14.4-2 HREM IMAGE PROCESSING APPLIED TO GaAs / AIAs INTERFACES. By <u>A.F. de Jong</u>, Philips Research Laboratories, 5600 JA Eindhoven, The Netherlands; and W. Coene<sup>1</sup>, University of Antwerp, RUCA, B-2020 Antwerp, Belgium. 'Senior Research Assistant for the National Fund for Scientific Research (Belgium).

To determine the quality and the exact position of interfaces from High Resolution Electron Microscopy (HREM) images, comparison with simulated images is required. In the case of GaAs / AIAs interfaces, the different layers are commonly distinguished by the difference in mean intensity between the GaAs and AIAs images. However, the mean intensity of a lattice image is influenced by surface damage resulting from specimen preparation and by inelastic scattering processes. This makes calculation of the mean intensities, and hence comparison between experimental and simulated images, extremely difficult.

Alternatively, we distinguish the layers by differences in the fine pattern of GaAs and AlAs lattice images, typically imaged away from Scherzer defocus. To determine interface quality and position via this approach image processing is used. The principal difficulty is that both the relevant information about the interface and the unwanted information about background contrast are non-periodic. Image processing techniques which can be used to extract the relevant information, and make comparison with calculated data possible, are investigated using both experimental and simulated images. Results indicate that, when carefully used, filters in reciprocal space can be applied to suppress background contrast while retaining (non-periodic) fine features in the lattice images. As a next step, correlation procedures can be applied to distinguish the differences in fine pattern between the different layers, and compare experimental and simulated images.

14.4-3 STRUCTURAL ANALYSES OF METASTABLE PHASES IN Li<sub>2</sub>O-TiO<sub>2</sub> SYSTEM BY ED AND HREM. By <u>J Zou</u>\*, F H Li, D Y Yang, Y D Jiang and K H Kuo±, \*PO Box 2724, Beijing, China, Institute of Physics, Academia Sinica, Beijing, China, ±Institute of Metals Research, Academia Sinica, Shenyang, China.

When the quenched R phase of  $\text{Li}_2^{\text{Ti}}_3^{0}_7$  is heated to about 450 °C, it transforms to a metastable phase, called H (J C Mikklsen, Jr., J Cryst. Growth, 1979, <u>147</u>, 659). The electron diffraction (ED) patterns of H phase show that it in fact consists of two phases, called  $H_1$  and  $H_2$ , both belonging to the trigonal system. Their parameters of hexagonal unit cell are  $a_1 = 0.514$ ,  $c_1 = 7.02$  nm for the  $H_1$  phase and  $a_2 = 0.514$ ,  $c_2 = 0.936$  nm for  $H_2$  phase. The space group of  $H_1$  is R3c determined by ED and high resolution electron microscopy (HREM). And probable space groups of  $H_2$  are P3, P3, P321, P3m1 and P3m1. The intergrowth of  $H_1$  and  $H_2$  along [001] axis has been observed frequently. This can be explained as the result that a equals to a and both H phases have the same  $\frac{1}{2}$ fundamental stacking layer of spacing 0.234nm. Furthermore, the rutile  $\operatorname{TiO}_2$  layers sandwiched in H phases has been found. The orientation relationship between them is as follows:

<0 1 0>(TiO<sub>2</sub>)//<0 1 0>(H); <0 0 1>(TiO<sub>2</sub>)//<1 1 0>(H).

14.4-4 OBSERVATION OF STRUCTURES OF VACUUM CO-DEPOS-ITED B1-Mn FILMS BY HIGH RESOLUTION ELECTRON MICROSCOPY. By <u>T. Yamada</u> and K. Yoshida, Dept. of Appl. Phys., Fac. Eng., Kobe University, Rokkodai, Nada, Kobe 657, Japan.

It was found that vacuum co-deposited Bi-Mn films are not crystalline when their composition is in a range 85-65 at.% Mn, and a new metastable crystal phase, Nn<sub>3</sub>Bi, appears when they are heated at about 180 °C. Its basic crystal structure was derived from their lattice images (Authors, Acta. Metall. 1986, <u>34</u>, 969); its refinement by computer simulation is now in progress.

Structures of the films in a neighbouring range, 60-38 at.% Mn, were investigated. They were prepared by codeposition of Bi and Mn at  $10^{-7}$  Torr. They were observed by an electron microscope, JEM-200CX. Both high resolution lattice images and Energy Dispersive X-ray Spectra (EDS) of a specimen can be obtained.

Bright-field images of as-deposited films show almost uniform contrasts over the specimen, and very small crystalline regions at places. Their diffraction patterns show diffuse halos superposed with spotty Debye-Scherrer rings, the latter being well indexed as those of Bi type lattice. The more the Bi content, the stronger the rings. However, measurements of film thicknesses by Tolansky method surely show that these films contain about 50 at.<sup>3</sup> Mn atoms. EDS observations using Mn characteristic X-ray also prove that Mn atoms are uniformly distributed over all parts of the films, including the crystalline regions. A film of 38 at.<sup>3</sup> Mn shows a few weak diffraction spots very near to the incident beam and, in its high resolution micrographs, lattice fringes of 7.5 Å are occasionally observed at boundaries of the small crystalline regions. Mn atoms, as many as 38 at.<sup>3</sup>, seem to hide themselves in the amorphous parts of the films and also in the Bi type crystalline regions, and may react with the Bi type lattice to form long periods at these boundaries. Heating effects of these films are to be investigated and their high resolution electron micrographs will be shown.

14.4-5 NEW STRUCTURES OF ALKALI NIOBIUM TUNGSTEN OXIDES DERIVED BY *HREM* AND X-RAY POWDER DIFFRACTION. By <u>M. Lundberg</u> and M. Sundberg, Department of Inorganic Chemistry, Arrhenius Laboratory, University of Stockholm, Sweden.

A new tunnel structure of a fully oxidized compound with the general formula  $K_x Nb_{\delta+x} M_{\Theta-x} O_{47}$  (1  $\leq$  x < 3) has been deduced from high resolution electron micrographs. For x = 2 the monoclinic unit cell parameters are a = 18.882(5), b = 3.9572(5), c = 12.378(2) Å,  $\beta$  = 102.93(3)^{\circ}. The space group is P2/m. The structure has been confirmed by simulated image calculations and by X-ray powder diffraction studies. The polyhedral framework is built up of octahedra and pentagonal columns in such a way that four-, five, and six-sided tunnels are formed (Fig. 1). The structure comprises features of both the  $W_{18}O_{49}$  and the tetragonal tungsten bronze (TTB) structure types.

Phases obtained for values of x = 0, 3 and 5 possess structures with a tripled TTB unit cell, while preliminary *IREM* studies of the sample x = 7 reveal the existence of a new TTB-related phase with the composition  $K_x$  (Nb,W)  $_{11}O_{31}$ .



Fig. 1. The crystal structure of K<sub>x</sub>(Nb,W)<sub>17</sub>0<sub>47</sub>. K atoms are not included.