Quantitative HRTEM analysis of rare earth hexaaluminate films on sapphire substrates

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In this contribution interfaces of sapphire and artificially grown hexaaluminates are analyzed with advanced methods of HRTEM. Rare earth hexaaluminates are of increasing interest for their luminescence properties, their application as laser matrix and structure characteristics. In our study, highly-oriented heteroepitaxial rare earth hexaaluminate films (LnHA) and rare earth magnesium hexaaluminate films (LnMHA) have been grown on single crystal sapphire substrates via chemical solution deposition.

Images have been recorded in a Philips CM 300 FEG-UT at the University of Bonn, and in a C_S-corrected FEI Titan T at the Ernst Ruska-Centre in Jülich. C_S-corrected electron microscopy is an ideal method for studying such interfaces, due to the reduced effect of delocalization [1]. As an auxiliary method exit-plane wave reconstruction from a focal-series has been applied. This is based on a combination of parabolic and maximum likelihood (PAMMAL) algorithm [2].

For further data analysis the software package *EWACS* (***E**lectron **WA**ve **C**omparison **S**uite*) is used. This program is based on semi-automated multi-slice simulations and comparison with experimental data. It has now been extended by the super-cell editor module *CrystalMan* which offers an intuitive and precise method for setting up interface structure models and defining a structure refinement process. The graphical user interface is shown in Fig.1 on the left. For the materials studied a possible refinement parameter is the translation vector that describes the relative position of the hexaaluminate film and the sapphire substrate. Here two possible interface types are expected as shown in Fig. 1 on the right.

A further interesting aspect of LnMHA with respect to LnHA is the appearance of reduced site occupancy factors (S.O.F.) of oxygen atom positions marked in Fig. 1b. This is due to the substitution of Al^{3+} ions by Mg^{2+} ions [3] in LnMHA. In the micrograph in Fig. 2 an experimental bright field image with negative C_S of a neodymium magnesium hexaaluminate film on sapphire is shown. The insets are simulated images with varying oxygen S.O.F. As a result the expected reduced site occupancy of oxygen is observed. The orientation relationship between substrate and film is $(0001)_{HA} \| (0001)_S$ and $[2\bar{1}\bar{1}0]_{HA} \| [1\bar{1}00]_S$, similar to lanthanum hexaaluminate as reported in [4].

Beneath these major points of interest the so-called geometrical parameters are determined simultaneously, i.e. the specimen tilt $\tau = (\tau_x, \tau_y)$ specimen thickness t. This is essential since these parameters have strong influence on HRTEM data, i.e. the intensity distribution experimental and simulated images, especially at ultra high-resolution.

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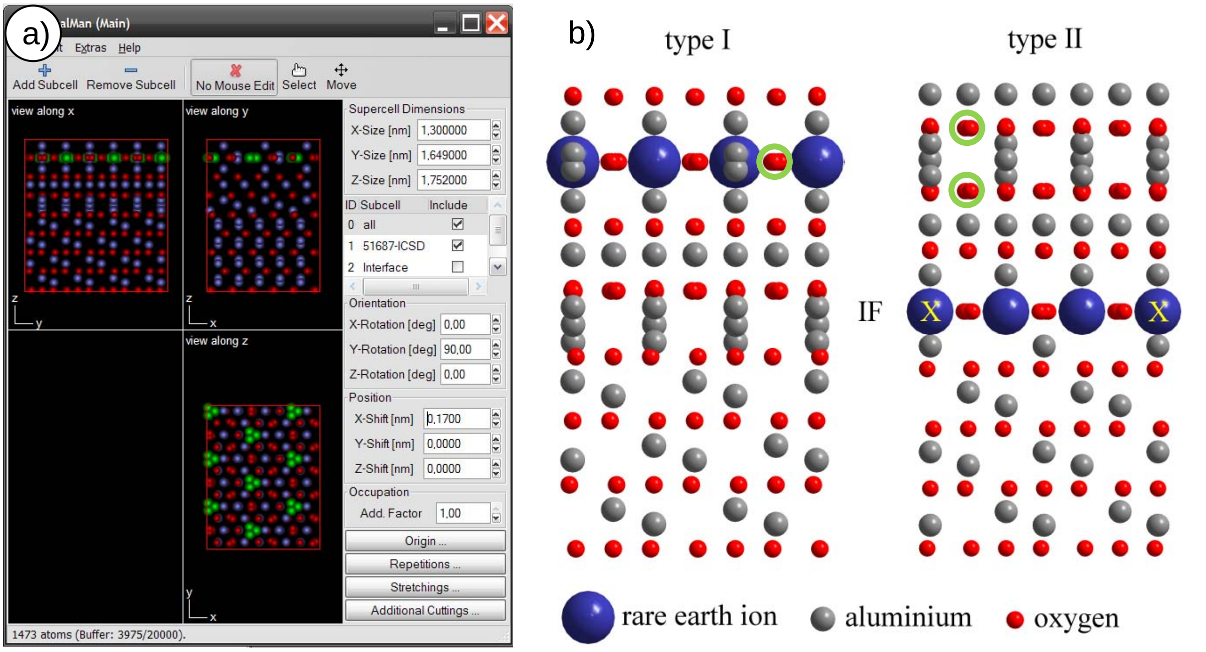

