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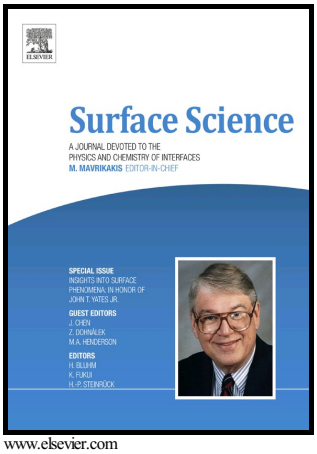

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Surface structure of bulk 2H-MoS_2(0001) and exfoliated suspended monolayer MoS_2: A selected area low energy electron diffraction study

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Abstract

We have used selected area low energy electron diffraction intensity-voltage (μLEED-IV) analysis to investigate the surface structure of crystalline 2H molybdenum disulfide (MoS_2) and mechanically exfoliated and suspended monolayer MoS_2. Our results show that the surface structure of bulk 2H-MoS_2 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 MoS_2 shows a large interlayer relaxation compared to the MoS_2 sandwich layer terminating the bulk surface. The Debye temperature of MoS_2 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 μLEED-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: MoS_2, μLEED-IV, 2-D material, surface structure

1. Introduction

Molybdenum disulfide (MoS_2), 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]. MoS_2 has three common polytypes: 1T-MoS_2, 2H-MoS_2 and 3R-MoS_2. The 2H-MoS_2 polytype is the most stable configuration [3]. The present study investigates 2H-MoS_2; its crystal structure is shown in Fig. 1. MoS_2 consists of covalently

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