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Excitonic and electronic transitions in Me–Sb_2Se_3 structures

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Full Research Paper

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Abstract

The optical anisotropy of the Sb_2Se_3 crystals was investigated at 300 and 11 K. Excitonic features of four excitons (A, B, C, and D) were observed in the optical spectra of the Sb_2Se_3 single crystals and in the photoelectric spectra of the Me–Sb_2Se_3 structures. The exciton parameters, such as the ground (n = 1) and excited (n = 2) state positions and the binding energy (Ry), were determined. The effective mass of the electrons at the bottom of the conduction band (m_c* = 0.67m_0) as well as the holes at the four top valence bands (m_{v1}* = 3.32m_0, m_{v2}* = 3.83m_0, m_{v3}* = 3.23m_0 and m_{v4}* = 3.23m_0) were calculated in the Γ-point of the Brillouin zone. The magnitude of the valence band splitting V_1–V_2 due to the spin–orbit interaction (Δ_{so} = 35 meV) and the crystal field (Δ_{cf} = 13 meV) were estimated in the Brillouin zone center. The energy splitting between the bands V_3–V_4 was 191 meV. The identified features were discussed based on both the theoretically calculated energy band structure and the excitonic band symmetry in the Brillouin zone (k = 0) for crystals with an orthorhombic symmetry (*Pnma*). The photoelectric properties of the Me–Sb_2S_3 structures were investigated in the spectral range 1–1.8 eV under E||c and E⊥c polarization conditions and at different applied voltages.

Introduction

Antimony selenide (Sb_2Se_3) is an inorganic semiconductor compound with interesting photoelectric properties. This material has a high absorption coefficient (≈10^5 cm^{-1}) in the region of maximum solar energy radiation [1,2] which is corroborated by a 6.5% rapid increase in solar cell efficiency when Sb_2Se_3 is present [3-5]. Interestingly, this high absorption coefficient is 10^3 times higher than the absorption in silicon [5-7] and encompasses a wide portion of the spectrum ranging from 1.0 eV to 2–3 eV. The crystalline structure of Sb_2Se_3 is quite uniform and stable which minimizes the energy loss due to radiation [3,7,8]. In combination, the binary arrangement (Sb, Se), high crystalline stability, low toxicity and low deposition temperature (melting point ≈611 °C) reduce the production costs [3-10]. It has been shown that Sb_2Se_3 has many applications in photovoltaic devices and thermoelectric systems where it can be used as a thin film [11], in thermovoltaic and switch devices [12], in