[MS36-03] Synthesis, Superstructure and Vacancy-Ordering in 2H-Cu0.52TaSe2

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Transition metal dichalcogenides MX2, (M = Ta, Nb, Ti, V, Mo; and X = S, Se, Te) are of interest due to their layer-type structural and electronic properties [1-3]. The transition metal (M) has trigonal prismatic or octahedral coordination by six chalcogen atoms. These MX6 groups are interconnected to form three-atom thick slabs of composition MX2. Interaction between atoms within a slab are mainly covalent. Slab to slab interactions are weak, and in general of Van der Waals type. Guest atoms or molecules (G) can be filled into the existing vacant sites between weekly bonded MX2 layers and form stoichiometric or non-stoichiometric intercalated compounds (GxMX2). 'x' varies from zero up-to a maximum filling of one. Depending upon the availability of sites, the intercalated atoms or molecules occupy either tetrahedral or octahedral sites within the Van der Waals gap. For non-stoichiometric intercalated compounds, superstructures may arise due to the vacancy ordering or ordering of intercalated atoms in the Van der Waals gap. 6R-CuxTa1+yS2 forms an eightfold (2a0 • 2b0 • 2c0) superstructure and average maximum filling of x+y = 0.375 of Cu and additional Ta are allowed over octahedral and tetrahedral sites in the Van der Waals gap [4]. 2H-Co0.33NbS2 forms a threefold (√3a0 • √3b0 • c0) superstructure and one-third of the octahedral sites occupied by cobalt ions in the Van der Waals gap [5]. Here, we present the synthesis of 2H-Cu0.52TaSe2 by iodine vapor transport method for the first time and discuss the formation of a fourfold superstructure (2a0 • 2b0 • c0) which arises due to the vacancy ordering of intercalated copper sites in the Van der Waals gaps.

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