

## On the Application of APFIM to Investigation of Site Occupancy of Pt in $\beta$ -NiAl

Krystyna Stiller\*, Johan Angenete\*

\*Dept. of Experimental Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden

Ordered intermetallic  $\beta$ -NiAl alloys belong to an important group of advanced materials, used in high temperature applications. Due to their high Al content, the alloys provide good oxidation resistance and are therefore used as protective coatings on nickel base superalloys to minimise the environmental degradation due to high temperature oxidation.

Under the last decades, small additions of Pt to such coatings have been extensively used since this proves to have a beneficial effect on the time during which the coating is able to produce a protective layer of alumina ( $\text{Al}_2\text{O}_3$ ) [1,2]. Some of the proposed mechanisms behind this improvement of the oxidation properties of the coatings are based either on the influence of Pt on the diffusion behaviour of Ni and Al in the material or on its stabilisation of the  $\beta$ -NiAl phase [3-5]. At present, there is still no consensus in this matter, due to contradictory experimental results and the limited amount of thermodynamical and diffusion data for the NiAlPt system.

One of the possible ways of bringing more clarity in this issue is to investigate the site occupancy behaviour of Pt in  $\beta$ -NiAl. An uneven distribution of Pt on Ni or Al sites may explain its alleged influence on the diffusivity of Ni and Al. The atom probe technique, with its high spatial resolution, is ideally suited for such investigations and it was therefore used to study the platinum site occupancy in a stoichiometric, polycrystalline  $\beta$ -NiAl alloy containing 1 at% Pt.

The APFIM specimens were prepared using the Focused Ion Beam method [6], to avoid thin oxide film on the tip produced by the standard electropolishing procedure. The analyses were performed along the  $\langle 100 \rangle$  direction of the specimen in order to resolve pure  $\{001\}$  Ni and Al planes (Fig. 1). The other possible direction for resolution of pure Ni and Al planes,  $\langle 111 \rangle$ , was not used because of the observed retention of Pt on the  $\{111\}$  planes.

Due to the difference in evaporation field of Al and Ni, the reconstructed Ni planes appeared somewhat blurred while the Al planes were clearly visible. The Pt atoms were observed both in and between the Al planes (Fig. 2). This was interpreted as a sign for Pt location both on Ni and Al sites.

Calculation of the chemical environment around the Pt atoms (i.e. in slabs with thickness corresponding to a half a distance between the adjacent Ni or Al planes) indicated that Pt atoms were quite evenly distributed between Al and Ni sites.

A more detailed statistical method, termed stacked profile, by which it was possible to calculate the average chemical environment of all Pt atoms, was developed [7]. In these calculations, slabs with two lattice parameters width around each Pt atom were extracted from the original dataset. These subsets were put together in a new coordinate system, with the Pt atoms at the origin. This resulted in a very dense dataset, in which accurate chemical profiles (based

on over 60,000 atoms/Å) could be determined. This closer look on the occurrence of Ni and Al atoms around the Pt atoms revealed a very slight preference for Pt to occupy Al sites (Fig. 3).

#### References

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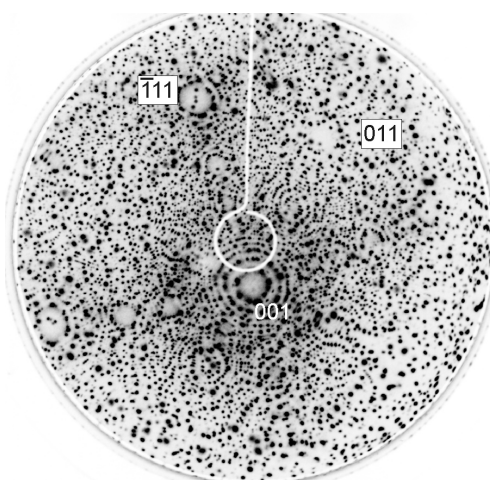


Fig. 1. Typical FIM image close to the  $\{001\}$  pole. The image was acquired in Ne at about 20 K during DC evaporation at approximately 13 kV.

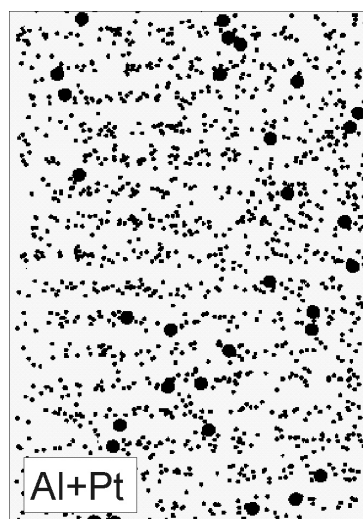


Fig. 2. Atom map, showing Al planes and Pt atoms (large black dots).

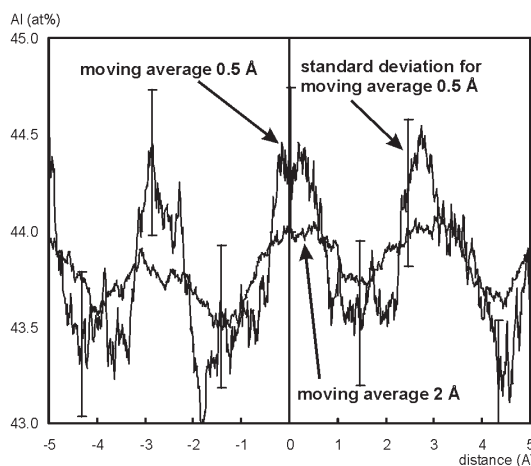


Fig. 3. Stacked profile over 797 Pt atoms, placed at  $z=0$ . The composition was calculated over two different moving averages, 0.5 and 2 Å wide. The error limits are given by the standard deviation for the 0.5 Å calculation.