

SURFACE SCIENCE LETTERS

**COMMENTS ON "A RE-INTERPRETATION OF THE LEED
STRUCTURES FORMED BY IODINE ON W(110)" BY
P.A. DOWBEN AND R.G. JONES**

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In this paper, the adsorption of iodine on W(110) surfaces is re-examined. It is shown that a model based on regularly spaced anti-phase boundaries can explain the LEED patterns and the relative Auger intensities.

Recently, Dowben and Jones (DJ) [1] have re-examined the LEED structures formed by iodine adsorption on W(110) studied earlier by Avery [2]. In this new interpretation, DJ use non-coincident adatom nets which change size in response to changes in surface coverage, while Avery used a model based on regularly spaced anti-phase boundaries.

The purpose of these comments is to discuss DJ's criticism on Avery's model and to modify this model in order to take into account this criticism.

The first point developed by DJ [1] to reject Avery's [2] model is that similar behaviour has been found for adsorption of halogens and halocarbons on Fe (100) [3-8], and for iodine on W(100) [9,10], and that this behaviour has been successfully interpreted using non-coincident nets. However, those systems could very well be interpreted using models based on anti-phase domains. Very similar LEED patterns have been interpreted this way. Huber and Oudar [11] have given a first approach of this model that has been applied to many systems: sulfur on (110) molybdenum [12], platinum [13] and palladium [14], metals on (100) surfaces of metals [15], and carbon monoxide on (100) metal surfaces [16,17]. The existence of walls between anti-phase domains has been used to explain the non-commensurate structures of rare gases adsorbed on the basal plane of graphite [18-21] and also proposed for the reconstruction of the (100) surfaces of platinum and gold [22].

The second point developed by DJ [1] is that "the anti-phase boundaries have to move and/or rotate relative to each other in a precise manner if the overlayer structure is to produce sharp continuously moving beams in the LEED pattern". To understand this point, it has to be recalled that the

patterns are observable only at low temperature; at room temperature and above, the structure disappears, indicating a high degree of disordering and a large mobility of the adatoms. An examination of the LEED patterns published by Avery [2] indicates that the LEED beams are not sharp, but rather broad, and that disorder coexists with the ordered structures. In fact, the models proposed by Avery are rather schematic, the real surface might not be so perfect as in the ideal model. The last point, the coverages predicted by Avery [2] for the different surface structures using the anti-phase boundaries, are inconsistent with the experimentally determined values. It is the purpose of this paper to modify the models proposed by Avery [2] in order to obtain coverages compatible with the experimental data.

The first two phases are the γ and α phases which are respectively splitted $p(2 \times 2)$ and $p(2 \times 1)$ structures. Fig. 1 shows possible models for these structures assuming that iodine is molecularly adsorbed at these high coverages and low temperatures as suggested by Avery [2]. The coverages are then 0.75 and 0.5, respectively. It has to be noted that DJ [1] do not give any interpretation of the γ phase.

At higher desorption temperatures, the β_1 phase appears. The iodine is dissociated in this phase. Four different structures of the β_1 phase are represented in fig. 2, the coverages being 0.5, 0.47, 0.45 and 0.43 for the β_1 phases appearing at 530, 600, 650 and 700 K, respectively.

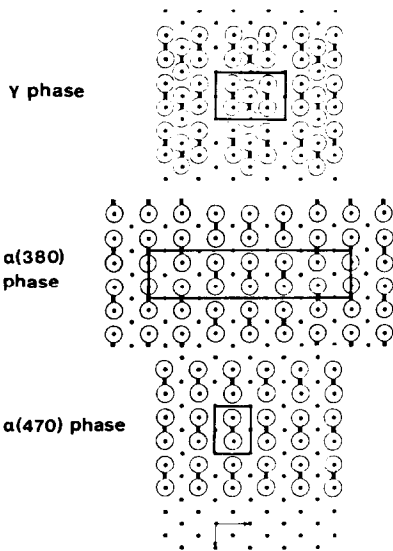


Fig. 1. A representation of the (2×2) γ phase, the $c(6 \times 2)$ $\alpha(380)$ phase and the $p(2 \times 1)$ $\alpha(470)$ phase. The joint open circles represent the iodine molecules and the dots the tungsten surface atoms. The respective position of the iodine molecules and of the tungsten surface atoms is arbitrary.

