Ion Scattering Simulations of Misfit Dislocations at the Single Crystal Fe_2O_3/Al_2O_3 interface

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We have investigated the buried interface of α-Fe_2O_3(0001)/ α-Al_2O_3 (0001) using ion scattering techniques and high resolution transmission electron microscopy (HRTEM). Molecular dynamics (MD) calculations were performed to understand the formation of misfit dislocations and the interface structural features. Ion scattering simulations were carried out using VEGAS code which uses Monte Carlo simulations based on Moliere screened potential to calculate the hitting probabilities. Atomic positions generated during the MD calculations were used in these simulations and the results were compared with experimental results. Combination of MD and VEGAS simulations with RBS and HRTEM measurements show promising results in understanding the interface structures of this single crystal Fe_2O_3/Al_2O_3.

1. Introduction

High quality single crystal iron oxide thin films are extremely important in several applications including catalysis, magnetic thin films and integrated microwave devices [1]. The structural and chemical properties of the surfaces and the film-substrate interface are vital in growing such high quality films. Recently, several high-quality well-oriented single crystal iron oxide films with various stoichiometries have been synthesised using Molecular Beam Epitaxial (MBE) growth and the structural properties have been analysed by various surface and bulk sensitive techniques [2].

High-energy ion scattering techniques (RBS and channelling) have been widely used to characterise interfacial solid-solid interaction, determine crystal structure at buried interfaces and analyse for extended defects that may arise in growth procedures. When single crystal α-Fe_2O_3 thin films are deposited on α-Al_2O_3 (0001) substrates using oxygen plasma assisted molecular beam epitaxy, a periodic distribution of basal dislocations occurs due to lattice mismatch along the interfaces. Such misfit dislocations were investigated using RBS and high resolution transmission electron microscopy (HRTEM) [3]. HRTEM measurements showed that these dislocations lie at the interface about 7.0 nm apart and the interface peaks that were seen in ion scattering experiments are consistent with the HRTEM results [3]. Molecular dynamics (MD) calculations were carried out to understand the formation of misfit dislocations and the interface structural features of this system [4].

This paper describes ion scattering simulations, which were carried out using VEGAS code. This code uses Monte Carlo simulations based on the Moliere screened potential to calculate the hitting probabilities and is described elsewhere [5]. Atomic positions generated during the MD calculations were used in the ion scattering simulations and the results were compared with experimental surface peak areas.

2. Results of Ion Scattering Simulations and Discussion

The relaxed cluster, which has been generated in the one-dimensional MD calculations, contained a very large number of atoms. The current VEGAS code can handle only up to 2200 atoms in a cluster. The big cluster around one dislocation has been divided into a number of small clusters for ion scattering simulations. Such a small cluster before and after relaxation (results of MD calculations) is shown in Figure 1.

We have used atomic positions of such small crystal clusters generated by MD calculations in VEGAS code with appropriate boundary conditions and obtained hitting probabilities. Figure 2 (a) shows the displacement of a particular atomic row from its original position. The hitting probability of an incident ion due to that particular atomic row (marked by arrow) is shown in Figure 2 (b). The hitting probability of an incident ion initially decreases from one at the surface and increases again at the interface due to rearrangement of atoms. The hitting probability of an incident ion due to substrate atoms is high at the interface and then decreases systematically as expected.

