PS12.01.10 A NEW METHOD OF THE IDENTIFICATION OF CRYSTALLINE-AMORPHOUS INTERFACES BY QUANTITATIVE EVALUATION OF HREM IMAGES. N.I. Borgardt and B. Plikat*, Moscow Institute of Electronic Technology, 103498 Moscow, Russia, *IV. Physikal. Institut der Universitat Gottingen, Bunsenstr. 13-15, 37073 Gottingen, Germany

Identification of the atomic structure of interfaces between amorphous and crystalline phases by quantitative evaluation of HREM-images of cross-sectional samples is not straight-forward. This is due to the fact that the projected potentials of the atoms in the amorphous layer overlap randomly if the distance between them exceeds the length of short range order (about 1,5 nm). As a result, the contrast of interface steps can be blurred to different extends.

Intensity fluctuations caused by the random overlap of the projected potentials of the atoms in the amorphous layer can be eliminated if the two-dimensional intensity distribution of a homogeneous region of the interface is averaged along the interface. A theoretical analysis shows that the shape of the intensity profiles obtained by this method depends on:

i.) the distribution of steps at the interface and

ii) the averaged distribution of the amorphous layer atoms in the vicinity of the crystal boundary atoms.

Properties of the interface structure can be obtained by comparison of theoretical and experimental intensity profiles for various defocus settings. In order to simulate stepped interfaces the EMS multislice program [1] was supplemented to take into account the short range order of the amorphous layer. For this purpose the averaged distribution of atoms in the amorphous layer as a function of the distance to the interface is calculated from the radial distribution function as obtained from X-ray or neutron scattering. Comparisons of experimental images of a c-Si/a-SiO$_2$ interface and simulations based on the proposed method were carried out.

1. Stadelman P.A. (1987) Ultramicroscopy 21, 131

PS12.01.11 INVESTIGATION OF STORED ENERGY IN TiN-FILMS BY THIN FILM DIFFRACTION H. Wulff, C. Eggs* E.-M.-A.-University, Institute of Physical Chemistry, 17489 Greifswald, Germany* E.-M.-A.-University, Department of Physics, 17489 Greifswald, Germany.

Thin TiN films were deposited using a Hollow Cathode Arc Evaporation Device (HCAED) for studying the influence of low energy ion bombardment on film growth and film properties. Films were deposited at various nitrogen gas flows and negative substrate voltages at a defined discharge power, and investigated by thin film x-ray diffraction and x-ray photoelectron spectroscopy.

From the broadening and shifting of x-ray lineprofiles the dislocation densities and the concentration of interstitials in the films were calculated. With the energies of individual dislocations and interstitials a calculation was made of the energy stored in the films caused by low energy ion bombardment. The results were compared with investigations of the energy transfer to the substrate during titanium respective titaniumnitride deposition in HCAED [1].

[1] H.Steffen, H. Kersten, H.Wulff, J.Vac.Sci.Technol. A 12 (1994) 2780

PS12.01.12 THE INTERFACIAL STRUCTURE AND THE PREFERRED ORIENTATION OF LAYERED PEROVSKITE SrBi$_2$Ta$_2$O$_9$ THIN FILMS GROWN ON THE Pt ELECTRODE. Jeong Soo Lee*, Hyun Ha Kim*, Hyun Ja Kwon*, Seshu B. Desu#, *LG Electronics Research Center, 16, Woomyeon-dong, Seocho-gu, Seoul 137-140, Korea, #Department of Materials Science and Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061-0237, USA

The influence of the Pt bottom electrode orientation on the growth of ferroelectric SrBi$_2$Ta$_2$O$_9$ (SBT) films was interpreted in terms of the atomic matching at the interfaces. The symmetry of SBT can be described as either an orthorhombic (SBT$_{orth}$) or a pseudo-tetragonal (SBT$_{tet}$) structure. The preferred orientations of the SBT layers were determined by comparing the experimentally observed x-ray $\theta-2\theta$ diffraction profiles with the simulated powder diffraction one. A highly (00l) prefer oriented SBT$_{tet}$ film was grown when the Pt layer was mainly (001) oriented. There are three kinds of SBT$_{tet}$ (00l) plane with different atomic configurations. All these atomic planes match pretty well with the Pt (001) plane both energetically and crystallographically if the following orientation relationship is satisfied; Pt (001) // SBT$_{tet}$ (00l) // SBT$_{orth}$ (00l), Pt [100] // SBT$_{tet}$ [100] // SBT$_{orth}$ [110], and Pt [010] // SBT$_{tet}$ [010] // SBT$_{orth}$ [$\bar{1}$10] The mismatches in the [100] and [010] directions of the SBT$_{tet}$ are quite small (-0.74%). The (110) and (105) SBT$_{tet}$ peaks were predominantly found when the Pt electrode was (111) oriented. It was calculated that the Pt (111) plane exhibits a relatively good matching with either one of the two kinds of SBT$_{tet}$ (110) plane or the SBT$_{tet}$ (105) plane. The following orientation relationships are proposed; i) Pt (111) // SBT$_{tet}$ (110) // SBT$_{orth}$ (010), Pt [$1\bar{1}0$] // SBT$_{tet}$ [$\bar{1}$10] // SBT$_{orth}$ [100], and Pt [112] // SBT$_{tet}$ [$00\bar{1}$] // SBT$_{orth}$ [$00\bar{1}$], ii) Pt (111) // SBT$_{tet}$ (105) // SBT$_{orth}$ (1l5), Pt [$\bar{1}$10] // SBT$_{tet}$ [010] // SBT$_{orth}$ [$\bar{1}$10], and Pt [112] // SBT$_{tet}$ [$50\bar{1}$] // SBT$_{orth}$ [$55\bar{1}$].

PS12.01.13 CORRELATION BETWEEN SURFACE AND VOLUME: A METHOD OF THE CRYSTAL HABITUS DESCRIPTION A. M. Ivanov and Yu. M. Smirnov *Tver State University, 170000 Tver, Russia*

The habitus and morphology of crystals are subject to considerable changes by the melt supercooling. In [1] we described a method enabling the analysis of the volume and surface changes during the crystal growth. The method is based on the comparison of the flux densities of extensive quantities. These quantities are presented by surface (area) A and volume V.

The main equation is
$$\frac{J_A}{J_V} = \frac{\Delta A}{\left(\Delta V\right)^{2/3}\left(\Delta \overline{V}\right)^{1/3}} ,$$

where J_A, J_V are the flux densities, ΔA, ΔV are the changes of A and V at the interval of time, and ΔV is the averaged volume of the crystal.
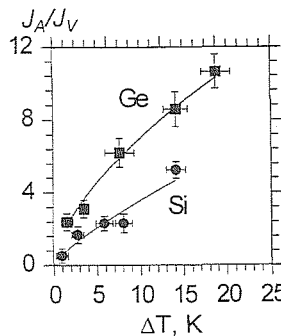
Shown in the figure is the dependence of the defined parameter on the melt supercooling ΔT for germanium (Ge) and silicon (Si). The J_A/J_V increases with supercooling and morphology in the following order: antiskeleton - face form - skeleton - dendrite.

This method was applied to the study of ceramics [2] prepared from natural raw materials. The samples were interpreted as conglomerates