport study [4] shows the in-plane magnetization is asymmetric about the two interfaces of LMO and SMO. At one interface, the magnetization is sharply enhanced, and at the other interface, the magnetization is suppressed. Using a combination of STEM, EELS, and Nanoarea electron diffraction (NED), we investigated the origin of this asymmetry. For the Ruddleson Popper manganites, electron diffraction performed with a liquid nitrogen cooled stage shows the crystal structure is modified upon cooling to ~100 K.

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Interfacial magnetism by resonant X-ray reflectivity

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The X-ray Resonant Magnetic Reflectivity (XRMR) technique yields the magnetization density across ultra-thin magnetic samples, with specificities that establish the technique as a complement to macroscopic techniques or polarized neutron scattering. The technique is sensitive to the orientation and the amplitude of the magnetic moment with a spatial resolution below the nanometer, distinguishing contributions from different chemical elements. The presentation will have an emphasis on some experimental and analytical methodologies and then turn to two recent applications. In a first example, XRMR allowed the direct analysis of the layer resolved spin structure in the fcc Fe films on Cu(001) providing the magnetic structure in the coverage regime above four monolayers, which is commonly referred to as ''antiferromagnetic'', but whose detailed structure was never solved [1]. Meyerheim *et al.* found a new model characterized by

units of strongly coupled spins, whose relative orientation can vary easily involving noncollinearity of the spins. In a second example, an antiferromagnetic NiO/CoO thin layer over Pt, it was demonstrated that the soft-x-ray resonant magnetic reflectivity measured over a wide angular range provides a direct way to probe out-of-plane magnetic profiles [2]. Tonnerre *et al.* obtained the extension and structure of the magnetic ordering induced by an ultrathin Co FM layer, over a few oxide atomic layers in the antiferromagnetic layer.

[1] H.L. Meyerheim, J.-M. Tonnerre, L. Sandratskii, H.C.N. Tolentino, M. Przybylski, Y. Gabi, F. Yildiz, X.L. Fu, E. Bontempi, S. Grenier, J. Kirschner, *Physical Review Letters* ***2009***, *103,* 267202. [2] J.M. Tonnerre, M.D. Santis, S. Grenier, H.C.N. Tolentino, V. Langlais, E. Bontempi, M. Garcia-Fernandez, U. Staub, *Physical Review Letters*, ***2008,*** *100,* 157202.

Keywords: X-ray_resonant_magnetic_scattering, interfacial_ magnetism, metallic_thin_films

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High energy X-Ray surface and interface scattering

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Using a focused high energy x-ray beam (E < 100 keV) we have developed a dedicated instrument for High Energy MicroDiffraction (HEMD) for surface and interface scattering at beamline ID15A (ESRF, Grenoble, France). The high energy of the beam allows us to access deeply buried structures including interfaces. The instrument is also equipped with a beam deflector unit which allows us to incline the x-ray beam with respect to flat liquid surface and interfaces, sufficient to reach large perpendicular momentum transfer for atomic or molecular resolution [1].

The instrument has been used for a wide range of structural investigations on deeply buried interfaces. Examples including such diverse materials as ice, ionic liquids, alcohols, metal- semiconductor/ insulator interfaces, hydrophobic interfaces, will be presented in order to demonstrate the high performance and capabilities of high energy microbeams in structural investigations of buried interfaces.

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Keywords: surface, interface, high-energy x-rays

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High resolution STEM study of InGaAs/InAlAs and Si/Ge heterostructures

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Si/Ge and InGaAs/InAlAs based heterostructures are studied as perspective materials for high frequency generators, detectors and optoelectronic devices. Two types of heterostructures were investigated: a) $In_xAl_{1-x}As/In_yGa_{1-y}As/In_xAl_{1-x}As$ on InP substrate with different layer thickness and different content; b) Si/Ge heterostructures having 2 to 12 Ge layers thickness and deposited at low temperatures. The heterostructures were formed by MBE. In the present study we show an application of high-resolution scanning/transmission electron microscopy for the determination of structural parameters and defects in heterostructures. The Cs corrected TITAN 80-300 TEM/STEM (FEI, US) equipped with HAADF detector (Fischione), EDXS (EDAX, US) and GIF (Gatan, US) systems were used in the study. In both systems the interfaces were atomically flat and tetragonal lattice distortions was the most typical mechanism of crystal lattices mismatch reduction. Low density of 60^0 misfit dislocations, microtwins (MTs), stacking faults (SFs) and second phase precipitates were found at $In_xAl_{1-x}As/In_yGa_{1-y}As$ interfaces Fig.1. These precipitates were identificate as wurtzite inclusions in sphalerite matrix. The inverted piramids started to form in the Ge layers associated with SFs, when thickness exeeded 10 monolayers. The MT and SF were revealed mostly by bright field HREM demonstrating poor contrast in HAADF STEM mode. The structure-properties relations were discussed.

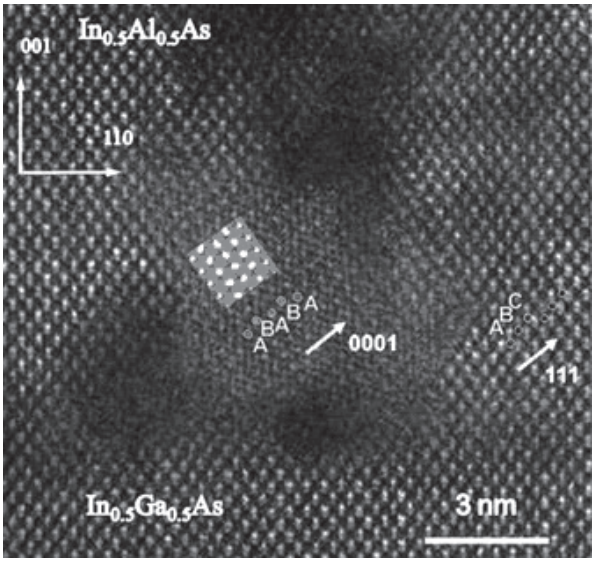

Fig. 1. HR STEM image of $In_{0.5}Al_{0.5}As/In_{0.5}Ga_{0.5}As$ interface. The model of wurtzite structure is in the insert. The sequence of layers typical for wurtzite (ABABAB) and sphalerite structures (ABCABC) are shown.

Keywords: heterostructures, STEM, defects.

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Spatial resolution of electronic structure through modeling reflectivity spectra

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X-ray absorption spectroscopy has become an important tool in understanding the electronic structure of materials. Resonant absorption edges in the soft x-ray regime are especially interesting as they allow the study of the lighter elements, such as in organic or organo-metallic substances, as well as important *L*-edges of the 3*d* transition metals important in magnetic and oxide systems. Measurements of soft x-ray absorption spectra are inherently surface sensitive, and are plagued by issues such as extinction (in electron yield measurements) or self absorption (in fluorescence yield measurements), which make accurate determination of the optical constants difficult. More accurate optical constants can be obtained by modeling the reflectivity spectra, while being somewhat less surface sensitive compared to electron yield.

Soft x-ray reflectivity from single crystals, thin films, or superlattice structures contains depth dependent information that can be exploited