Structure of extended defects in epitaxial $CuInS_2$/Si(111)

R. Hunger[a], D. S. Su[b,d], A. Krost[c], D. Ellmer[a], H. J. Lewerenz[a], R. Scheer[a]

a: Bereich Physikalische Chemie, Hahn -Meinter-Institut, Abt. CG, Glienicker Strae 100, D-14109 Berlin, Germany
b: Humbold-Universität zu Berlin, Institut für Physik, Kristallographie, Invalidenstraße 110, D-10115 Berlin, Germany
c: Otto-von-Guericke-Universität Magdeburg, Postfach 4120, D -39016 Magdeburg, Germany
d: Fritz-Haber-Institut der MPG, Faradayweg 4 -6, D-14195 Berlin, Germany

Abstract

$CuInS_2$ films grown epitaxially on Si (111) substrates exhibit a number of extended defects such as stacking faults, coherent and incoherent twin boundaries, and micro twins. These de fects are partly induced by the interface strain due to the lattice or thermal mismatch between Si and CuInS2. The appearance and density of the planar defects depend on film stoichiometry: in Cu -rich films, coherent twin boundaries form on (-1-1-2) surfaces but are absent on (-1-12). The density of incoherent twin boundaries and dislocation lines is small. Film growth appears to apply a step flow mechanism on [1-10] steps with the result of defect free regions laterally extending up to 1.3 µm. Incoherent twin boundaries and stacking faults are co ncentrated near the interface region. For cu -poor films, the density of stacking faults and dislocation lines on the /112) plane is much higher. Stacking fault and twin formation is also found on (-1-12) p lanes. The film volume free of planar defects is smaller. This difference between Cu -rich and Cu-poor CuIn2S films is discussed in relation to the different point defects induced by the stoichiometry deviation. A model for the formation of stacking faults is proposed.