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MICROSTRUCTURES AND ELECTRICAL PROPERTIES OF
SrRuO₃ THIN FILMS ON LaAlO₃ SUBSTRATES

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Author(s):

F. Chu - CMS
T. E. Mitchell - CMS
M. Hawley - CMS
G. Landrum - CMS
Q. X. Jia - STC
X. D. Wu - STC

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Microstructures and Electrical Properties of SrRuO₃ Thin Films on LaAlO₃ Substrates

F. Chu, Q. X. Jia, G. Landrum*, X. D. Wu, M. Hawley, and T. E. Mitchell
Materials Science and Technology Division, Los Alamos National
Laboratory, Los Alamos, NM 87545, U. S. A.

Abstract

Conductive oxide SrRuO₃ thin films have been deposited using pulsed laser deposition on LaAlO₃ substrates at different substrate temperatures. Structural and microstructural properties of the SrRuO₃/LaAlO₃ system have been studied using x-ray diffraction, scanning electron microscopy and scanning tunneling microscopy. Electrical properties of SrRuO₃ thin films have been measured. It was found that the film deposited at 250°C is amorphous-like, showing semiconductor-like temperature dependence of electrical conductivity. The film deposited at 425°C is crystalline with very fine grain size (100~200Å), showing both metallic and semiconductor-like temperature dependence of the electrical conductivity in different temperature regions. The film deposited at 775°C shows a resistivity of 280 μΩ.cm at room temperature and the residual resistivity ratio of 8.4. The optimized deposition conditions to grow SrRuO₃ thin films on LaAlO₃ substrates have been found. Possible engineering applications of SrRuO₃ thin films deposited at different temperatures are discussed. Bulk and surface electronic structures of SrRuO₃ are calculated using a semi-empirical valence electron linear combination of atomic orbitals approach. The theoretical calculation results are employed to understand the electrical properties of SrRuO₃ thin films.

*Present address: Department of Chemistry and Materials Science Center,
Cornell University, Ithaca, New York, 14853-1301, U. S. A.

Introduction

Conductive solids are very useful in electronic devices, serving as contacts, metallization, and interconnects. Except metals, some oxides are metallic, while most are insulating [1]. Among conductive oxides, SrRuO_3 , which crystallizes in perovskite structure with lattice parameters of $a=0.556$ nm, $b=0.555$ nm, and $c=0.786$ nm, has recently been found possible engineering applications in different fields. For example, the relatively high conductivity and structural compatibility of SrRuO_3 with ferroelectric or high dielectric constant materials make it promising as a bottom electrode for dynamic random memory capacitors [2-5]. In addition, highly thermal and chemical stabilities of SrRuO_3 make it attractive as a buffer layer for growth of high-temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ thin films on different substrates [6-7].

It has been observed experimentally that the electrical resistivity of bulk SrRuO_3 is a strong function of microstructure. Polycrystalline SrRuO_3 has a resistivity of $1130 \mu\Omega\cdot\text{cm}$ at room temperature [8] whereas single crystalline SrRuO_3 has a room temperature resistivity of $280 \mu\Omega\cdot\text{cm}$ [9]. SrRuO_3 thin films have been deposited using either off-axis sputtering or pulsed laser deposition on different substrates, e.g. SiTiO_3 [10], LaAlO_3 [3,6], MgO with Pt or BaTiO_3 [4,7] buffer layer, and Si with yttria stabilized zirconia (YSZ) as a buffer layer [5]. However, microstructural and electrical properties of these SrRuO_3 thin films have not been systematically studied. This investigation is crucial for SrRuO_3 thin films to be used as a bottom electrode in microelectronic devices, because the device performance is strongly related to the microstructure and electrical resistivity of the films.

It is our intent, in this paper, to study the relationship between the microstructures and electrical properties of SrRuO_3 thin films deposited on a specific substrate, LaAlO_3 , at different substrate temperatures. In Section 2, the experimental procedure and calculation method are described. The experimental results on microstructures and electrical properties and the calculation results are presented and discussed in Section 3. Conclusions are drawn in Section 4.

Experimental Procedures and Calculation Method

Pulsed laser deposition (PLD) with a XeCl excimer laser ($\lambda=3008\text{\AA}$) was used to deposit SrRuO_3 thin films on LaAlO_3 substrates. The SrRuO_3 target was prepared by mixing appropriate molar ratios of SrCO_3 and Ru metal powder, grinding, heating in air at $1200\text{ }^\circ\text{C}$ for 12 hours, regrinding and heating, and repressing into disks [6]. Single crystal (100) LaAlO_3 ($a=0.3793\text{ nm}$) wafers were employed as substrates. Before deposition, the substrates were cleaned in a sequence of acetone, methanol, and deionized water. In the deposition process, the *in situ* PLD operated at an energy density of 2 J/cm^2 and repetition rates of 10-20 Hz. The oxygen pressure was experimentally optimized and maintained at 200 mTorr during film deposition in order to keep the stoichiometry of the films. The deposition temperatures were varied from room temperature to $850\text{ }^\circ\text{C}$. The nominal film thickness was in the range of 100 - 1500 nm.

The structural properties of the SrRuO_3 thin films were characterized using a combination of x-ray diffraction (XRD), scanning electron microscopy (SEM), and scanning tunneling microscopy (STM). A Siemens D5000 four circle x-ray diffractometer with $\text{Cu K}\alpha$ radiation was employed to examine the crystallographic orientation and crystallinity of the thin films. A JEOL JSM-6300FXV field emission gun scanning electron microscope was used to study the surface morphology and microstructure of the thin films. A Nanoscope III STM was employed to measure the surface roughness of the thin films.

The electrical properties of the thin films were studied by measuring their electrical resistivity. The resistivity of the SrRuO_3 thin films was measured using a standard four-probe technique, in which the SrRuO_3 thin films were patterned by ion milling to form a bridge of $500\text{ }\mu\text{m}$ in width and 2.5-7.5 mm in length. Au contact pads were deposited on the patterned SrRuO_3 thin films by rf sputtering in vacuum.

The electronic structures of the bulk and surface of SrRuO_3 were calculated using the extended Hückel implementation of the tight-binding method. The extended Hückel theory is a semi-empirical valence electron Linear Combination of Atomic Orbitals (LCAO) approach [11]. The band

structure and the density of states of the bulk and thin film of SrRuO_3 were obtained, which can be used to understand the electrical conducting behavior of the systems. The details of the calculations will be published elsewhere [12].

