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Surface electronic structure of single-crystalline zirconium diboride thin films[1] Y. YAMADA-TAKAMURA, F. BUSSOLOTTI, A. FLEURENCE, S. BERA, R. FRIEDLEIN, JAIST — Single-crystalline thin films of zirconium diboride (ZrB_2) with a simple crystal structure consisting of alternating hexagonal close-packed Zr and honeycomb B layers have been epitaxially grown on Si(111) by chemical vapor epitaxy. Oxide layers formed upon exposure to air can be removed by heating in ultra-high vacuum resulting in oxide-free and atomically-flat surfaces making the ZrB_2 films ideal for the epitaxial growth of heterostructures in other setups. The electronic structure of the as obtained ZrB_2(0001)-(2×2) surface has been studied using angle-resolved ultraviolet photoelectron spectroscopy. Along the $\bar{\Gamma}\bar{M}$ direction two parabolic features in the vicinity of the Fermi level are clearly resolved. While the dispersion of these Zr-derived surface states is similar to those observed at (1x1) single crystal surfaces and calculated dispersion curves for a Zr-terminated slab model, a pronounced intensity change at the zone boundary is a strong indication of a back-folding of electronic bands into the reduced Brillouin zone. The origin of the (2×2) reconstruction is likely the presence of Si atoms on the surface. A flat band at 0.25 eV is accordingly assigned to localized Si-derived states

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