14. X–13 NEW TECHNIQUES IN SYMMETRY ANALYSIS.

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Space Group Determination

Dynamic extinction rules for 2_1 screw axis and glide planes are studied by Gjønnes and Moodie (Acta Cryst. 19 (1965) 65). To determine the crystal space groups by dynamic extinction (GM line), we have investigated the dynamic extinction rules when plural number of screw axes and/or glide planes coexist and when these symmetry elements are combined with various lattice types. Based upon the rules, we have given the tables which list the GM lines expected at various incident-beam orientations for all the space groups. It has been found that 185 space groups can be identified by GM lines [M. Tanaka, H. Sekii and T. Nagasawa, Acta Cryst. A39 (1983) 825]. The indistinguishable space-group pairs have to be identified from the intensity change of the forbidden reflections by varying crystal orientation.

An example of space-group determination using the dynamic extinction with the aid of the tables is demonstrated for a magnetic-super conductor $ErRh_4B_4$. Its point group was found to be 4/mmm. A_2 and B_2 GM lines were observed in the 0k0(k=odd) reflections at [100] electron incidence. The space groups No. 129, 130, 137 and 138 are found to be possible ones by referring the tables. At $[03\bar{1}]$ incidence, A_2 and B_2 GM lines were observed in the h00(h=odd) reflections, and no GM line in the 013 reflection. The space group was determined as No. 137, $P4_2/nmc$, by consulting the tables. A_3 GM line was observed in the $11\bar{3}$ reflection at [332] incidence, this GM line being also expected from the space group.

Glide planes, especially those whose translation vector is perpendicular to the specimen surface, can be identified from the GM lines appearing in the higher order Laue-zone (HOLZ) reflections. When the HOLZ GM lines are utilized with the GM lines in the 0-th Laue zone reflections, the space groups can be unambiguously and quickly determined.

Techniques for Obtaining CBED Patterns

CTEM CBED patterns are obtained by converging the incident beam with a condenser-objective lens on a specimen area of about 10 nm diameter.

BRCBED CBED patterns can be also obtained by rocking the parallel incident beam instead of the convergent beam [M. Tanaka, JEOL News 16E (1978) 13]. A CBED pattern appears on the CRT and the corresponding microscopic image simultaneously appears on the fluorescent screen. The advantages of BRCBED are as follows:

1) The area from which a CBED pattern is taken can be more easily identified than by CTEM.
2) Specimen contamination is insignificant.
3) Specimen damage is greatly reduced.
4) Electrical signal processing is possible.

Wide Angle Patterns The diameter of a non-overlapping disk in a CBED pattern is limited by the Bragg angle of the nearest reflection. To find the symmetry of a pattern obtained from a crystal of a large lattice parameter, a wide-angle CBED pattern of a larger disk diameter than that determined by the Bragg angle is necessary. Wide-angle bright field pattern and wide-angle dark field pattern are obtained by displacing the specimen from the focus of the incident beam in CTEM and obtained by the double rocking method in BRCBED [M. Tanaka, R. Saito, K. Ueno and Y. Harada, J. Electron Microsc. 29 (1980) 408]. The wide-angle whole pattern can be obtained by a hollow-cone incident beam which is formed with an annular aperture in CTEM and also formed by electrically deflecting and rotating the incident beam [Y. Kondo, T. Ito and Y. Harada, Jpn. J. Appl. Phys. Lett. 23 (1984) in press, M. Tanaka, H. Takayoshi, M. Terauchi, Y. Kondo, K. Ueno and Y. Harada, Jpn. J. Appl. Phys. 23 (1984) in press].

14. X–14 HIGH ENERGY ELECTRON DIFFRACTION FROM SURFACES.

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The technique of reflection high energy electron diffraction (RHEED) offers many advantages over other surface structure techniques. The geometry is ideally suited to the study of dynamic changes that occur in thin film growth, particularly in the growth of semiconductor layers by molecular beam epitaxy (MBE). Unlike its low energy counterpart (LEED) it is capable of giving quantitative structural information from surfaces that are rough, polycrystalline, disordered or even amorphous. Furthermore, RHEED also offers the possibilities of forming surface images from the diffracted beams. It also offers a high degree of precision in the determination of lattice spacing parallel to the surface, which is particularly important for the detection of strain in thin films. The main drawback to its widespread acceptance in surface studies has been our inability to perform a detailed structure determination for a well ordered single crystal surface (c.f. LEED). Recent advances in the theory of RHEED may improve the situation, although it will be demonstrated that the intensities of diffracted beams are very dependent on crystal perfection. Layer growth processes in MBE can also be monitored quantitatively (Neave et al. Appl. Phys. (1983) A31, 1) and the measurement of the scattered electron beam intensity offers the possibilities of determining film thickness during growth to sub-monolayer accuracy as well as the composition of III-V semiconductor alloy films.

14. X–15 ION-BEAM CRYSTALLOGRAPHY OF METAL-SILICON INTERFACES.

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Metal-silicon and silicide-silicon interfaces have been the subject of a rapidly growing number of studies, due to their great technological importance and the fascinating physical questions involved. Many metals have been found to mix readily with silicon, even at room temperature or below, and several models have been suggested to explain this behaviour. Furthermore, the abruptness of the metal-silicon or silicide-silicon interface, and the composition near the interface are key questions in understanding such issues as Schottky Barrier height formation or thin film adhesion.

Rutherford Backscattering Spectrometry, using 1-2 MeV ion beams is a well known standard technique for film analysis with 50-200 Å depth resolution. If, however, the depth resolution is improved to values less than ∿10 Å, this technique becomes suited for studies of ultrathin films and 2D structures, i.e. surfaces and interfaces. Such resolutions have recently been obtained in three ways. (I) When single crystals are studied, the ion beam can be aligned with a crystal axis, thereby shadowing all atoms below the topmost layers. (II) When the ion beam energy is reduced to ∿50-200 keV, an electrostatic energy analyser can be used instead of the widely used surface barrier detectors. The much better energy resolution of these analysers has resulted in a depth resolution of typically 3 Å, while even better resolutions are possible. Since the excellent quantitative properties of RBS are still valid in this medium energy regime, a high resolution RBS technique is obtained, which is not limited to crystalline layers. (III) Surface sensitivity can also be obtained by reducing the ion beam energy to values below typically 10 keV, using ion trapping and neutralization. However, buried interfaces