Results and Discussion

1. *Structural Properties of SrRuO_3 Thin Films*

XRD pattern of θ - 2θ scan on the SrRuO_3 thin film deposited at 775°C on a LaAlO_3 substrate is shown in Fig. 1. Note that for SrRuO_3 , the lattice parameters satisfy $a \sim b$ and $a \sim b \sim c/\sqrt{2}$, so the (220) and (004) peaks may overlap. Therefore, Figure 1 shows that the SrRuO_3 thin film is **c-axis** or/**a+b-axis** oriented with respect to the substrate normal. The detailed crystallographic study using transmission electron microscopy for this feature of the system will be published elsewhere [13]. Figure 2 demonstrates the XRD ω -rocking curve of the (004)/(220) reflection of the SrRuO_3 thin film, showing that the full width at half maximum (FWHM) is about 0.72° . The very narrow ω -rocking curve suggests that the SrRuO_3 thin film deposited at 775°C is well **c-axis** or/**a+b-axis** oriented with respect to the substrate. The in-plane orientation of the SrRuO_3 film with respect to the (100) LaAlO_3 substrate is measured by XRD ϕ -scan on both the SrRuO_3 (404) and the LaAlO_3 (101) reflections. Figure 3 shows the typical XRD ϕ -scans on both the (404) reflection of the SrRuO_3 thin film deposited at 775°C and the (101) reflection of the LaAlO_3 substrate. It is reasonable to have the 45° rotation between the basal plane of SrRuO_3 and that of LaAlO_3 , as shown in Fig. 3, because the compatibility of the lattice parameters of the two systems: $a_{\text{SrRuO}_3} \sim a_{\text{LaAlO}_3}/\sqrt{2}$. The lattice mismatch is less than 4% with such a growth pattern [$\langle 001 \rangle_{\text{SrRuO}_3} // \langle 011 \rangle_{\text{LaAlO}_3}$ and $(001)_{\text{SrRuO}_3} // (100)_{\text{LaAlO}_3}$].

The effect of deposition temperature on the crystallinity of the SrRuO_3 thin films can be demonstrated by the plot of the FWHM values of both the ω -rocking curve on the (004)/(220) reflection and the ϕ -scan on the (404) reflection of the SrRuO_3 films deposited at different temperatures. Figure 4 shows the values of these FWHMs of the SrRuO_3 thin films as a function of deposition temperature. It can be seen from Fig.

4 that the values of the FWHM decrease monotonically with increasing deposition temperature. It is physically plausible to have smaller FWHMs, i.e., better crystallized thin films, at higher deposition temperatures. However, it is remarkable that well aligned SrRuO_3 thin films can be grown on LaAlO_3 substrates by PLD at a deposition temperature as low as 450°C . It is possible that the energetic ions in the laser plume enhance the texture of the thin films, compensating for the lack of sufficient thermal energy supplied by the low temperature substrates. In addition, it is expected based on Fig. 4 that the optimized SrRuO_3 thin films in terms of crystallinity can be grown in the range of $650\text{--}800^\circ\text{C}$.

The degree of the crystallinity of the SrRuO_3 thin films grown on LaAlO_3 substrates can also be studied by SEM. Figure 5 shows the surface morphology and microstructure of the SrRuO_3 thin films deposited on LaAlO_3 at different temperatures. First of all, it can be seen from Fig. 5 that the surfaces of the films deposited at different substrate temperatures are very clean and smooth, and no particles are detected. The smoothness of the film makes the SrRuO_3 system very promising as a bottom electrode material in high capacity thin film capacitors because of the lack of microshort from the particles. Furthermore, it can be seen from Fig. 5 that the grain size of the films increases with increasing deposition temperature. Epitaxial growth of SrRuO_3 on LaAlO_3 by PLD occurs at deposition temperatures higher than 650°C [13], although a well textured SrRuO_3 film can be obtained at a deposition temperature as low as 450°C .

Finally, the smoothness of the thin films can be quantitatively measured by STM. Figure 6 shows the r.m.s. surface roughness of the SrRuO_3 thin films on LaAlO_3 deposited at different temperatures. It can be seen from Fig. 6 that the SrRuO_3 thin films deposited at temperatures higher than 650°C are extremely smooth, having r.m.s. surface roughness less than 0.2 nm within a testing area of $0.1 \times 0.1\text{ }\mu\text{m}^2$.

2. *Electrical Properties of SrRuO_3 Thin Films*

Room-temperature electrical resistivities of the SrRuO_3 thin films deposited at different substrate temperatures by PLD are shown in Fig. 7. It can be seen from Fig. 7 that the deposition temperature has a strong

impact on the room temperature resistivity of the SrRuO_3 thin films. The higher the deposition temperature of the films, the more conductive the films are. The room temperature resistivity decreases more than three orders in magnitude when the deposition temperature increases from 250°C to 775°C . The SrRuO_3 thin film deposited at 775°C by PLD with the optimized crystal structure is highly conductive with a room temperature resistivity of around $280\ \mu\Omega\cdot\text{cm}$. This value is very close to that of bulk single crystal SrRuO_3 [9], lower than $340\ \mu\Omega\cdot\text{cm}$ of sputtered SrRuO_3 films [10], and much lower than $1130\ \mu\Omega\cdot\text{cm}$ of bulk polycrystalline SrRuO_3 [8]. It is physically plausible to believe that the room temperature resistivity of the SrRuO_3 thin films is directly related to the crystallinity of the films, because, as analyzed above, deposition temperature has a strong influence on the crystallinity of the films. It has been shown above that the crystallinity of the films increases with increasing deposition temperature and the SrRuO_3 thin films become highly textured when deposited above 450°C . It is especially worthwhile to note that the grain size of the films increases with increasing deposition temperature, as shown in Fig. 5. It is believe that the reduced grain boundary scattering from crystallized films enhances the conductivity of the films. On the other hand, the room temperature resistivity of the polycrystalline SrRuO_3 can be as high as $1130\ \mu\Omega\cdot\text{cm}$, presumably due to strong grain boundary scattering. Therefore, it is very clear that only the crystalline-like SrRuO_3 thin films should be used as electrode materials, and the other forms, either polycrystalline or amorphous, are of too high resistivity and should be excluded from consideration. In addition, a very weak dependence of the film resistivity on the oxygen pressure during film deposition in the range of 50 to 200 mTorr for a given deposition temperature indicates that the films are completely oxidized under our optimized PLD process conditions.

Temperature dependence of the electrical resistivity of the films deposited at different substrate temperatures by PLD is shown in Fig. 8. It can be seen from Fig. 8 that the films deposited at different substrate temperatures have different temperature dependence of electrical resistivity (ρ -T characteristic). The SrRuO_3 films deposited at 250°C has a semiconductor-like characteristic in resistivity, as shown in Fig. 8 (a).