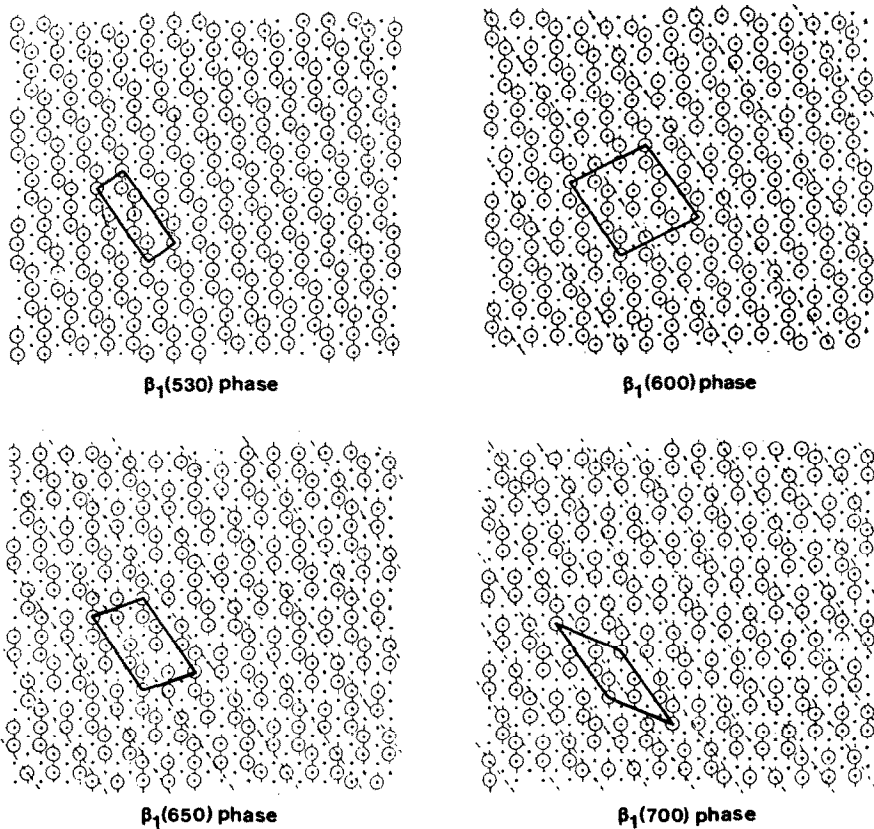


Fig. 2. The β_1 phases. The iodine is atomically adsorbed.

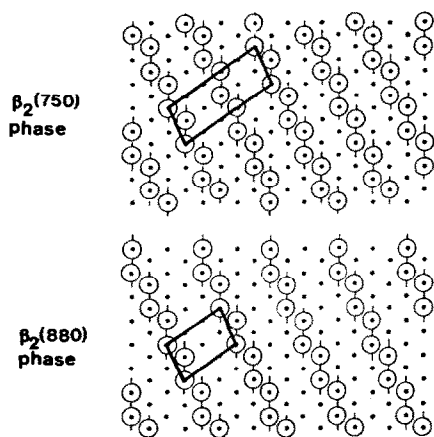


Fig. 3. The β_2 phases.