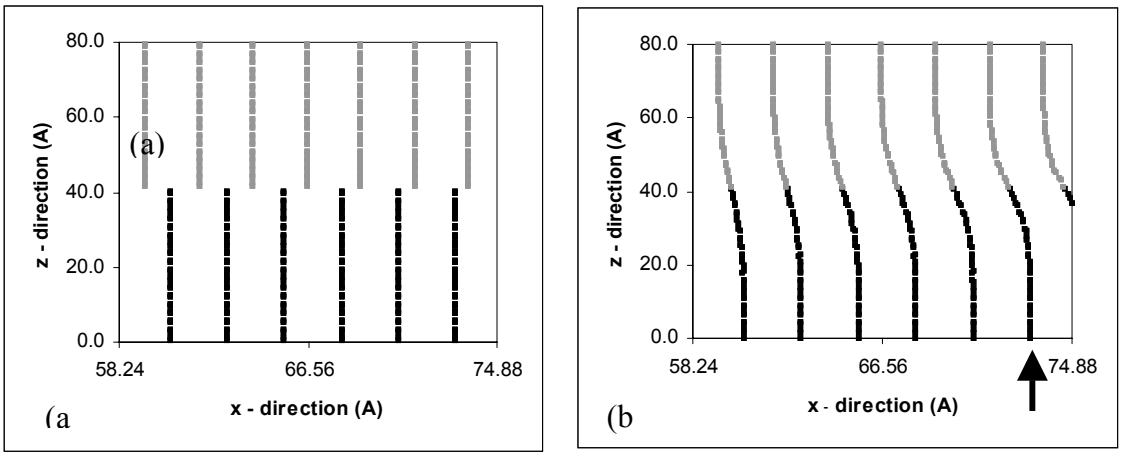

Fig.1: Position of atoms in a small cluster (a) before and (b) after relaxation (from MD calculations). The black and grey dots represent Fe and Al atoms respectively. Bending of atomic rows at the interface is clearly visible.

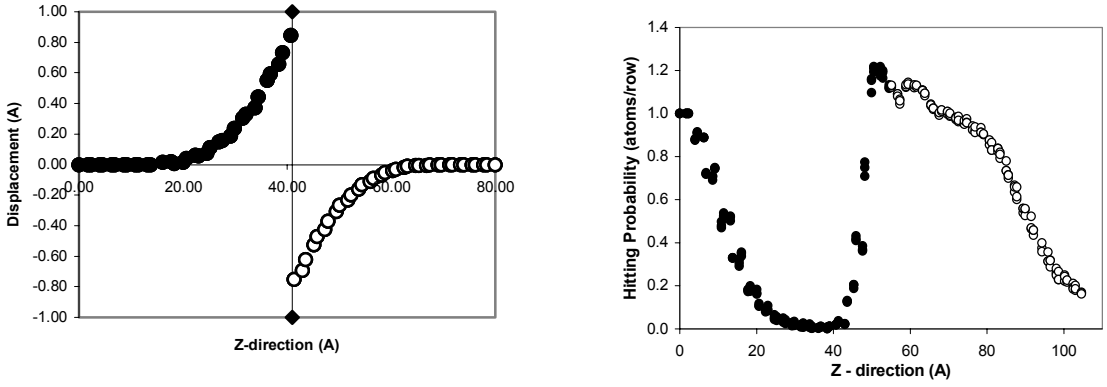

Fig 2: (a) Displacement of Fe and Al atoms at the interface of a particular row indicated by an arrow in Figure 1. (b) Calculated hitting probability of an incident ion due to Fe and Al atoms from the ion scattering simulations. The shaded and unshaded circles represent Fe and Al atoms respectively.

Ion scattering simulations were carried out for a number of similar clusters around one dislocation and hitting probabilities of an incident ion in terms of atoms/row due to Fe atoms at the surface and interface and Al atoms at the substrate were calculated. Results of these simulations (theoretical surface and interface peaks area) along with the experimental surface and interface peaks area (from the channelling measurements) are summarised in Table 1. Experimental channelling spectra and associated surface and interface peaks area were reported elsewhere [3].

In summary, combination of MD and the ion scattering simulations with RBS and HRTEM measurements show promising results in understanding the interface structures of this single crystal Fe_2O_3/Al_2O_3. Some differences have been observed between the experimental and theoretical simulations, in particular interface peaks corresponding to Fe and Al atoms. The two-dimensional MD calculations and ion scattering simulations are in progress and will be discussed in a later publication.

Table 1: Summary of experimental (from the channelling measurements) and theoretical (from ion scattering simulations) values surface and interface peaks area.

Experimental Surface and Interface Peaks area (from the channeling measurements)

Sample Description	***Peak Description***	***Peak area (atoms/row)***
70 nm thick Fe_2O_3 film	Fe – Surface Peak	3.9
on Al_2O_3 substrate	Fe – Interface Peak	4.3
	Al – Interface Peak	7.3
Pure Al_2O_3 substrate	Al – Surface Peak	6.2

Theoretical Surface and Interface Peaks are (from Ion Scattering Simulations)

Sample Description	***Contributing atom***	***Hitting Probability (atoms/row)***
10 nm thick Fe_2O_3/Al_2O_3 cluster	Fe at surface	3.8
	Fe at interface	1.5
	Al at interface	8.2
10nm thick Al_2O_3 cluster	Al	6.1

Acknowledgments

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