However, the ρ -T characteristic is composed of three distinguished regions if the SrRuO_3 thin film is deposited at 450°C , as shown in Fig. 8 (b). The ρ -T curve of the film is semiconductor-like below 93K, metallic-like in the range of 93K to 160K, and virtually constant above 160K. The SrRuO_3 films deposited above 650°C show metallic resistivity vs. temperature behavior, where the kink at about 160 K represents the Curie point of SrRuO_3 which becomes ferromagnetic below this temperature [14]. These unique ρ -T characteristics of the SrRuO_3 thin films deposited at certain temperatures may provide new features in development of novel electronic devices. Further work is underway to investigate such properties on the SrRuO_3 thin films.

Another well-known direct measurement of film perfection, the residual resistivity ratio (RRR), is also studied for the SrRuO_3 thin films. Based on the analysis of temperature dependence of resistivity, it is found that the RRR of SrRuO_3 thin films on LaAlO_3 substrates increases with increasing deposition temperature. The RRR of the SrRuO_3 films is 3.4 and 8.4, respectively, while increasing deposition temperature from 650°C to 775°C . Note that a RRR of around 12 has been reported for bulk single crystalline SrRuO_3 [9] and a RRR of less than 3 has been measured for SrRuO_3 thin films epitaxially grown by sputtering [10]. The higher RRR value for the PLD deposited SrRuO_3 thin films on LaAlO_3 substrates can be attributed to the higher crystallinity of the films at higher deposition temperatures by PLD.

3. *Theoretical Calculations*

Although it has been experimentally found that bulk SrRuO_3 , as one of few conductive oxides, is electrically conductive, the physical mechanism for conductivity has never been explained based on electronic structure calculations. Figure 9 (a) shows the total density of states (DOS) for bulk SrRuO_3 in the experimental geometry, while Fig. 9 (b) shows the energy levels of the $[\text{Ru}(\text{OH})_6]^{2-}$ model of the Ru coordination environment in SrRuO_3 . It can be seen from Fig. 9 that the Fermi level of bulk SrRuO_3 cuts through the conduction band, so that the DOS at Fermi level, $N(E_F)$, is of a significant value, i.e. the bulk SrRuO_3 is electrically conductive. In addition, the contribution of the d-electrons from Ru substantially

determines the conductivity of bulk SrRuO_3 . However, the $N(E_F)$ is not very high, as shown in Fig. 9, therefore, it is expected that bulk SrRuO_3 still has a relatively high resistivity at room temperature ($280 \mu\Omega\cdot\text{cm}$).

In order to study the electrical properties of SrRuO_3 thin films, the electronic structure of the SrRuO_3 (001) surface was determined using a two dimensional slab model. This model used a slab made up of five atomic planes: $\text{RuO}_2\text{-SrO-RuO}_2\text{-SrO-RuO}_2$. The total DOS and projected DOS of the surface atoms is shown in Fig. 10. The most striking features can be seen from Fig. 9 and 10 are that the DOS of the SrRuO_3 (001) slab is very similar to that of the bulk SrRuO_3 and the position of Fermi level, E_F , of the SrRuO_3 (001) slab is almost the same as that of the bulk SrRuO_3 . The major difference is the presence of the peak appearing below -12 eV in SrRuO_3 (001) slab, which is composed almost entirely of surface states. These are the so-called "dangling bonds" states which arise when the bulk material is cleaved and some bonds are broken. Due to the fact that these states appear ~ 1 eV above E_F (which is still in much the same position as it is in the bulk), we would not expect the conductivity of this perfect SrRuO_3 (001) surface to be significantly different from that of the bulk.

It is very important to point out that the model system employed in these slab calculations are much thinner than the films reported in this work (100-150 nm). In a real SrRuO_3 thin film, there are many more layers, this would give rise more bulk-like electronic structure and electrical behavior. Since there is no significant perturbation of the DOS near E_F by the formation of the SrRuO_3 (001) surface, we would expect these films with the optimized crystal structure to exhibit a conductivity close to that of the bulk single crystalline SrRuO_3 , as pointed out above based on the experimental results. Furthermore, we do not believe that the observed semiconductor-like and temperature-independent behavior of the SrRuO_3 thin films deposited at certain temperatures can be explained in terms of the electronic structure of a perfect film. These anomalous electrical properties of SrRuO_3 thin films must be due to more macroscopic phenomena, such as grain boundary scattering.

Conclusions

The structural and electrical properties of SrRuO_3 thin films deposited on LaAlO_3 at different substrate temperatures by PLD have been studied. The following conclusions can be drawn from the investigation:

(1) Microstructure dependence on deposition temperatures has been revealed. The films have a better crystallinity, i.e. higher textured crystalline with a larger grain size and a smaller surface roughness, when grown at higher deposition temperatures. Although a well aligned SrRuO_3 thin film can be grown at 450°C , the optimized SrRuO_3 thin films on LaAlO_3 substrates should be grown by PLD at above 650°C .

(2) Room temperature resistivity dependence on deposition temperature has been examined. The SrRuO_3 thin film deposited at 775°C has an optimized electrical resistivity of $280\ \mu\Omega\cdot\text{cm}$, which is very close to that of the bulk single crystalline SrRuO_3 . It also has a RRR value of 8.4, which is much higher than those of polycrystalline bulk and sputterly grown thin film SrRuO_3 . In addition, it has the lowest surface roughness. All of these make this optimized film a very attractive bottom electrode material.

(3) Temperature dependence of electrical resistivity (ρ -T characteristic) of the SrRuO_3 thin films deposited at different substrate temperatures has been determined. The SrRuO_3 films deposited at 250°C has a semiconductor-like characteristic in resistivity. However, the ρ -T characteristic is composed of three distinguished regions if the SrRuO_3 thin film is deposited at 450°C : semiconductor-like below 93K, metallic-like in the range of 93K to 160K, and virtually temperature-independent above 160K. The SrRuO_3 films deposited above 650°C show metallic behavior, where the kink at about 160 K represents the Curie point of SrRuO_3 . These unique ρ -T characteristics of the SrRuO_3 thin films deposited at certain temperatures may provide new features in fabrication of novel electronic devices.

(4) The electronic structures of the bulk and (001) slab of SrRuO_3 have been calculated using the extended Hückel implementation of the tight-binding method. Electrons of SrRuO_3 perovskite fill the Fermi surface in

such a way that $N(E_F)$ is of a significant value, which results in the conductivity of SrRuO_3 . More importantly, the DOS and the position of Fermi level of thin film and bulk SrRuO_3 are basically the same, which result in the conductivity of thin film close to that of bulk single crystals. Furthermore, anomalous electrical properties of the SrRuO_3 thin films grown at different deposition temperatures should be understood in terms of more macroscopic phenomena, such as grain boundary scattering, instead of electronic structure.

