

THIN-FILM GROWTH DYNAMICS AND MICROSTRUCTURE OF Cd-DOPED LEAD TELLURIDE ALLOYS

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Thin films based on $\text{Pb}_{0.9}\text{Cd}_{0.1}\text{Te}:\text{Pb}$ (3 at.%) alloys were fabricated using the physical vapor deposition (PVD) technique onto mica-muscovite substrates. The research focused on the correlation between deposition parameters, film thickness, microstructure, and defect dynamics. Particular attention was paid to the morphological evolution of grains and the mechanisms governing the nucleation and growth of crystalline phases in systems with significant lattice mismatch.

Experimental observations using scanning electron microscopy (SEM) demonstrated that all deposited films exhibit granular surface structures with grains ranging from tens to several micrometers in size. Interestingly, the average grain size inversely correlates with film thickness. For example, the thinnest films (~270 nm) exhibited the largest grains (up to 70 μm), while thicker films (~400 nm) formed more homogeneous but finer grains (~20 – 25 μm). This grain size distribution is linked to stress-induced fragmentation processes occurring during film condensation and solidification.

The observed growth mode aligns with the Volmer-Weber (VW) mechanism, which typically arises in systems characterized by a substantial lattice mismatch. In this case, the mismatch between the lattice parameters of $\text{Pb}_{0.9}\text{Cd}_{0.1}\text{Te}:\text{Pb}$ ($a \approx 0.643$ nm) and mica ($a \approx 0.518$ nm) was estimated at approximately 19%, favoring three-dimensional island growth rather than layer-by-layer epitaxy. This was further supported by experimental identification of nucleation centers and boundary structures, indicating independent island formation.

Microstructural irregularities such as compositional inhomogeneities and distinct faceted formations were detected by SEM and energy-dispersive X-ray spectroscopy (EDS). Local phase separations revealed regions highly enriched with cadmium or lead, suggesting partial decomposition of the solid solution or cadmium segregation during cooling. These secondary phases potentially alter local conductivity and thermoelectric behavior, which is critical for device integration.

From a theoretical perspective, density functional theory (DFT) simulations were employed to analyze atomic configurations and energetics of $\text{Pb}_{1-x}\text{Cd}_x\text{Te}$ ($x = 0.07 - 0.08$) solid solutions. Calculations showed that cadmium atoms prefer three-coordinated positions within the PbTe lattice, as this configuration minimizes the system's total energy. Substitution of lead atoms by cadmium reduces the lattice constant and introduces local strain, which contributes to the fragmentation of grains during growth. Furthermore, surface positioning of Cd was less energetically favorable, indicating a tendency for Cd to diffuse into the film interior during annealing.

Additionally, SEM images showed evidence of layer-by-layer overgrowth in certain regions, suggesting localized van der Waals epitaxy. These regions were characterized by well-formed terraces and step-like morphologies, particularly at lower deposition thicknesses. This duality in growth behavior indicates a complex interplay between lateral surface energy minimization and vertical stress relaxation mechanisms.

1. Kostyuk O, Dzundza B, Yavorsky Y and Dashevsky Z 2021 *Physics and Chemistry of Solid State* 22, 45.
2. Ilchuk H, Nykyrui L, Kashuba A, Semkiv I, Solovyov M, Naidych B, Kordan V, Deva L, Karkulovska M and Petrus R 2022 *Physics and Chemistry of Solid State* 23, 261.