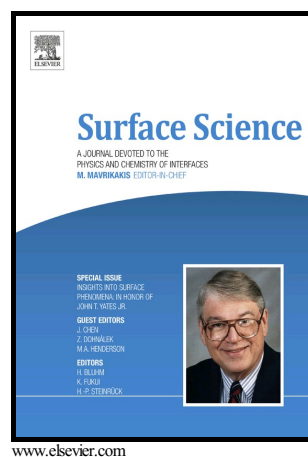


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Surface structure of bulk 2H-MoS₂(0001) and exfoliated suspended monolayer MoS₂: A selected area low energy electron diffraction study

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Abstract

We have used selected area low energy electron diffraction intensity-voltage (μ LEED-IV) analysis to investigate the surface structure of crystalline 2H molybdenum disulfide (MoS₂) and mechanically exfoliated and suspended monolayer MoS₂. Our results show that the surface structure of bulk 2H-MoS₂ is distinct from its bulk and that it has a slightly smaller surface relaxation at 320 K than previously reported at 95 K (Van Hove et al., 1977). We concluded that suspended monolayer MoS₂ shows a large interlayer relaxation compared to the MoS₂ sandwich layer terminating the bulk surface. The Debye temperature of MoS₂ was concluded to be about 600 K, which agrees with a previous theoretical study (Su et al., 2015). Our work has shown that the dynamical μ LEED-IV analysis performed with a low energy electron microscope (LEEM) is a powerful technique for determination of the local atomic structures of currently extensively studied two-dimensional (2-D) materials.

Keywords: MoS₂, μ LEED-IV, 2-D material, surface structure

1. Introduction

Molybdenum disulfide (MoS₂), a layered transition metal dichalcogenide, is an indirect-gap semiconductor with an optical band gap matching well with the solar spectrum [1]. Due to this important property, it may be used for electrodes in high efficiency photoelectrochemical (PEC) cells [2]. MoS₂ has three common polytypes: 1T-MoS₂, 2H-MoS₂ and 3R-MoS₂. The 2H-MoS₂ polytype is the most stable configuration [3]. The present study investigates 2H-MoS₂; its crystal structure is shown in Fig. 1. MoS₂ consists of covalently

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