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ANOTHER MODEL FOR THE CONDENSATION OF GOLD ON TANTALUM (100)

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Recently, Huber and Oudar [1] have proposed a new model for the interpretation of the LEED diagrams. They propose a high symmetry of the coincidence mesh. Biberian and Huber [2] have applied this model to interpret some of the diagrams obtained during the adsorption of a metal on a (100) face of a metal. In the case of lead adsorbed on gold (100), they interpret the $\begin{pmatrix} 2 & \bar{1} \\ 1 & 1 \end{pmatrix}$ (c($3\sqrt{2} \times \sqrt{2}$)45°) structure with a model in which the adsorbed atoms form double rows (see fig. 1). In this model all the adatoms are identical and are in the four-fold symmetry sites. The diagram is very similar to the one observed by Elliot [3] in the case of gold adsorbed on tantalum (100), but with a splitting of the beans in the [11] direction. Elliott [3] propose a model (see fig. 6a in ref. [3]) with double chains, but it is quite surprising that the chains being so distant, and the interaction between the gold atoms being small compared to the gold–tantalum interaction, the chains can

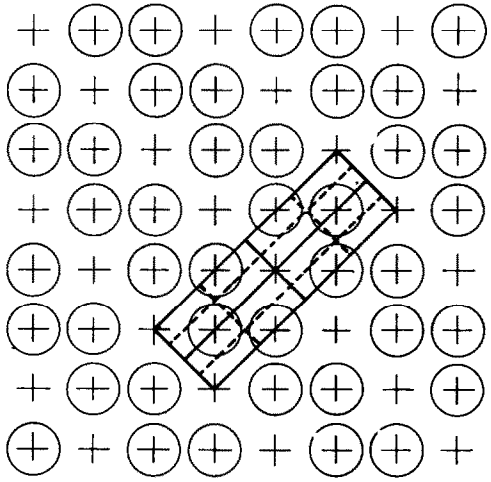

Fig. 1. The position of the gold atoms on tantalum (100), respecting the C2mm symmetry of the c($3\sqrt{2} \times \sqrt{2}$)45° or $\begin{pmatrix} 2 & \bar{1} \\ 1 & 1 \end{pmatrix}$ structure. There is formation of hexagons of gold atoms. The open circles represent the gold atoms, and the crosses, the four-fold symmetry sites.

be so different in terms of the position of the gold atoms onto the tantalum (100) surface.

We propose here that the structure is a $\begin{pmatrix} 2 & \bar{1} \\ 1 & 1 \end{pmatrix}$ (c($3\sqrt{2} \times \sqrt{2}$)45°), but with a splitting due to antiphase domains [4]. The gold atoms having a diameter of 2.88 Å, and the tantalum–tantalum distance on the (100) surface being 3.30 Å, there is no stoichiometric problem for the adsorption of the gold atoms in the four-fold symmetry sites. It is even quite possible, that due to the above remark, the gold atoms move slightly from their proposed position, but respecting the symmetries of the C2mm bidimensional space group to be at the closest possible distance from each other, that is 2.88 Å (see fig. 2). This might cause a deformation of the first layer of tantalum, always with respect of the C2mm space group symmetries, and be at the origin of the antiphase domains which create the splitting of the extra beams. This model corresponds to an occupation of 2/3 of the four-fold symmetry sites of the (100) tantalum. This value is in agreement with the AES measurements [3].

After the completion of the first monolayer, the diffraction diagram is identical. Elliott [3] proposes a new mesh, smaller than the first one, but giving the same diffraction spots (see fig. 6b of ref. [3]). Then according to this model, the adsorbed gold is a dense monolayer of pseudohexagonal structure. This structure persists up to 16 layers of gold, and after an annealing of the crystal at an elevated tempera-

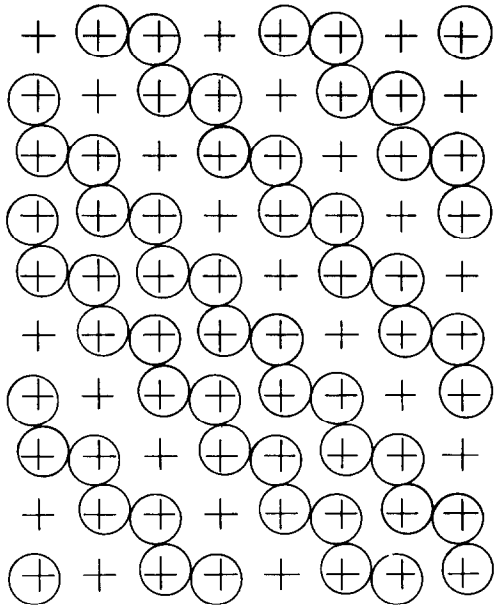

Fig. 2. The same model, but the gold atoms are moved at the closest possible distance, respecting the symmetries of the coincidence mesh. There is formation of chains. We have represented two possible antiphase domains.

ture, a (1 × 1) structure appears, but with broad and diffuse spots. AES indicates 1/2 a monolayer of gold.

Using the model proposed here, we can see on fig. 1 that there is a four-fold symmetry site in each hexagon of gold atoms, and the adsorption of a gold atom on this site does not change the coincidence mesh, but only the contain. One can argue that we should have a (1 × 1) structure because all the sites are occupied, but as proposed before, it is probable that the chains are deformed because of the gold–gold interaction.

So this model suggests a growth of the gold layer with (100)gold//(100)tantalum. An annealing of the crystal creates a desorption of diffusion of gold and restores a (1 × 1) structure with a coverage of half a monolayer. This can be obtained by breaking the chains and the creation of two-dimensional islands of (1 × 1) gold of small size. This explains the broadening of the diffraction spots.

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