Direct Structure Determination of Epitaxially Grown Films

M. Sowwan,[1] Y. Yacoby,[1] J. Pitney,[2] R. MacHarrie,[2] M. Hong,[2] J. Cross,[3,4]
D. A. Walko,[5] R. Clarke,[6] R. Pindak,[7] E. A. Stern[4]
[1]Racah Institute of Physics, Hebrew University, Jerusalem, Israel
[2]Bell Laboratories, Lucent Technologies, Murray Hill, NJ, U.S.A.
[3]PNC-CAT, Advanced Photon Source, Argonne National Laboratory, Argonne, IL, U.S.A.
[4]Physics Department, University of Washington, Seattle, WA, U.S.A.
[5]MHATT-CAT, Advanced Photon Source, Argonne National Laboratory, Argonne, IL, U.S.A.
[6]NSF FOCUS Center, Department of Physics, University of Michigan, Ann Arbor, MI, U.S.A.
[7]National Synchrotron Light Source, Brookhaven National Laboratory, Upton, NY, U.S.A.

Introduction

Epitaxially grown films are physically exciting because their properties are often substantially different from the properties of the bulk materials, and they are important because of the role they play in various microelectronic and optoelectronic devices. Determination of their atomic structure, particularly close to the film substrate interface, is essential for understanding their properties. During the past few years, we have developed a new direct method [1] based on coherent Bragg rod analysis (COBRA) to determine their structure. In the last year, the method has been brought to fruition and applied to two systems: Gd_2O_3 grown on (1 0 0) GaAs and $BaTiO_3$ grown on (1 0 0) $SrTiO_3$.

Structure of Gd_2O_3 Grown on (1 0 0) GaAs

Gd_2O_3 has been shown to be a very effective passivation layer for GaAs, allowing the formation of high-quality field effect transistors in GaAs [2]. To determine the atomic structure of these films, we measured their x-ray diffraction along 13 symmetry-inequivalent substrate-defined Bragg rods. We then used COBRA to determine the complex scattering factors along the Bragg rods and Fourier-transformed the scattering factors into real space to obtain the electron density and structure of the system.

The results confirm the finding of Kortan et al. [3] that the film is a single domain and, in addition, show that the film substrate interface and the film surface have transition regions of about five Gd_2O_3 layers, probably resulting from interface and surface roughness. The results reveal two rather surprising features.

First, the stacking order of the layers in the film is different from the stacking order of the corresponding layers in bulk Gd_2O_3. In both Gd_2O_3 and GaAs, the structure repeats itself every four layers. Figure 1 shows the in-plane Gd positions in four consecutive Gd_2O_3 layers, along with the positions of Ga and As in four consecutive layers of the GaAs substrate. Notice that the relative positions of the Gd and Ga/As atoms remain approximately the same in all four layers. Second, the COBRA-determined electron density shows that the Gd atoms in the first three Gd_2O_3 layers in Rows 1, 2, 4, and 5 are displaced so that they overlap exactly the in-plane Ga/As positions. As the distance from the interface increases, the positions relax to the positions expected from bulk Gd_2O_3.

The way the Gd_2O_3 conforms to the GaAs structure may be at the bottom of the fact that this material forms an excellent passivation layer for GaAs.

Structure of $BaTiO_3$ Grown on (1 0 0) $SrTiO_3$

$SrTiO_3$ is an incipient ferroelectric, while $BaTiO_3$ is ferroelectric at room temperature. We have investigated the structure of epitaxially grown BaTiO3 on (1 0 0) $SrTiO_3$. The diffraction intensities were measured along the $SrTiO_3$ defined Bragg rods. Then we used COBRA to obtain the complex scattering factors along the Bragg rods. Fourier-transforming them yielded the 3-D electron density and atomic structure of the system. The results show that the vertical Ba-Ba distances are larger than in Bulk $BaTiO_3$; otherwise, almost all atoms are in centro-symmetric positions within the experimental accuracy of 0.1 Å. The exceptions are the oxygen atoms in the Sr and Ba planes parallel to the interface. Close to the interface on both $SrTiO_3$ and $BaTiO_3$ sides, the O atoms in the Sr and Ba planes are displaced by up to 0.3 Å. These displacements are shown in Fig. 2 as a function of layer number.

