

研究论文

H原子在W低指数面上的吸附位和吸附态

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摘要 应用原子和表面簇合物相互作用的5参数Morse势及由5参数Morse势组装推广的LEPS方法对H-W低指数表面吸附体系进行了研究, 并获得了全部临界点特性. 计算结果表明, 低覆盖度下, H原子优先吸附在W(100)面的内层吸附位二层桥位B', 获得156 meV的垂直振动频率, 随着覆盖度的增加, H原子稳定吸附在表层的五重洞位(二层顶位)、桥位及顶位. 内层吸附位的优先吸附, 对与其邻近的表面吸附位的临界点性质有一定影响. 在W(110)面上只存在三重洞位的稳定吸附态, 垂直振动频率为151 meV. 在W(111)面上存在三种稳定吸附态, 子表面吸附位H₁, 桥位B'和顶位T, 分别获得104, 200, 259 meV的垂直振动频率. 在低覆盖度下, H原子优先吸附在子表面吸附位H₁.

关键词 [H-W表面吸附体系](#) [内层吸附](#) [5-MP](#) [LEPS势](#)

分类号

Adsorption Sites and States for H Atom on W Low-index Surfaces

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Abstract The adsorption of H atom on W low index surfaces was investigated with the 5-parameter Morse potential (5-MP) and the extended LEPS (constructed by 5-MP). All critical characteristics of this system were obtained. The calculated results show that H atom preoccupies the twofold bridge site of the subsurface on the intact W(100) surface at low coverage, and obtains the perpendicular vibration frequency of 156 meV. The H-atom adsorption on bridge site, top site and fivefold hollow site (the top site on the second W layer) were observed at high coverage. The preoccupancy of the subsurface adsorption site affects the critical characteristics of the adsorption sites adjacent to the subsurface adsorption site. On (110) surface H atom occupies the three-fold hollow site and produces the vibration frequency of 151 meV. On (111) surface there exist three stable adsorption states, the subsurface adsorption site H₁, the bridge sites and top sites, with the eigenvibration of 104, 200 and 259 meV, respectively. H atom preoccupies the H₁ site at low coverage.

Key words [H-W surface adsorption system](#) [subsurface adsorption](#) [5-MP](#) [LEPS](#)

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