

## Structure and Energy of Equilibrated Ni-Al<sub>2</sub>O<sub>3</sub> Interfaces

H. Meltzman\* and W.D. Kaplan\*

\* Department of Materials Engineering, Technion – Israel Institute of Technology, Haifa 32000, Israel

The structure, chemistry and properties of metal-ceramic interfaces have been the focus of many research studies, largely due to potential technological applications [1]. At the same time, the thermodynamic properties of metal-ceramic interfaces are of fundamental importance, defining equilibrium segregation and the thermodynamic work of adhesion. For the most part, solid-liquid interfacial energies for metal-ceramic systems have been studied, while it is clear that it is the solid-solid interfacial energy which is important for most applications. The complexity of the solid-solid interface structure, together with the experimental challenge of measuring solid-solid interfacial energy often inhibits quantitative treatments of interfacial phenomenon.

One of the most studied types of metal-ceramic interfaces is that between FCC metals and  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> (sapphire). These interfaces are usually produced either by diffusion bonding of a pre-determined orientation [2], or by thin film deposition such as molecular beam epitaxy (MBE) [3]. It should be noted that these preparation techniques do not necessarily produce equilibrated interfaces. The as-bonded or as-deposited interface states often reflect a metastable interface structure and orientation, rather than a thermodynamically equilibrated state. The question of whether the examined interface is equilibrated or not, and whether it reflects the minimum energy configuration of the interface is rarely addressed, although this is a significant driving force for microstructural evolution of interfaces.

One way to equilibrate metal-ceramic interfaces is to dewet thin metallic films on ceramic substrates, which is essentially a disruption of the film driven by the minimization of surface and interfacial energy [4-6]. This process of film agglomeration results in a very large number of isolated particles, which can be investigated separately to achieve very good statistics (Fig. 1). Transmission electron microscopy (TEM) samples can be prepared with a quality good enough for atomistic structure analysis [7], and from the shape of the particles TEM data can provide the means to determine the solid-solid interface energy [4].

In addition to being a good metal-ceramic model system, Ni-alumina interfaces can be found in numerous technological applications. In contrast to the large technological importance of this system, Ni-alumina interfaces were not experimentally studied to the same extent as other metal-alumina interfaces. This is perhaps due to the relatively high melting temperature and/or because of the relatively large surface energy of Ni, which requires an extremely pure environment for model studies [8-9].

Given the importance of the Ni-Al<sub>2</sub>O<sub>3</sub> system, and the questions raised by numerous atomistic simulations of this system, the goal of the present work is to determine the structure and energy of Ni equilibrated in contact with (0001) sapphire. Samples are based on very pure thin Ni films which were dewetted in the solid-state (and under controlled impurity levels and oxygen partial pressure) to reach equilibrium, from which both the interface structure and energy can be determined. For

interface structural analysis, TEM samples were characterized using a monochromated and aberration corrected TEM (Titan 80-300 S/TEM). Two different zone-axes were used to acquire TEM data for subsequent exit wave reconstruction, which was conducted using TrueImage (FEI) from which an atomistic model of the interface was constructed. From the TEM analysis it was found that the interface structure is incoherent, and has reconstructed to form a 2-D interface Bravais lattice of  $2.5\sqrt{3}R30$ . The concept of interfacial reconstruction as an alternative mechanism to semi-coherent interfaces for absorbing strain energy will be discussed.

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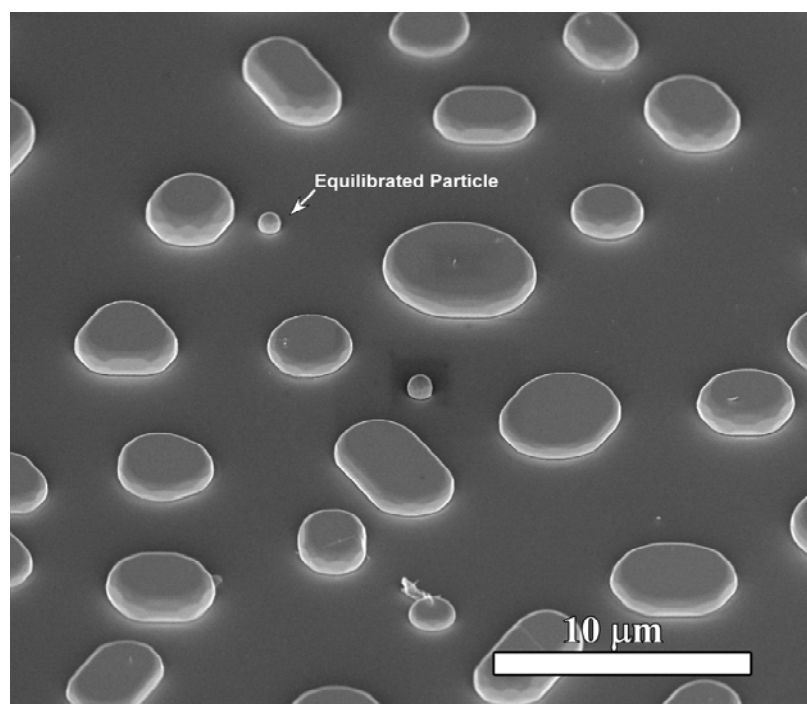


FIG. 1. Secondary electron SEM micrograph of Ni particles dewetted on (0001) sapphire. The smaller particles (arrowed) reached equilibrium and were used for subsequent TEM analysis.