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Figure Captions

Fig. 1 X-ray diffraction of θ - 2θ scan on the SrRuO_3 thin film deposited at 775°C on a LaAlO_3 substrate.

Fig. 2 X-ray ω -rocking curve on the (004)/(220) reflection of the SrRuO_3 thin film deposited at 775°C on a LaAlO_3 substrate.

Fig. 3 X-ray diffraction ϕ -scans on both the (404) reflection of the SrRuO_3 thin film deposited at 775°C and the (101) reflection of the LaAlO_3 substrate.

Fig. 4 Crystallinity of the SrRuO_3 thin films as a function of deposition temperature, showing the FWHMs for the ω -rocking curve (tilt of c-axis or/and a+b-axis) on the SrRuO_3 (004)/(220) reflection and for the ϕ -scan (in-plane twist misalignment) on the SrRuO_3 (404) reflection.

Fig. 5 SEM micrograph of the SrRuO_3 thin films on LaAlO_3 deposited at (a) 250°C , (b) 450°C , (c) 650°C , and (d) 775°C .

Fig. 6 Deposition temperature dependence of the surface roughness of the SrRuO_3 thin films.

Fig. 7 Room-temperature resistivity of the SrRuO_3 thin films as a function of deposition temperature.

Fig. 8 Temperature dependence of the normalized resistivity of the films deposited at different deposition temperatures: (a) 250°C , (b) 450°C , and (c) 650°C and 775°C .

Fig. 9 (a) Solid line: the total DOS for bulk SrRuO_3 in the experimental geometry. Filled area: the contribution of Ru to the total DOS. The horizontal dashed line indicates the position of the calculated Fermi level (E_F). (b) The energy levels of the $[\text{Ru}(\text{OH})_6]^{2-}$ model of the Ru coordination environment in SrRuO_3 . Due to the small size of the distortion from octahedral coordination, many levels are nearly degenerate and appear as a single level.

Fig. 10 The calculated DOS of the 5 atomic layer model of the SrRuO_3 (001) surface. The shaded area indicates the contribution of surface atoms to the total DOS: (a) surface Ru's, (b) surface O's. The horizontal dashed line represents the position of Fermi level, E_F .

