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In situ studies of metal–semiconductor interactions with synchrotron radiation

D. E. Sayers,[a]* P. T. Goeller,[b] B. I. Boyanov[a] and R. J. Nemanich[a]

[a]Department of Physics, North Carolina State University, Raleigh, NC 27695, USA, and [b]Department of Materials Science, North Carolina State University, Raleigh, NC 27695, USA. E-mail: sayers@pymvds.physics.ncsu.edu

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The capabilities and performance of a UHV system for *in situ* studies of metal–semiconductor interactions are described. The UHV system consists of interconnected deposition and analysis chambers, each of which is capable of maintaining a base pressure of approximately 1×10^{-10} torr. The deposited materials and their reaction products can be studied *in situ* with RHEED, XAFS, AES, XPS, UPS and ARUPS. Results from a study of the reaction of 0.7- and 1.7-monolayer-thick films of cobalt with strained silicon–germanium alloys are presented. The signal-to-noise ratio obtained in these experiments indicates that the apparatus is capable of supporting *in situ* EXAFS studies of ~0.1-monolayer-thick films.

Keywords: EXAFS; metal–semiconductor contacts; silicon–germanium alloys; molecular-beam epitaxy.

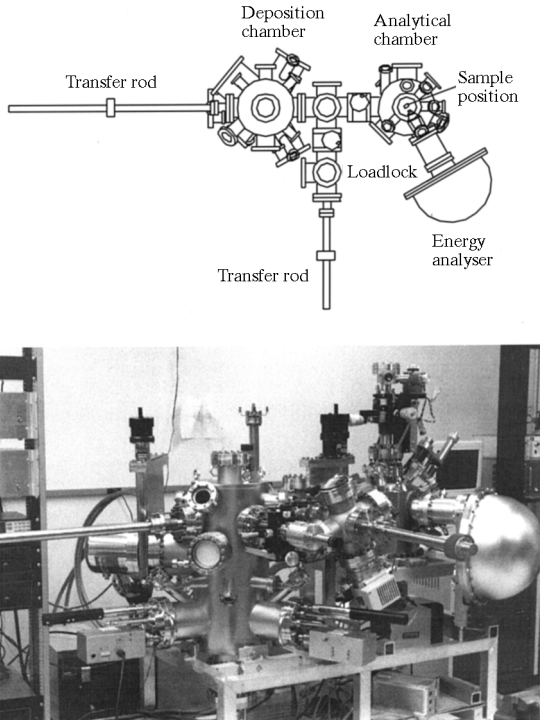

Figure 1
An overview of the experimental apparatus.

1. Introduction

The composition and structure of the interface between thick metal films (>500 Å) and various semiconductors have been studied extensively, but little is known about ultra-thin [1−10 monolayer (ML)] films. An understanding of the interface is essential for obtaining epitaxial growth, good contact morphology and uniform overlayer thickness. In order to facilitate the study of monolayer and sub-monolayer coverage of metals on semiconductors *in situ*, a UHV electron beam deposition system coupled with an analytical chamber has been developed and installed at beamline X-11A at the National Synchrotron Light Source.

2. Equipment

The system consists of interconnected growth and analytical chambers (Fig. 1). The entire system is assembled on an aluminium frame with wheels, which allows the equipment to be transported between beamlines at the NSLS. The growth chamber contains three single-pocket electron-beam evaporators, which provide the capability of depositing up to three materials simultaneously. The sample manipulator has five degrees of freedom. A heating stage mounted on the manipulator allows the sample to be heated from ambient temperature to 1473 K. Film growth can be monitored *in situ* with reflection high-energy electron diffraction (RHEED). The analytical chamber has the capabilities of AES, EXAFS, XPS and UPS. The sample manipulator in the analytical chamber is fully motorized, and also has five degrees of freedom: x, y, z translation, as well as polar

