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STRUCTURES OF FCC METAL/FCC OXIDE INTERFACES

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Resume. On a fait croître de façon épitaxiale avec une orientation cube-cube des îlots d’or sur un substrat de MgO. La théorie du réseau-0 prévoit la formation par les dislocations de discordance, d’un réseau carré de dislocations coins espacés de 9.9 nm et avec un vecteur de Burgers de 1/2 a, <110>. Les images sur fond clair et avec faisceaux de faible intensité n’ont pas révélé la présence de ces dislocations. Indirectement, néanmoins la création des dislocations de discordance se manifeste par une faible distortion en rotation des îlots; et l’interface peut être considérée comme constituée de zones cohérentes liées par des bandes incohérentes.

Abstract. Gold islands have been grown epitaxially on an MgO substrate in a cube-cube orientation. Applying the O-lattice theory, misfit dislocations are predicted to form a square network of edge-dislocations spaced 9.9 nm apart, and with a Burgers vector of 1/2 a, <110>. Bright-field and weak-beam images did not reveal the presence of such dislocations. Indirectly, however, the creation of misfit dislocations is shown to manifest itself through a slight rotational distortion of the islands, and the interface can be regarded as consisting of coherent domains bounded by incoherent bands.

1. Introduction. The CSL and O-lattice grain boundary models [1] have previously been shown to be widely applicable to cubic metals, and more recently to ionic solids [2]. Work described by Bonnet and Durand [3] also shows that the DSC-lattice construction can be used to obtain the Burgers vectors of phase boundary dislocations.

The object of the work presented here is to establish if such geometrical models are applicable to a metal-ceramic interface where Au islands are grown epitaxially on MgO (cube-cube orientation). The observations will also be compared to the lock-in model described by Fecht and Gleiter [4].

2. Geometrically Predicted Boundary Structure. The O-lattice, and consequently the misfit dislocation structure of the phase boundary, can be obtained as follows. According to Bollmann [1] the translation vectors, \([x_0]\), giving the positions of points of good fit (i.e. the O-lattice) are given by

\[
[x_0] = (I - A^{-1})^{-1} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} [x]
\]

where the vectors \([x]\) define the primitive reference lattice cell (see Fig. 1a). From Fig. 1a it can also be seen (choosing the MgO lattice as reference) that the appropriate two-dimensional reference matrix is given by

\[
[x] = \begin{bmatrix} a'/2 & a'/2 \\ a'/2 & -a'/2 \end{bmatrix}
\]
Fig. 1. a) Au and MgO hard sphere structures, and b) (110) lattice planes viewed along the [110] direction.

(with \( a' \) = lattice constant of MgO) and the transformation matrix, \( \mathbf{A} \), is the product of a rotation matrix, and a matrix describing the distortion necessary to transform the unit cell of the reference lattice into the unit cell of the other lattice. For the present case this distortion is simply the ratio of the lattice parameters, and the rotation is 0°. Hence

\[
\mathbf{A} = a \begin{bmatrix} \cos 0° & -\sin 0° \\ \sin 0° & \cos 0° \end{bmatrix}
\]

with \( a = a''/a' \) \( (a'' = \text{lattice constant of Au}) \).

This gives
Hence $a'$ with $a' = \frac{2(1-a)}{a'} = 7.0$ nm for the Au-MgO interface.

Interface misfit dislocations are expected to run along the boundaries of the Wigner-Seitz cell of the O-lattice, i.e. along $\langle 110 \rangle$ directions with a spacing equal to $\sqrt{2} \cdot 7.0$ nm = 9.9 nm.

Fig. 1a shows a hard sphere model of the MgO and Au structures. One possible interface structure configuration is depicted in Fig. 1b. The figure shows how lattice planes get gradually more and more out of register, until midway between points of near coincidence $1/2 \cdot a' \langle 110 \rangle$ edge misfit dislocation is accommodated. (The lattice planes are assumed continuous across the interface.) Such a dislocation structure is consistent with the DSC lattice calculations for fcc/fcc systems (Pieraggi [5]). Thus the interface would consist of coherent, square domains bounded by pure edge-dislocations. Such dislocations should be resolved on bright-field as well as on weak-beam images.