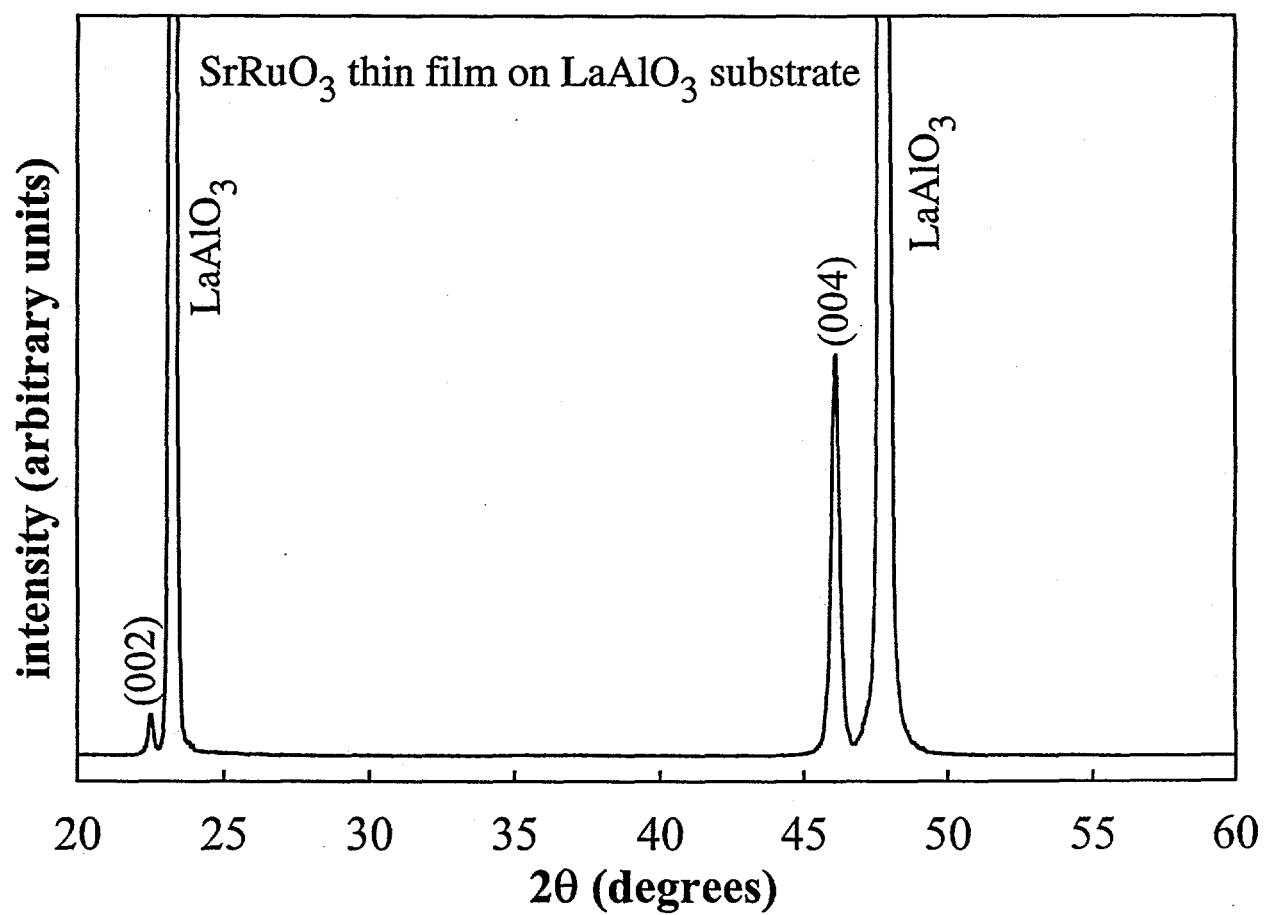


Figure 1

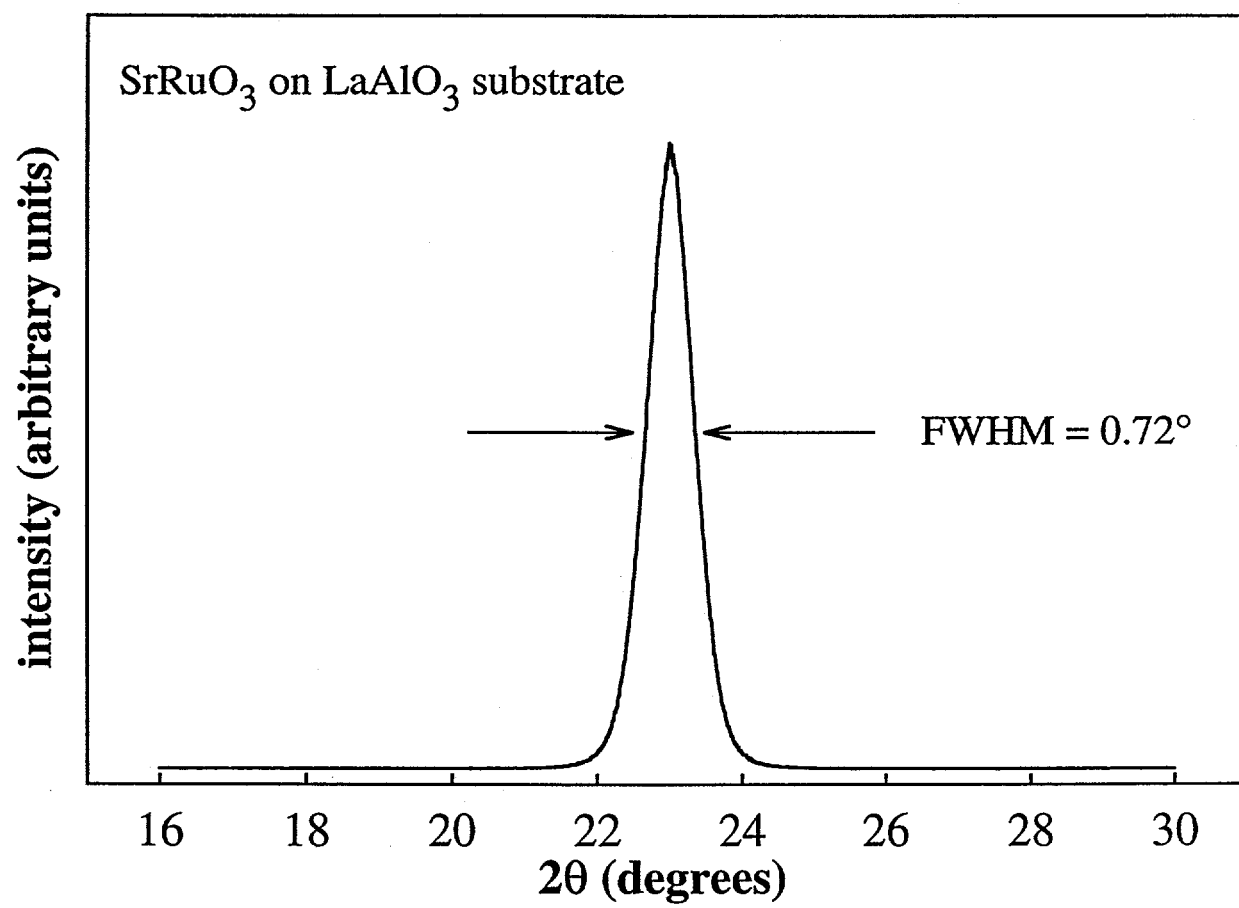


Figure 2

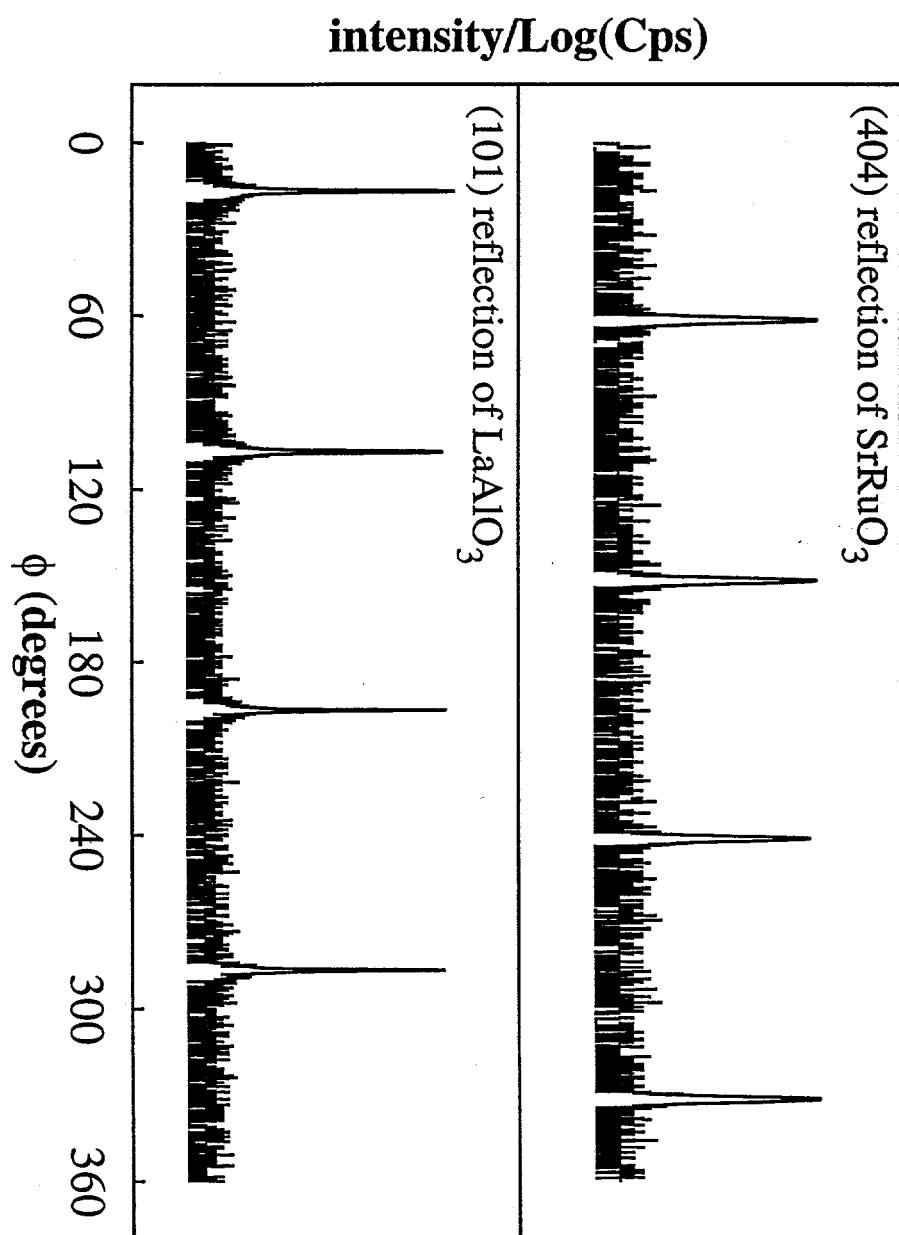


Figure 3