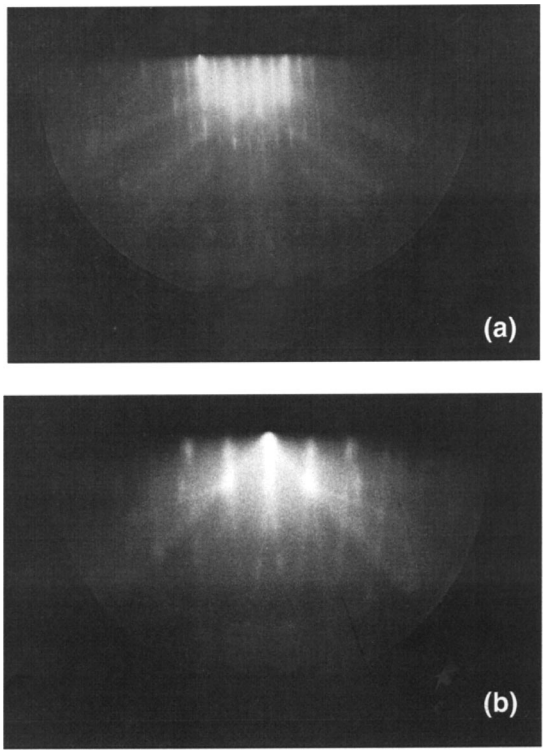

Figure 2
RHEED patterns: (*a*) 2×8 surface reconstruction of the $Si_{0.79}Ge_{0.21}$ substrate; (*b*) $3\sqrt{2} \times \sqrt{2}$ surface reconstruction of a 0.7 ML Co film annealed at 723 K. The electron beam azimuth is along the [110] and [100] directions of the Si(100) substrate, respectively.

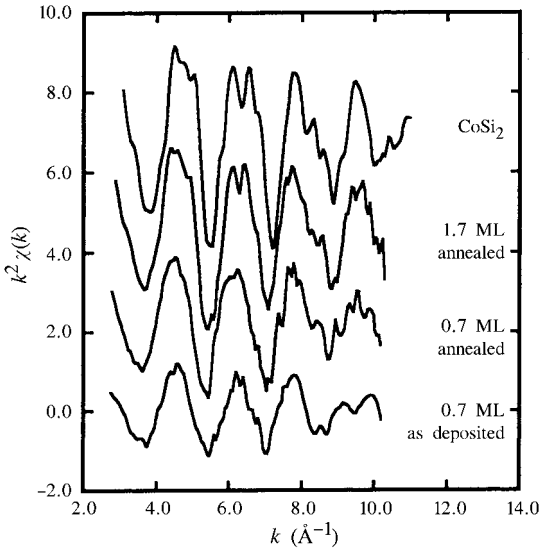

Figure 3
Normalized and k^2-weighted EXAFS data for the samples used in this study. The top trace represents the data for a 730 Å-thick $CoSi_2$/Si(100) film.

and azimuthal rotation for angle-resolved studies. The base pressure of both chambers is 1×10^{-10} torr.

3. Experimental

Metal films were deposited at room temperature on 800 Å-thick layers of strained epitaxial $Si_{0.79}Ge_{0.21}$ alloys grown at 823 K on *p*-type (boron-doped) Si(100) substrates. Cobalt coverage was confirmed *ex situ* with an estimated accuracy of ±0.2 ML with Rutherford backscattering. EXAFS data were collected *in situ* at the Co *K* edge (7709 eV) in total electron yield mode at beamline X-11A at the National Synchrotron Light Source (NSLS). Full details on the acquisition, processing and analysis procedures are given elsewhere (Boyanov *et al.*, 1997).

4. Results and discussion

The freshly prepared $Si_{0.79}Ge_{0.21}$ substrates exhibited a sharp 2×8 RHEED pattern. Immediately after Co deposition was initiated, a 2×1 RHEED pattern was observed, in agreement with results reported by other authors (Meyerheim *et al.*, 1991). After annealing for 10 min at 723 K, a $(3\sqrt{2} \times \sqrt{2})$ surface reconstruction identical to that reported by Stalder *et al.* (1992) was observed for both the 0.7 and 1.7 ML samples (Fig. 2). The corresponding EXAFS data are shown in Fig. 3. Data for a 730 Å-thick $CoSi_2$/Si(100) film are also included in this figure for comparison.

Analysis of the EXAFS data indicates that the first coordination shell of Co in the as-deposited 0.7 ML film consists exclusively of Si and Ge atoms in a 4:1 ratio, as would be expected from the stoichiometry of the $Si_{0.79}Ge_{0.21}$ substrate. The annealed 0.7 and 1.7 ML films have a $CoSi_2$-like structure. In both cases the first shell of Co consists predominantly of Si atoms, indicating a substantial preference for Co—Si bonding over Co—Ge bonding. Such preference for Co—Si bonding has significant implications for the control of misoriented grains in $CoSi_2$ films grown on SiGe substrates, which is discussed elsewhere (Boyanov *et al.*, 1997). The signal-to-noise ratio obtained in these experiments indicates that the apparatus is capable of supporting *in situ* EXAFS studies of ~0.1 ML-thick films, or equivalently, of heavy dopants at a concentration of $\sim 1 \times 10^{18}$ cm^{-3}.

5. Conclusions

The capabilities and performance of a UHV system for *in situ* studies of metal–semiconductor interactions have been described. Performance tests indicate that the apparatus is capable of supporting structural studies of the interaction of sub-monolayer metal films with semiconductor substrates. As the size of critical features in semiconductor devices continues to diminish, such studies are necessary in order to develop an understanding of the metal–semiconductor interface and the factors that contribute to obtaining good contact morphology, uniform overlayer thickness, and, in select cases, epitaxial growth.

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