s4.m1.o5 **Short and long-range order at surfaces probed by surface X-ray diffuse scattering.** M. Sauvage-Simkin[a,b], Y. Garreau[a], K. Aïd[a], N. Jedrecy[a,b], R. Pinchaux[a], *a: LURE, BP 34 , F-91898 0rsay-cedex , France; b: Laboratoire de Minéralogie-Cristallographie, Case 115, 4 Place Jussieu, F-75252 Paris-cedex 05, France.*
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Surface Structure analysis using the standard methods of 3D crystallography (model fitting with least square refinements or even direct methods) is now a well established field of research. Accurate models have been obtained for a large variety of reconstructed surfaces and interfaces. A recent development is concerned with periodicity breaking. Such faulted surfaces and interfaces resulting in incommensurate reconstructions are observed for instance either when the surface composition is not compatible with the stoichiometry constraints of the commensurate unit cell or when the strain stored in the interface limits the range of the periodic arrangement to sequences of variable lengths. Surface diffuse scattering is then produced.

A first example dealing with the 2xn ($2.5<n<3.3$) reconstructed surfaces of $In_xGa_{1-x}As$ alloys strained on a GaAs(001) substrate will be presented It will be shown that the details of the continuous diffuse scattering distribution measured in the direction of the discommensuration (k reciprocal axis) can be reproduced by a probabilistic distribution of indium depleted or indium enriched faults, using the phase matrix method based on nearest neighbour constraints. This analysis provides a unique access to the surface composition and cation distribution which show little dependence on the nominal concentration x of the disordered bulk alloy and reflects the indium surface segregation trend.

A second example of aperiodic interface is observed in the case of the Bi/Si (001) system. A local 2x1 supercell is formed by Bi dimers linked to the silicon substrate but the amount of strain prevents this structure to extend over more than 5 to 7 bulk unit cells and requires the introduction of missing Bi dimer defects. Incommensurate 2xn ($5<n<7$) are thus observed. Applying the same phase matrix method, one is able to interprete the diffuse scattering data in terms of the leading interactions governing the missing dimer distribution.

Notes

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