

Topic for a Master Thesis, Forschungszentrum Juelich

„Atomic arrangement in ultra-thin MBE grown $\text{Ge}_1\text{Sb}_2\text{Te}_4$ films using LEED-IV“

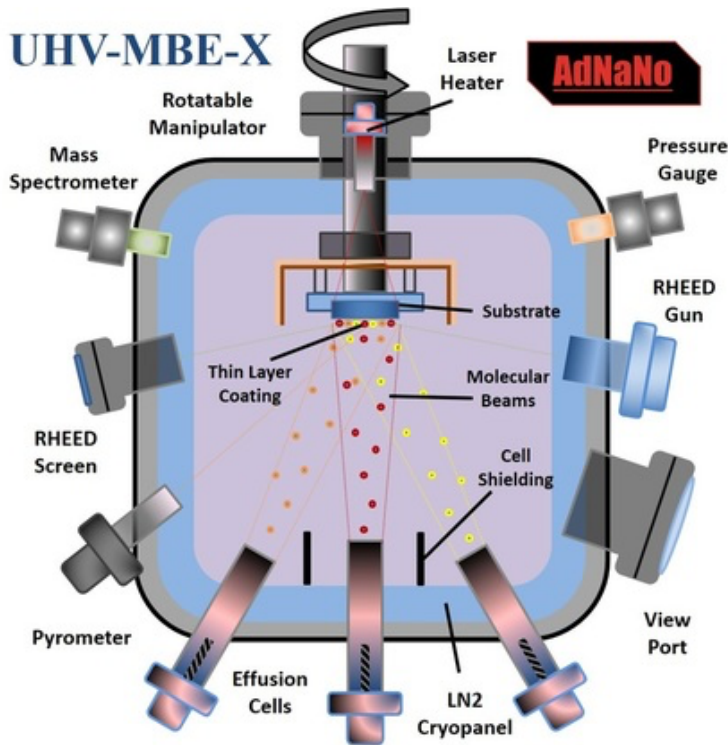


Fig. 1: MBE Setup in the NanoCluster, FZ Juelich

Phase Change Materials (PCMs) that incorporate Metavalent Bonding (MVB)^[2], a newly proposed type of chemical bonding that is characterized by a competition between electron localization and delocalization, often change their atomic arrangement when confined to thin films^[2,3]. It has been shown that the atomic arrangement in binary compounds like Sb_2Te_3 ^[2] and GeTe ^[3] is altered upon decreasing the film thickness, accompanied by an increased degree of electron localization and property changes. Studies of such effects in ternary compounds like $\text{Ge}_x\text{Sb}_y\text{Te}_z$ (GST-XYZ) are only rarely reported and structural data for such chalcogenides with various stoichiometries like GST-124 is desired. Such studies usually rely on X-Ray-Diffraction (XRD) to determine out of plane lattice parameters. However, XRD lacks accuracy, if the film thickness is decreased under a certain limit. Further, the determination of the atomic arrangement within the unit cell can not be done with XRD. Low Energy Electron Diffraction (LEED) Intensity vs. Electron Energy (LEED-IE) curves on the

other hand can obtain the atomic arrangement for thicknesses in the range of single unit cells, e.g., in the case of Sb_2Te_3 for thicknesses of single quintuples (5 atoms). Such films of excellent quality can be grown by Molecular Beam Epitaxy (MBE).

The aim of this thesis is the optimization of the MBE growth process for GST-124 and subsequent determination of the atomic arrangement using LEED-IE. For the former, techniques like RHEED, LEED, XRD, XRR, SEM and AFM can be used. A proper introduction for these techniques will be given by the staff of the FZ Juelich, so that measurement and analysis can be done by the student independently. The substrate preparation will be done by the student in the Clean Room of the Helmholtz Nano Facility.

After optimizing the growth conditions, films with decreasing thickness will be grown and (i) RHEED and (ii) XRD will be used to determine (i) in plane and (ii) out of plane structural changes of the unit cell. Last, the atomic arrangement of ultra thin GST-124 films will be determined using the fully dynamical LEED-IE^[1] Viperleed package. Proper assistance to the LEED-IE measurements and analysis will be given by the direct supervisor.

Note, that the everyday lab work will be done in the Forschungszentrum Juelich. A direct public transport connection between Aachen and the FZ can be used with the Deutschland Ticket. The second half of the thesis time period is paid according to the FZ Juelich regularities. Experience with ultra high vacuum and/or the stated techniques is preferred, but not necessary.

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[1] Viperleed package I, Florian Kraushofer et al., <https://doi.org/10.48550/arXiv.2406.18821>

[2] Confinement-Induced Phonon Softening and Hardening in Sb_2Te_3 Thin Films, Peter Kerres, <https://doi.org/10.1002/adfm.202307681>

[3] Scaling and Confinement in Ultrathin Chalcogenide Films as Exemplified by GeTe , Peter Kerres, <https://doi.org/10.1002/sml.202201753>