Effect of Post-Growth Cooling Conditions on Defect Structures in PVT Grown CdTe

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Introduction: During single crystal growth of compound semiconductor materials, it is very important to be able to precisely control the growth conditions in order not to introduce structural defects such as twins, dislocations, precipitates, inclusions, etc. Additionally, once the single crystal is solidified, it is necessary to cool the crystal down slow enough so as not to introduce thermal gradient stresses that could generate additional defects. In this work, crystals of CdTe grown by a 'contactless' PVT method were subjected to various post-growth cooling methods and their defect structures characterized by Synchrotron White Beam X-ray Topography (SWBXT).

Methods and Materials: CdTe crystals were grown by 'contactless' Physical Vapor Transport using Low Supersaturation Nucleation technique [1,2]. After growth, the ampoules were cooled down to room temperature at different rates using different methods:

G20 – Ampoule taken out of the furnace and allowed to cool in the air

G21 – Power to the furnace was switched off and the ampoule temperature dropped to 100°C in a 3 hour period

G22 – Ampoule pulled from the furnace and dipped in a bucket of cold water

G23 – Cool down at a constant rate of 10°C/hour

G24 – Cool down at a constant rate of 100°C/hour (wall contact occurred after about half the crystal was grown)

Growth rates vary in the following order: G22>G20>G24>G21>G23.

Wafers sliced from the boules were polished and imaged by SWBXT [3] in reflection geometry.

Results: Most samples are composed of one large grain and one or more smaller grains. The water-quenched sample G22 (Figure 1) exhibits a heavily twinned structure with a high density of dislocations (>10^6/cm^2) distributed in a dense subgrain network and severe peripheral distortion caused by strains. Sample G24 also contains a network of larger subgrains indicating a relatively lower density of dislocations (~10^5/cm^2). Air-cooled sample G20 exhibits a multiple twinned structure with a dense subgrain network of dislocations. Some distortion and deformation in the form of slip bands is observed in the peripheral regions. Furnace-cooled sample G21 also exhibits some deformation and strains in the periphery but the interior sections are characterized by a relatively low density of uniformly distributed dislocations. Slowest cooled sample G23 is composed of at least three twinned grains. While dislocation distribution is uneven with high densities in a subgrain network in the periphery and low densities uniformly distributed in the interior, overall dislocation density is the lowest among all the samples (~10^4-10^5/cm^2). In some regions, individual dislocations can be clearly resolved (Figure 2).

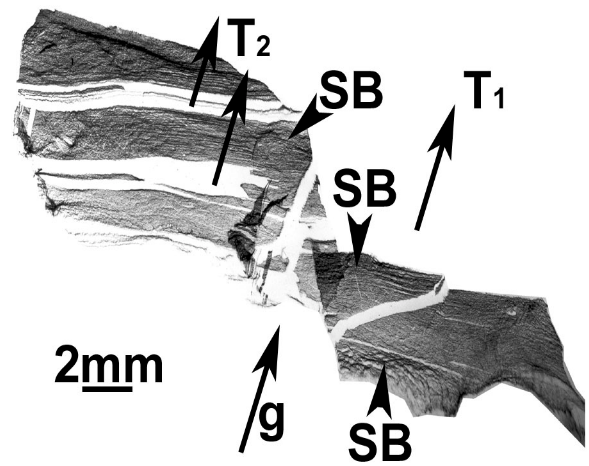

Figure 1. Reflection topograph from G-22 showing a high density of dislocations (>10^6/cm^2).(SB - subgrain boundaries, T - twins)

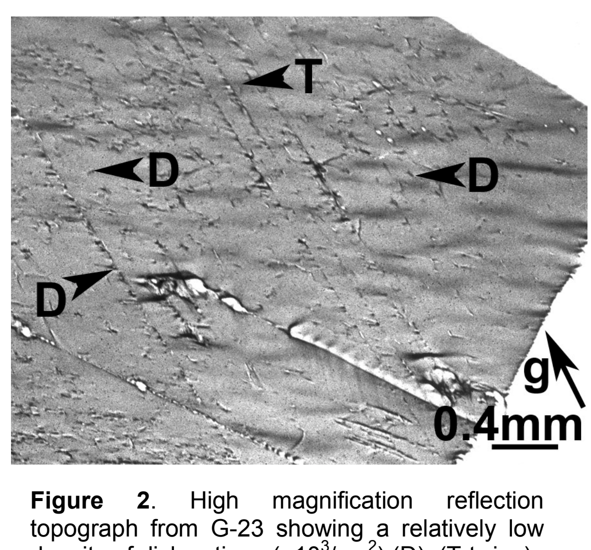

Figure 2. High magnification reflection topograph from G-23 showing a relatively low density of dislocations (~10^3/cm^2) (D). (T-twins)

Conclusions: Defect densities vary in the following order: G22>G20~G24>G21>G23. Clearly, the cooling rate has a strong influence on the overall defect content in CdTe single crystals. Thermal gradient stresses induced by higher cooling rates cause deformation leading to increase in dislocation densities.

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References: [1] W. Palosz, K. Grasza, D. Gillies, G. Jerman, J. Crystal Growth **169**, *20* (1996); [2] W. Palosz, M.A. George, E.E. Collins, K.-T. Chen, Y. Zhang, Z. Hu, A. Burger, J. Crystal Growth **174**, *733* (1997); [3] M. Dudley, Encyclopedia of Advanced Materials, **4**, *2950* (1994).