Poster

In-situ characterization of the epitaxial growth of BaTiO₃ thin films by pulsed laser deposition using synchrotron radiation

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Thin films of perovskites such as BaTiO₃ show different, exceptional behaviour compared to their bulk counterparts [1-5]. The understanding of property changes during the growth process itself is highly desirable. Here we focus on the *in-situ* characterization of BaTiO₃ thin films during the epitaxial growth by pulsed laser deposition (PLD) on different substrates. SrTiO₃, LaAlO₃ and MgO with a (0 0 1) crystal surface and GdScO₃ with a (1 1 0) crystal surface were used as substrate materials. *In-situ* X-ray diffraction (XRD) measurements were carried out using synchrotron radiation, in order to elucidate the growth process of BaTiO₃ thin films. In addition, the XRD experiments were simulated based on kinematic diffraction theory. The simulation results and the generated reciprocal space maps provide a deep insight into the crystal structure and the relaxation processes of BaTiO₃ thin films during the growth process. X-ray reflectometry measurements verify the results of the XRD measurements. The determined critical thickness of BaTiO₃ on a SrTiO₃ substrate is 65 Å. The critical thicknesses of BaTiO₃ on the LaAlO₃ and MgO substrates were estimated to be less than 16 Å and 36 Å, respectively. The critical thickness was found to be greater than 830 Å for the GdScO₃ substrate. A rich phase behaviour of BaTiO₃ thin films is observed, that differs strongly from that of bulk BaTiO₃.



Figure 1. XRD pattern of thin BaTiO₃ films deposited on a SrTiO₃ substrate. The diffraction intensity is shown as a function of the scattering vector (in units of the reciprocal lattice of SrTiO₃). With each growth step (GS) of the PLD process, the film reflections become more intense and sharper and thus characterise the growing BaTiO₃ film. The change in the position of the film reflections indicates ongoing relaxation.

- [1] Everhardt, A. S., Denneulin, T., Grünebohm, A. et al. (2020). Appl. Phys. Rev., 7, 011402.
- [2] Liu, R., Ulbrandt, J.G., Hsing, HC. et al. (2020). Nat. Commun., 11, 2630.
- [3] Guo, R., Shen, L., Wang, H. et al. (2016). Adv. Mater. Interfaces, 3, 1600737.
- [4] Sun, Z., Bai, Y., Liu, Ji. et al. (2022). J. Alloys Compd., 909, 164735.
- [5] Johnsson, M. & Lemmens, P. (2008). J. Phys.: Condens. Matter, 20, 264001.

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