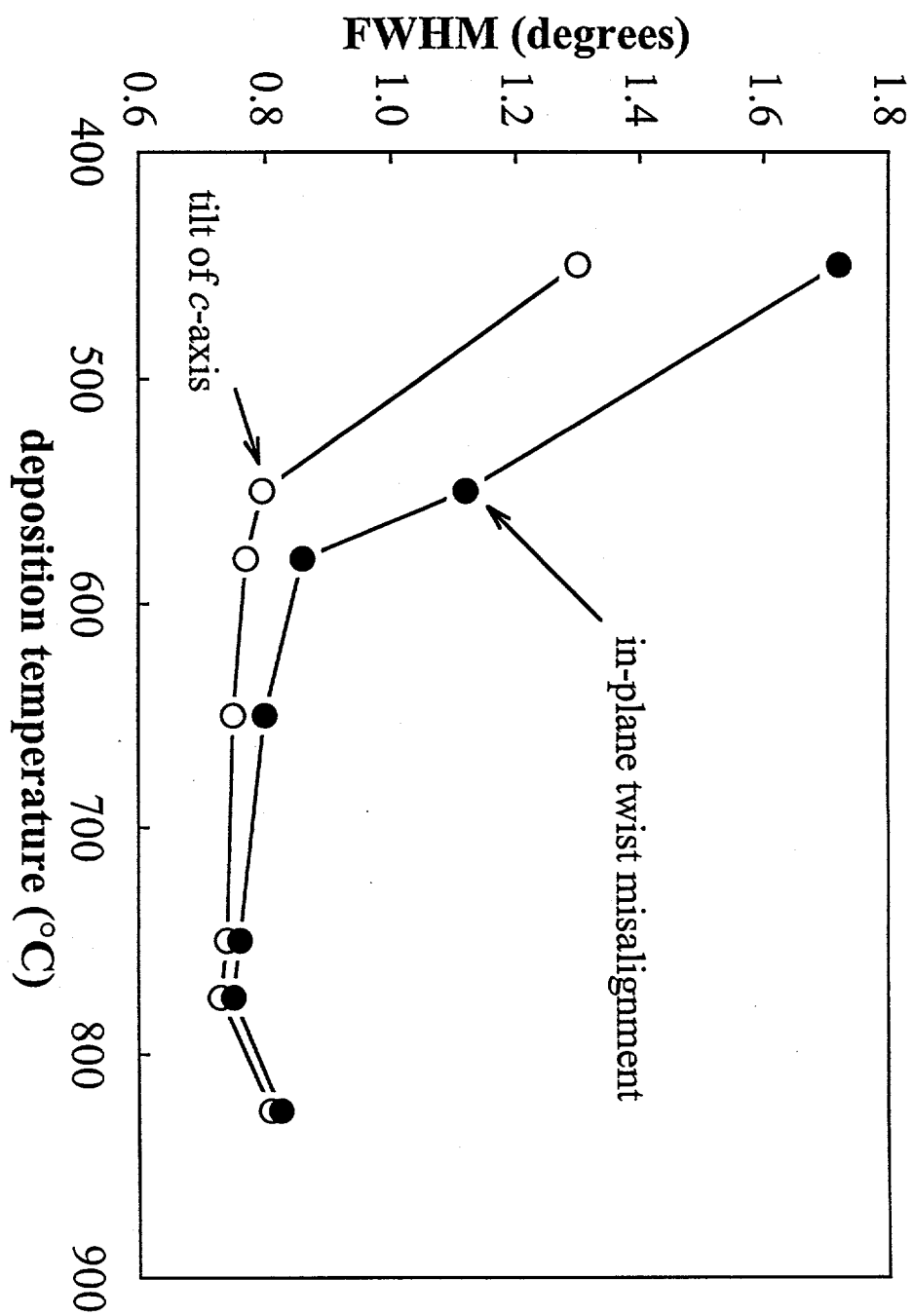


Figure 4

(a) SrRuO_3 deposited at 250°C on LaAlO_3

100nm
5KV 11mm

(b) SrRuO_3 deposited at 450°C on LaAlO_3

100nm
5KV 11mm

(c) SrRuO_3 deposited at 650°C on LaAlO_3