3. Specimen Preparation. Specimens suitable for face-on TEM observations of the interface were prepared as follows. 3 mm MgO discs were polished to optical flatness on one side, then dimpled and ion-beam thinned to electron transparancy on the other. The polished face was cleaned by a glow discharge prior to e-beam coating. Before and during deposition the vacuum was $7 \cdot 10^{-3}$ Pa and $7 \cdot 10^{-4}$ Pa, respectively. The Au was deposited at a rate of 0.05 nm/s until an average thickness of 25 nm was reached. The substrate temperature of $750^\circ$ C was retained for 5 mins after coating. Some samples were subsequently tempered for 2 hours at $350^\circ$ C and air. This annealing did not affect the results discussed below.

4. Results and Discussion. Fig. 2a shows a typical Au island with Moire fringes which are characteristic of epitaxial cube-cube growth. The dimensions of the islands studied were (120 ±10) nm, and the following imaging conditions were used in searching for the misfit dislocations: (i) illumination along the [001] zone axis, (ii) $g_{200}$ and $g_{220}$ two-beam bright field imaging, and (iii) ($g$, 4g) weak-beam imaging (with $g = (200)$ or $g = (220)$). Fig. 2 shows examples of such images. The two most noticeable features observed are:

1) The predicted regular array of misfit dislocations is not directly observed. This can be interpreted as follows. (i) The strain surrounding the dislocations is so small that no appreciable contrast can be seen. (ii) The spacing of the dislocation is so small that individual dislocations cannot be resolved, and (iii) no dislocations are present at all. For reasons discussed below, (iii) is not regarded as a plausible explanation for the present case.

2) The Moire patterns are rotated $(7.5 \pm 2.5)^\circ$ w.r.t. the MgO reference lattice. This corresponds to a real rotation of $(0.22 \pm 0.07)^\circ$ of the Au islands. The uncertainty is not caused by experimental errors (the accuracy in analyzing the diffraction pattern is $\pm 0.7^\circ$), but by scattering for different experiments. Six measurements were done for three different islands which resulted in the...
Fig. 2. a) shows 200 Moire cross-fringes (spacing 7.0 nm), illumination along [001], b) $g_{200}$ two-beam bright-field image (fringe spacing 7.0 nm), $g_{220}$ two-beam bright-field (fringe spacing 4.9 nm), and d) a weak-beam image, $s = 0.02$ A$^{-1}$. Only weak thickness fringes are seen.
different rotation angles. Such rotations can also be confirmed by convergent beam reflections, as shown in Fig. 3.

Similar rotations of Moire patterns as a result of microstructural distortions have previously been observed in Pt/Au, Sn/SnTe, Ag/MoS₂ and Cu/ Ni systems (see [6, 7] for a review). For a strongly bound system, as Au/MgO, one expects that the rotation involves a distortion of the lattice unit cell of the Au island. Such a distortion causes the creation of misfit dislocations and relaxation of misfit strain. Therefore, misfit dislocations have to be present at the studied metal/ceramic interface.

With this theory in mind, and referring to the model described in the introduction, the TEM observations can be interpreted as being an indirect confirmation of the presence of misfit dislocations. In the vicinity of the dislocation core, however, there is a loss of coherency, and the lattice planes are not continuous as depicted in Fig. 1b. The reduction in coherency strain is sufficient to render the dislocations invisible. The interphase can therefore be thought of as consisting of coherent, however small, domains bound by incoherent bands.

Such observations are consistent with the lock-in model described by Fecht and Gleiter [4]. According to this model, a low energy configuration is reached when low index planes and close-packed directions (⟨100⟩, ⟨110⟩) of the two phases are parallel. The close-packed directions on the surface of the ionic crystals are separated by valleys, and it is interesting to note from the hard sphere model of Fig. 1a that the valleys defined by the row of Mg ions running in ⟨110⟩ directions are wider than the valleys parallel to the closer packed ⟨100⟩ directions. The four Au atoms of the primitive unit cell may form a lock-in configuration by sitting on top of four Mg lock-in atoms. As the Au
island grows in the $\langle 110 \rangle$ directions, the $\langle 110 \rangle$ planes perpendicular to the interface will become more and more out of register (Fig. 1b). However, as the Au atoms are capable of sliding along $\langle 110 \rangle$ valleys, both coherency strain and the degree of coherency will be reduced. It should also be noted that during this sliding process the Au atoms have to overcome a certain potential barrier.

References