Figure 1. (a) The *CrystalMan* module of the *EWACS* package. (b) Two possible interfaces (IF) types for the rare earth magnesium hexaaluminate (HA) films on sapphire (S) are shown on the right side. The X mark expected rare earth ion vacancies for the corresponding atom column. The green circles mark that type of oxygen position which is supposed to have reduced site occupancy.

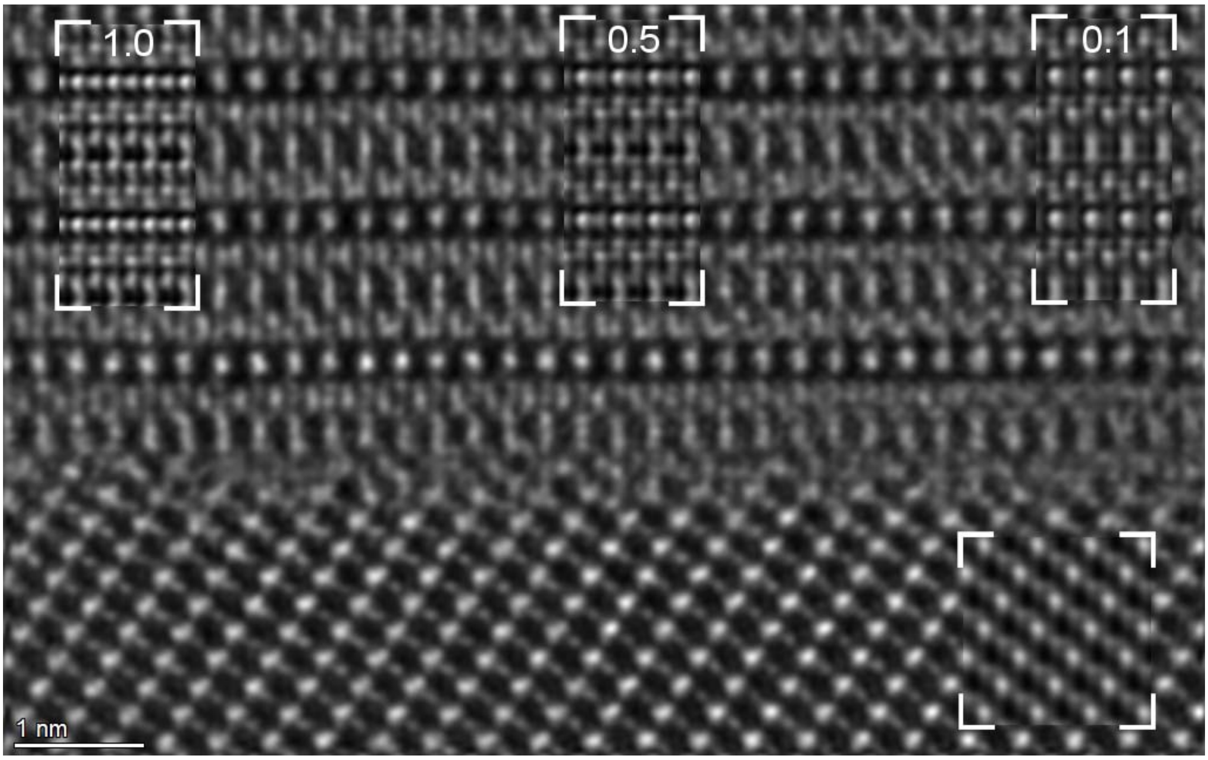

Figure 2. Bright field image of a hexaaluminate film in $[1\bar{1}00]_{HA}$: Neodymium magnesium hexaaluminate on sapphire recorded in a C_S-corrected FEI Titan T. The insets show simulated images near optimum defocus condition. The simulation includes a specimen tilt of τ = (-0.7°, 0.3°), specimen thickness t is ca. 6 nm. Numbers 1.0, 0.5 and 0.1 are S.O.F. of oxygen positions marked in Fig. 1b.

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