Surface Structure of Stripe ordered 1x2 phase on (Ba, Ca)(Fe_{1-x}Co_x)_2As_2

GUORONG LI, VON BRAUN NASCIMENTO, XIAOBO HE, AMAR B. KARKI, RONGYING JIN, JIANDI ZHANG, WARD PLUMMER, Louisiana State University — Low energy electron diffraction (LEED) and scanning tunneling microscopy/spectroscopy (STM/S) have been utilized to investigate the geometric structure of the stripe 1x2 surface phase of (Ba, Ca)(Fe_{1-x}Co_x)_2As_2 iron pnictides. STM images show that the surface consists of competing ordered and disordered regions. The 1x2 phase appears on the surface of all compounds but coexist with (√2 x √2)R45° phase on the surface of Ba122. Quantitative structural analysis of LEED-I(V) using the fractional spots of the 1x2 phase on both parent compounds as well as Ca(Fe_{0.925}Co_{0.075})_2As_2 gives a similar surface structure with a termination layer of 50% Ca/Ba atoms. The surface Ca/Ba layer has a large inward relaxation ~ 0.5 Å and the underneath As-Fe-As layer displays a buckling distortion. The Pendry Rp factor (~ 0.24) obtained in the structural refinement is excellent for all three systems.

1Research is supported by NSF DMR-1002622

Guorong Li
Louisiana State University

Date submitted: 19 Dec 2011

Electronic form version 1.4