MAX-PLANCK-INSTITUT FÜR METALLFORSCHUNG
Abteilung Dosch
Stuttgart

MAX-PLANCK-GESELLSCHAFT

MPI-MF Abteilung Dosch

In-situ X-ray Study of $Fe_3Al(110)$ Subsurface Superlattice Disorder during Oxidation

Vedran Vonk, Claus Ellinger, Navid Khorshidi, Alina Vlad [1]

Dr. A. Stierle

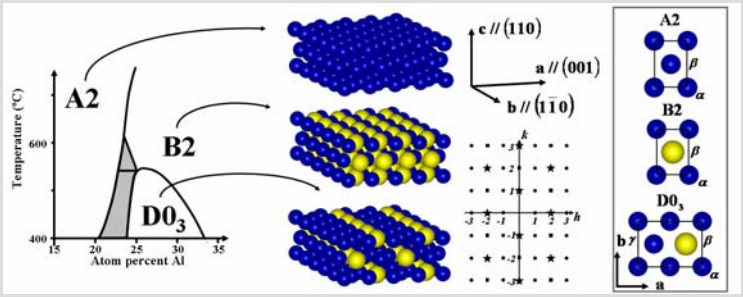
Abstract

We report an in situ x-ray investigation of the $Fe_3Al(110)$ surface during oxidation with a special focus on its impact onto the superlattice order. Upon oxidation at 10^{-6} mbar of molecular oxygen at a temperature of 573 K, the long-range superlattice order disappears completely in an extended subsurface region, without affecting the surface roughness nor the crystallinity. These findings can be understood by preferential surface segregation of Al in the presence of oxygen. We argue that this unavoidable subsurface disordering process should render these materials more brittle and vulnerable to aggressive environments, which is important for the use of iron-aluminium alloys as structural materials.

Motivation

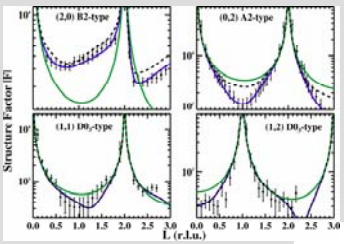
Iron-aluminides are promising materials as future light-weight replacements of steel, because of their potentially favourable density-strength ratio, their use in deep draw processes, and for their high-temperature stability [2]. However, in order to be used in high-temperature structural applications it is necessary that a protective oxide scale is formed on the surfaces of these materials to prevent them from further corrosion. Here, we present a combined In-situ Surface X-ray Diffraction, X-ray Reflectivity ,and Auger Electron Spectroscopy study of the clean and oxidized $Fe_3Al(110)$ surface.

Fe-Al Phase Diagram and the (110) Surface



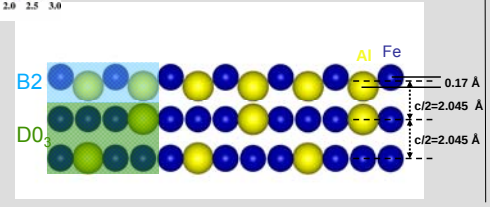
Body-centred-cubic fundamental lattice with decoration of Fe (blue) and Al (yellow) over the lattice sites α, β, and γ.
The (110) surface in the $D0_3$ phase distinguishes between three types of Crystal Truncation Rods, which probe A2 (■), B2 (★), and $D0_3$ (●) types of order.

Surface X-ray Diffraction of clean $Fe_3Al(110)$



The experimental data show the largest discrepancy with a bulk-termination model calculation on the B2-type rod. The best fit consists of a B2-type top-layer on a D03 bulk crystal.

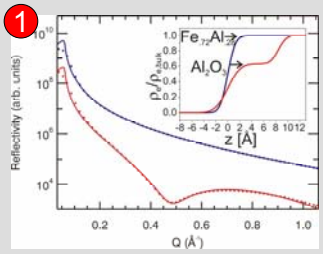
Best fit with vacancies
Best fit without vacancies
Bulk terminated

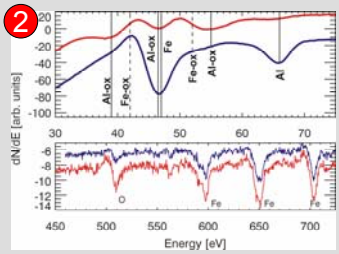


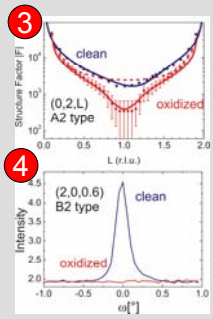
Oxidation

After the oxidation procedure (573K, 10^{-6} mbar O_2 for 30 minutes):

1. X-ray Reflectivity shows 8.4 Å thin oxide layer.
2. AES shows only the formation of aluminium oxide
3. A2-type CTR shows a pronounced dip.
4. Intensity on $D0_3$ and B2-type CTRs vanished.

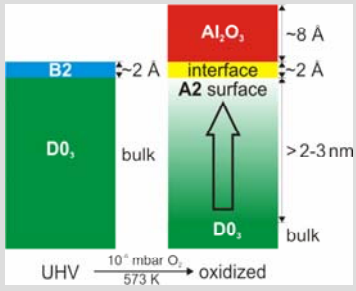






A disorder profile, which describes a gradual transition from the bulk to the surface, explains the vanishing of the $D0_3$ and B2 type CTRs without affecting the A2-type CTR too much. Here a "β-roughness" profile is chosen [3]. The particular dip in the A2 rod is well reproduced by an interfacial layer between the substrate and the film containing many vacancies, which can be seen as a sort of roughness.

Summary of Results



The clean surface comprises a topmost atomic layer with in-plane B2-type order on a $D0_3$ (and B2) ordered bulk crystal. Upon oxidation the superlattices disappear gradually in an extended subsurface region and a thin smooth aluminium-oxide forms having a disordered interface to the substrate.

Conclusions and Outlook

Preferential surface segregation is enhanced by the presence of oxygen. Due to compositional changes in an extended subsurface region it is to be expected that the material has become more brittle. In order to prevent this possible deterioration, the effects of oxidation under different thermodynamic conditions and post-annealing on the formation of oxides and their interfaces to the substrate will be explored.

Collaborations

(1) European Synchrotron Radiation Facility, Grenoble, France
(2) Ångström Quelle Karlsruhe, Germany

References

[1] V.Vonk et al. Phys. Rev. B **78** (165426) 2008
[2] C.G. McKamey *et al.* Mater. Res. **6** (1991) 1779
[3] I.K. Robinson Phys. Rev B **33** (1986) 3830