Acknowledgments

Y. Yacoby is grateful for the opportunity to spend a sabbatical year at the university of Washington. This project is supported by the US-Israel Bi-National Science Foundation (NSF) under Contract No. 1999-187. M. Sowwan is grateful for the Levy Eshkol Fellowship awarded him by the Israel Ministry of Science and Technology. Work at the University of Washington and

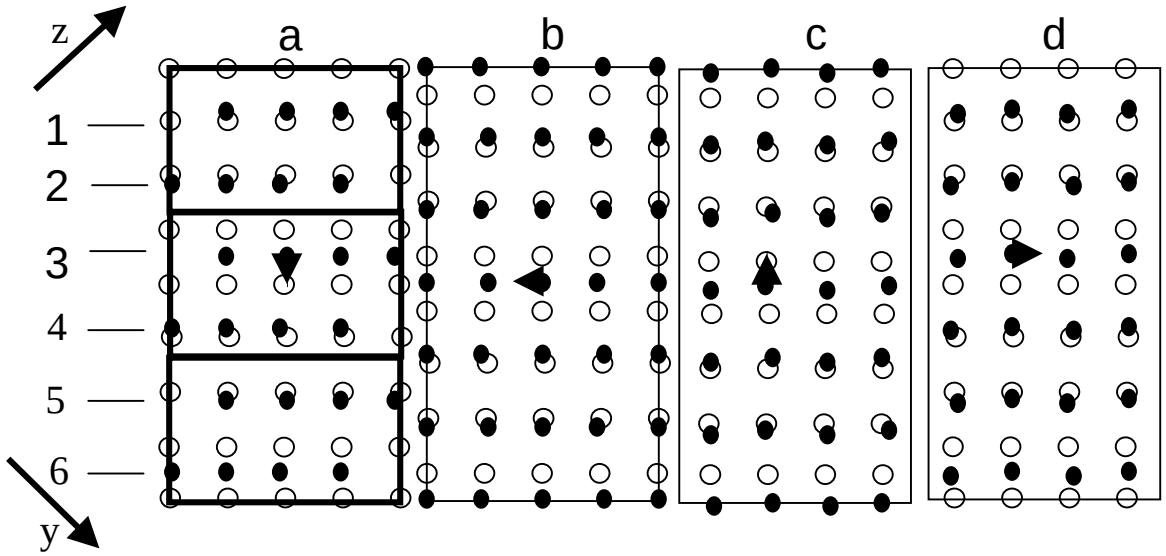

FIG. 1. Gd positions in four consecutive layers shown as dots. Notice that the positions in one layer can be approximately obtained from the positions in the previous layer by shifting them by the vector shown in that layer. (The last vector on the right shifts the positions from the last layer to the first.) The circles represent Ga and As positions in four consecutive layers of GaAs.

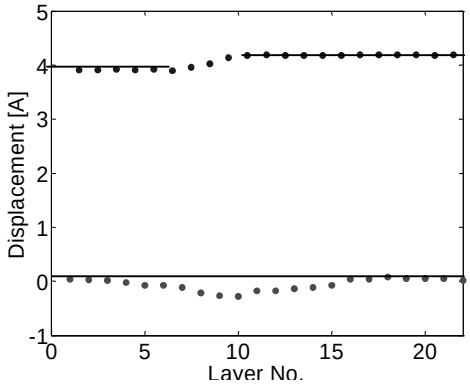

FIG. 2. Sr-Sr distances (left) and Ba-Ba distances (right) are indicated by blue dots. Vertical displacements of O atoms in the Sr and Ba planes are indicated by red dots. The lines are to guide the eye.

PNC-CAT was supported by U.S. Department of Energy (DOE) Grant Nos. DE-FG03-98ER45681 and DE-FG03-97ER45628. Work at MHATT-CAT was supported by DOE Grant No. FG02-99ER45743. Use of the APS was supported by the DOE Office of Science, Office of Basic Energy Sciences, under Contract No. W-31-109-ENG-38. R. Clarke acknowledges support from the NSF Frontiers of Physics Center, FOCUS.

References

[1] Y. Yacoby, R. Pindak, R. MacHarrie, L. Peiffer, L. Berman, and R. Clarke, J. Phys. Condensed Matter **12**, 3929 (2000).

[2] M. Hong, J. Kwo, A. R. Kortan, J. P. Mannaerts, and A. M. Sergent, Science 283, 1897 (1999).

[3] A. R. Kortan, M. Hong, J. Kwo, J. P. Mannaerts, and N. Kopylov, Phys. Rev. B **60**, 10913 (1999).