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A diffuse scattering in a single crystal of Cd0.9Zn0.1Te

Semiconductors with composition A1−xBxC find widespread applications in solid-state devices due to their tunable bandgap. Cd0.9Zn0.1Te is a very attractive ternary semiconductor material for x-ray and gamma-ray detectors. Single-crystal diffuse scattering provides very detailed information about the local structure. We have measured diffuse scattering in a single crystal of Cd0.9Zn0.1Te using a state-of-the-art laboratory diffractometer. Cd0.9Zn0.1Te single crystals were grown by the vertical Bridgman method in graphitized quartz ampoules from stoichiometric charges of high-purity (6 N) source components. A small amount of In (~1017 at/cm3) was added to the charge. As a result, the Cd0.9Zn0.1Te single-crystal ingot with a diameter of 20 mm and a length of 60 mm was obtained. A large-box atomistic simulation of a model crystal is used in conjunction with Monte Carlo modeling and the Kirkwood potential. A combination of structural relaxation in the presence of the dopant and thermal motion results in good qualitative agreement between the computed diffraction patterns of the model crystal and the measured x-ray patterns. The atoms are shown to displace predominantly in ⟨1,1,1⟩ and ⟨1,0,0⟩ type directions. So, we show that state-of-the-art laboratory equipment allows to record single-crystal diffuse scattering in addition to the Bragg peaks, making this technique accessible in a laboratory setting.

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