100nm
5KV 11mm

(d) SrRuO_3 deposited at 775°C on LaAlO_3

100nm
5KV 11mm

Figure 5

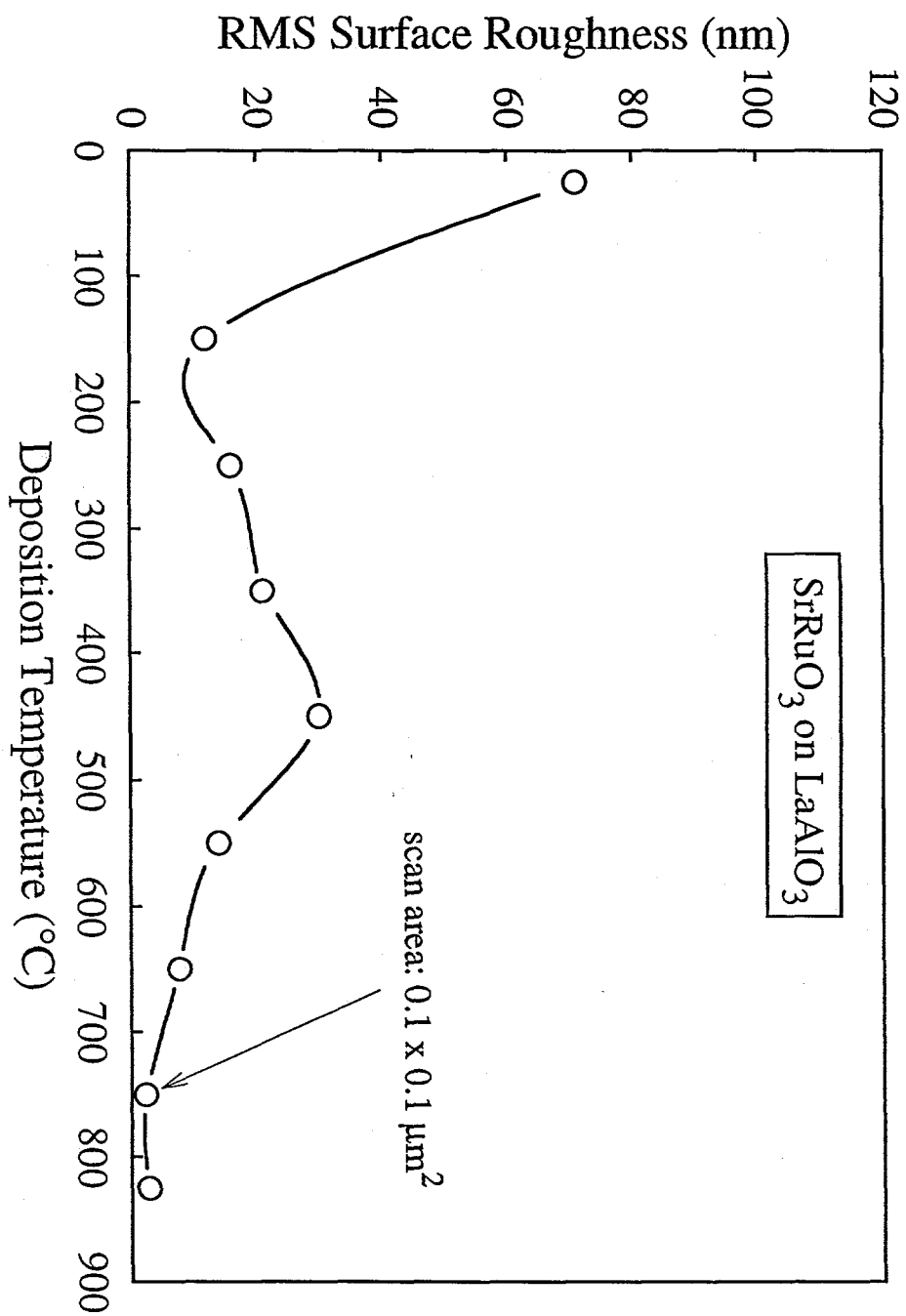


Figure 6

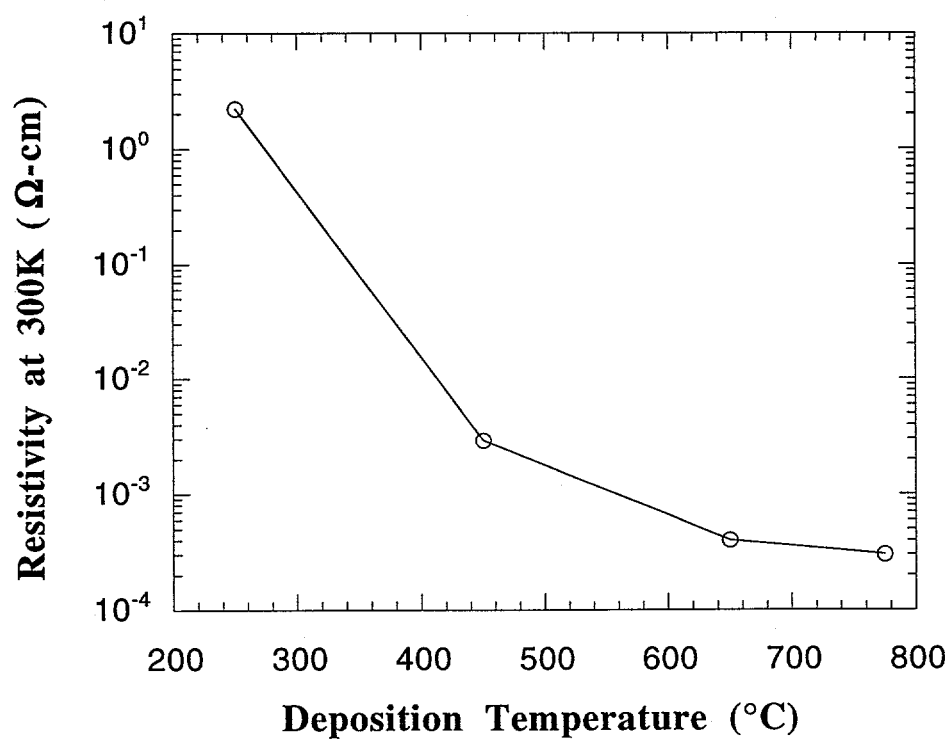


