Research Paper

ANALYSIS OF FORMATION OF OXIDE SURFACES

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Oxide consists of a diverse class of compounds and their properties cover all the aspects of material science and physics. Oxides range from superconductor to insulator while the bonding characteristics range from covalent on one hand to the highly ionic on the other. Oxides find a lot of applications from paints and pigments to sensors and catalysts. Oxide coatings on thin films can be related to condensed matter physics and thewhole field of thin film studies is of interest for future studies on clean and modified oxidesurfaces, because it opens up areas of study on the so-called polar surfaces.

Keywords: Oxide surface, Oxide coatings, Thin films, Polar surface

INTRODUCTION

The preparation of any stoichiometric compound surface compared with the elemental solid and in particular oxides is extremely difficult considering the preparation of different crystallographic orientations. The surface potential per unit charge for a polar surface is given by:

$$V = 2\frac{f}{s}\left[Nb(2a-1)+(1-a)b\right] \qquad ...(1)$$

where S is the area of surface unit cell, N is the number of layers separated by a distance b, a is the surface charge measured in units of the charge on a typical bulk layer. When N approaches to infinity the surface potential diverges so that cleavage of a rock salt structure in this direction is not possible.

Cleavage is not the most favorable method for preparation of ionic polar oxide surface. There are other methods for preparing surfaces of different surface orientation. For a polar surface the surface potential can have a finite value of thin film if the surface charge is reduced. For instance of the value of $a = 1/2$ in Equation (1). The reduction in surface charge is achieved by the following methods:

- Reducing the number of ions in the top most layers.
- Reducing the charge of each ion in the top most layers.

There are also many alternative methods for preparation of stable polar surface:

- Cutting the crystallographic plane mechanically and then polishing the surface.

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This method involves sputtering of surfaces and consecutively annealing in oxygen in order to replace oxygen vacancies induced via sputtering.

It is very difficult to prepare the polar surfaces as these surfaces have tendency to facet in the preparation process.

The other method is a somewhat different method of preparation in which Oxide films of varying thickness aregrown on metallic substrates (Wandelt, 1982). The structure of the oxide film depends on the geometry of the metallic substrate. It is this technique that allows preparation of non-polar as well as polar surfaces and it also involves the stabilization mechanisms for polar surfaces.

EXPERIMENTAL PROCEDURE

The structural quality of the film depends very strongly on therelation between the lattice constants of metallic substrate and oxide films. Therefore by controlling the lattice mismatch we can control the defect structure and defect density to a certain extent. Many techniques can be used for this surface.

In the first technique a metal single crystal is oxidized thereby forming a well ordered oxide film. The film can be defective if there is a large lattice mismatch between the metal and the oxide lattice constants. By using inert metal substrates less strained metal layers can be grown on which the metal to be oxidized is evaporated. During the deposition the oxidation can be done. The growth structure can exhibit a long range order and that to of high quality if the selections of lattice constants of inert substrates are done properly. The other technique involves of oxidation of alloy surfaces. The main advantage of this method is that it enhances the physical properties of alloy. For instance this technique can be used for growing well-ordered Al_2O_3 film on NiAl. Without melting substrate the Al_2O_3 film can be heated above 1000 °C due to which the ordering of layer can be done.Such a heat treatment leads to melting of the substrate before the oxide layer could be ordered in case of Al metal. This explains the reason as to why Al_2O_3 layers on Al are amorphous.

Vanishing of superstructure spot causes transition towards lower temperature while transition towards higher temperature causes partial loss of intensity but an increase in the diffusion rate of that particular superstructure. The superstructure has a pronounced resistivity for adsorption of various molecular species. At its maximum intensity, i.e., at 150 K, the superstructure is exposed to 5-8 * 10^{-8} torr carbon dioxide which is known to strongly chemisorb on thechromium oxide surface (Kuhlenbeck *et al.*, 1992). The superstructure was quenched immediately after the onsetof exposure. It could only be recovered by flashing the sample to the temperature at whichthermal desorption of the corresponding species takes place (Kuhlenbeck *et al.*, 1992).

The structural rearrangement on the clean sample takes place at the surface and the energetics of the structural rearrangementat the surface depends between interaction between adsorbates and substrates.

