LEED and Ab-Initio Study of the SmSi(111)-3x2 Reconstruction

CHRISTOPHER EAMES, STEVE TEAR, MATTHEW PROBERT, Dept of Physics, University of York, UK — The Si(111)3x2-Sm reconstruction that has been observed by STM produces a 3x1 pattern when viewed using LEED [1]. It has been suggested that similar behaviour for Si(111)3x2-Ba is due to the interference of the emergent electron amplitudes between adjacent registry shifted unit cells [2]. We have gathered LEED I(V) curves from this surface and here we present a quantitative comparison of these with a structural model that has been suggested in the literature [3] and with the results of our own ab-initio calculations done using the CASTEP [4] code.