Figure 7

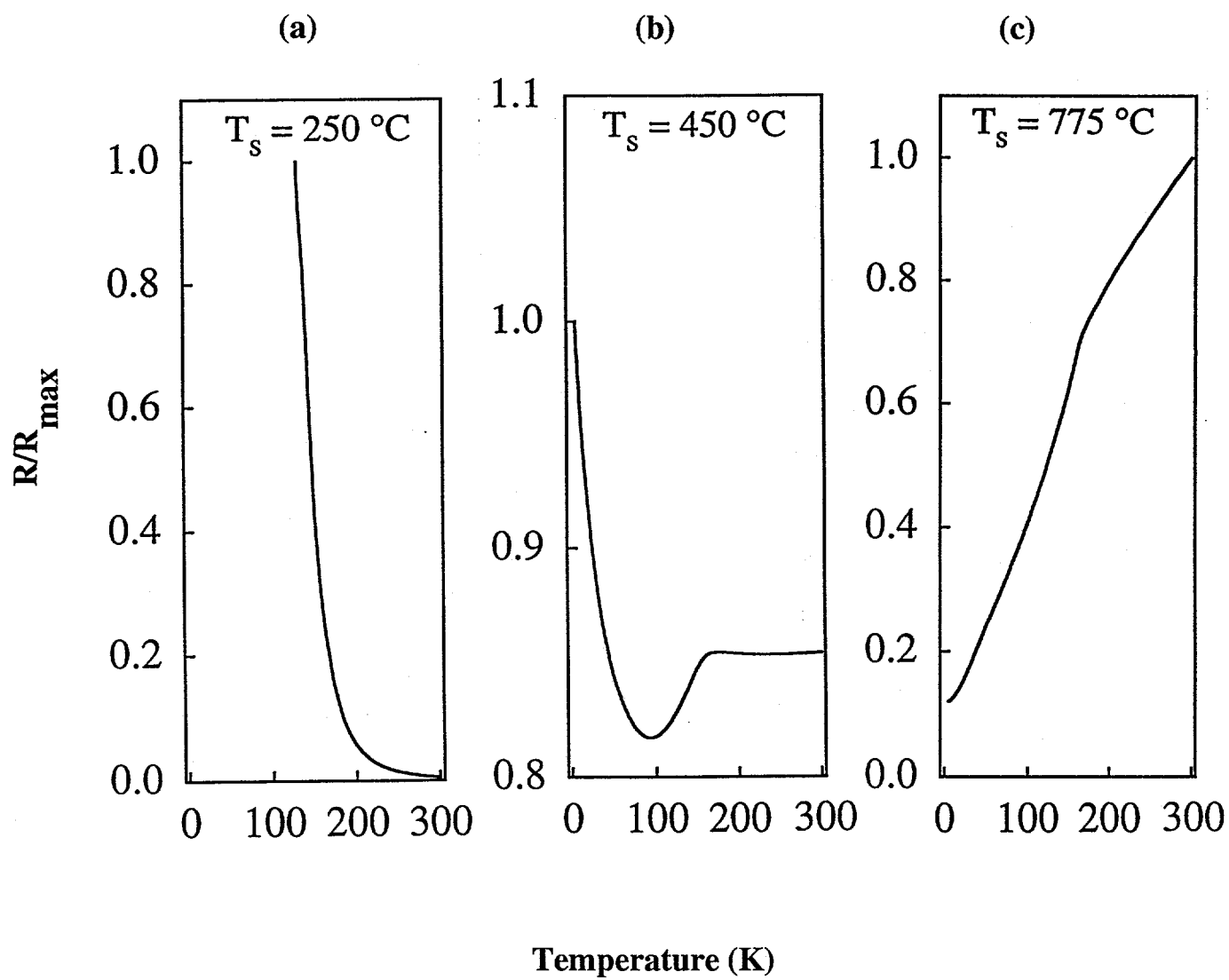


Figure 8

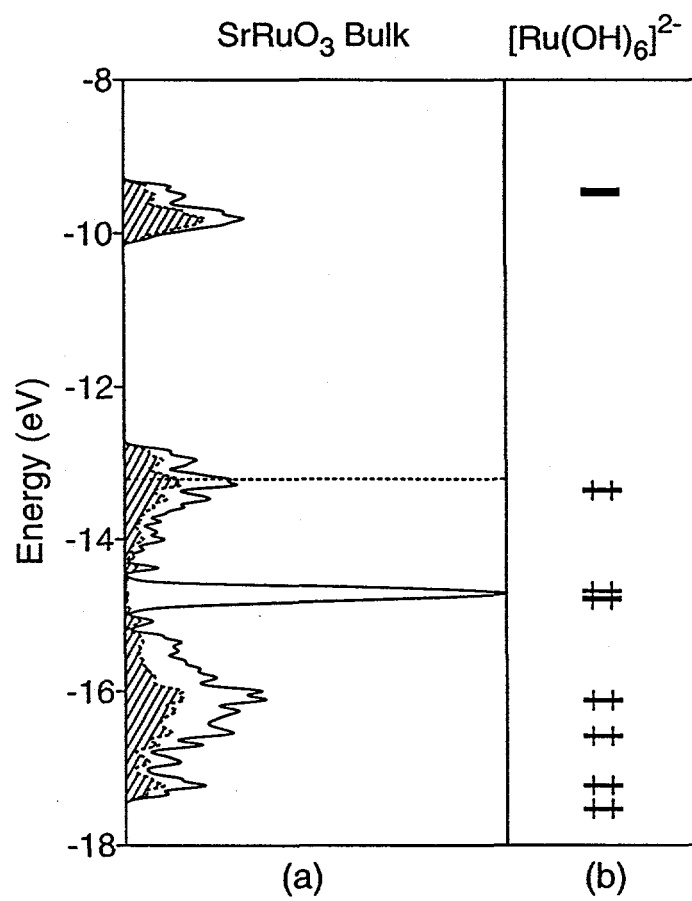


Figure 9

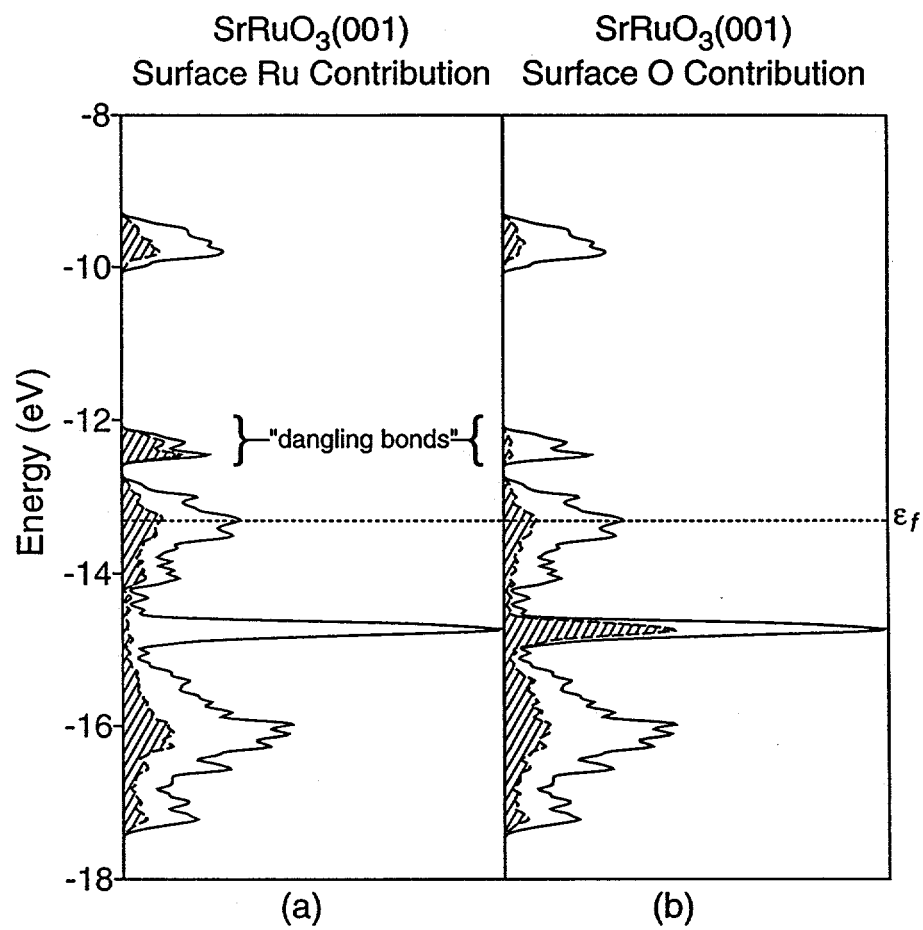


Figure 10