RESULTS AND DISCUSSION

The atomic structure cannot be resolved within the oxide layer. Therefore the arrangement of atoms within the surface is not clear.Ion scattering shows thatthe topmost surface is oxygen terminated (BertramsTh *et al.*, 1995).

High-resolution XPS indicates that there isan interface layer with Al exhibiting a chemical shift (Jaeger *et al.*, 1991). Angle resolved photoemission (ARUPS), where photoelectron spectra are recorded as a function of the direction of theelectronic band structure and thus of the symmetry of the electronic states, is indicativeof a hexagonal arrangement of the oxygen atoms within the oxygen sub lattice (Jaeger *et al.*, 1991). High Resolution Electron Energy Loss Spectroscopy (HREELS), where the inelastic electron scatteringby surface vibrations and electronic excitations is probed, points towards a structure similar to gamma form of Al_2O_3 with tetrahedral and octahedral Al sites being populated (Jaeger *et al.*, 1991). Al_2O_3 exhibits occupied levels only at a binding energy below the Fermi level (Jaeger *et al.*, 1991). The substrate within the interfacial regions has to be reconstructed for accommodating the oxide layer. To assure for the proper local site there should be a lateral motion between small fractions of atoms.

Due to the existence of interface layers the effective range of scattering path will increase.

Only by means of quantum chemical wave functions we can understand the bonding between oxidic substrate and an adsorbed atom.In the field of optical and electron spectroscopy the interpretation is hard. This fact is reflected by an increasing number of papers that contain both experimental and theoretical results. To treat the energetics of ionic crystals and surfaces properties like crystal structures, cohesive energies and phonon frequencies play a very significant role. Metal oxides, ionic crystals and adsorbed molecules are modelled by using a variety of pair potentials which includes structures of

Figure 1: LEED Patterns of Al_2O_3/NiAl
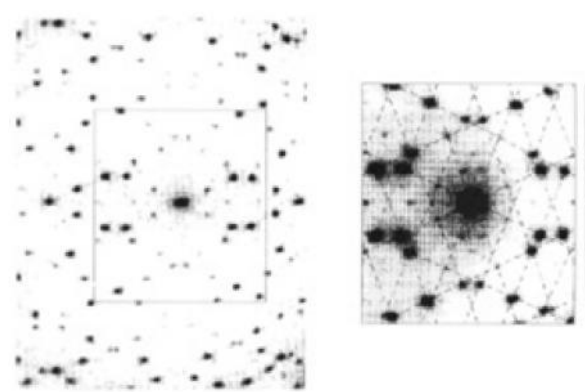
Source: Freund et al. (1993)

Figure 2: STM Topography of the Growing Al_2O_3 Film Near NiAl Edge
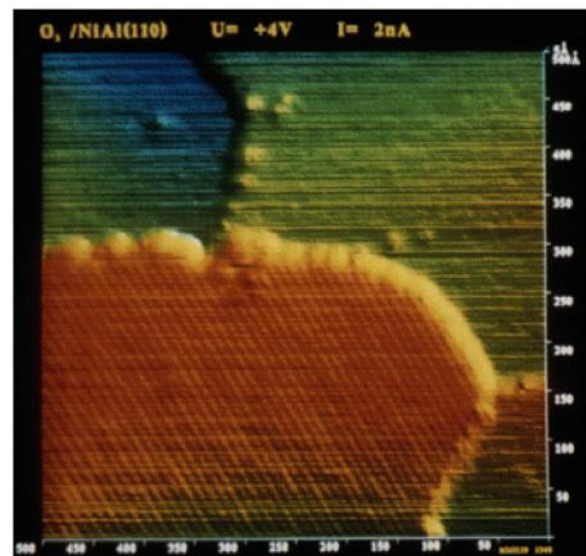
Source: Freund et al. (1993)

adsorbed monolayers, phase transitions between them, and the dynamics of adsorbed particles.

CONCLUSION

The main advantage of Interatomic potential simulating the static geometrical structures and dynamic properties of systems by using a large number of particles which consists of

bulk, surface ions and adsorbed molecules. However pair potentials include its use only when these properties cannot be changed by interaction of particles among each other in the system. This is true for a large extent of ions in the metal oxides but the bonding should be ionic in the transition metal oxides but not for those atoms which are at the metal surface.◐

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