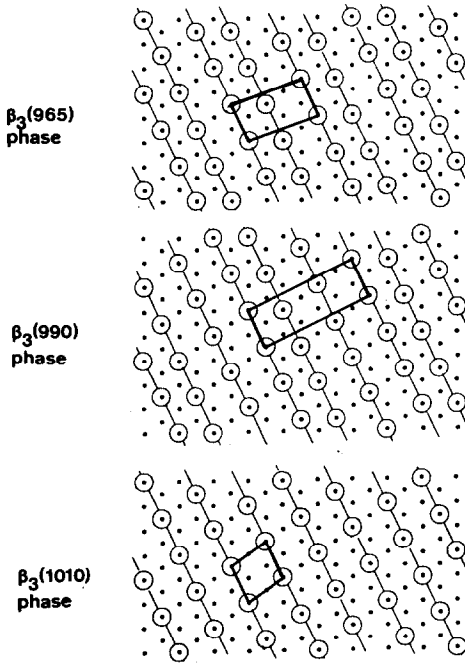


Fig. 4. The β_3 phases.

Two structures of the β_2 phase are shown in fig. 3: the $\beta_2(750)$ structure with a coverage of 0.40 and the $\beta_2(880)$ structure with a coverage of 0.33.

The low coverage phase β_3 is described in fig. 4. The coverages are 0.29, 0.27 and 0.25 for the 965, 990 and 1010 K structures, respectively.

Fig. 5 shows a comparison between the experimental coverage determined by AES [2] and the theoretical coverage deduced from this model. The agreement is excellent, better than the one found by DJ [1], especially for the $\alpha(380)$ phase.

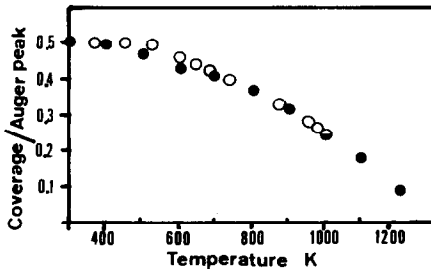


Fig. 5. A comparison between coverages determined by AES (●) and by coverages determined by the models described in the paper (○).

In conclusion, the model described here is in agreement with the LEED and AES data. At all coverages, the adsorption is two-dimensional, molecular below and atomic above 500 K. The various LEED structures are interpreted by anti-phase domains.

Note: The positions of the iodine atoms drawn in the figures are only schematic representations, the actual intramolecular, intermolecular or interatomic distances are not measurable in the figures because of possible relaxations to fill the voids in the anti-phase boundaries.

References

- [1] P.A. Dowben and R.G. Jones, *Surface Sci.* 105 (1981) 334.
- [2] N.R. Avery, *Surface Sci.* 43 (1974) 101.
- [3] R.G. Jones, PhD Thesis, Cambridge (1978).
- [4] P.A. Dowben and R.G. Jones, *Surface Sci.* 84 (1979) 449.
- [5] R.G. Jones and D.L. Perry, *Surface Sci.* 88 (1979) 331.
- [6] P.A. Dowben and R.G. Jones, *Surface Sci.* 88 (1979) 348.
- [7] R.G. Jones, *Surface Sci.* 88 (1979) 367.
- [8] P.A. Dowben and R.G. Jones, *Surface Sci.* 89 (1979) 114.
- [9] J.J. Laner and J. Morrisson, *Surface Sci.* 17 (1969) 469.
- [10] K.J. Rawlings, G.G. Price and B.J. Hopkins, *Surface Sci.* 95 (1980) 245.
- [11] M. Huber and J. Oudar, *Surface Sci.* 47 (1975) 605.
- [12] L. Peralta, Y. Berthier and J. Oudar, *Surface Sci.* 55 (1976) 199.
- [13] Y. Berthier, J. Oudar and M. Huber, *Surface Sci.* 65 (1977) 361.
- [14] L. Peralta, Y. Berthier and M. Huber, *Surface Sci.* 104 (1981) 435.
- [15] J.P. Biberian and M. Huber, *Surface Sci.* 55 (1976) 259.
- [16] J.P. Biberian and M.A. Van Hove, *Conf. on Vibrations at Surfaces*, Namur, 1980.
- [17] J.P. Biberian and M.A. Van Hove, to be published.
- [18] P.S. Schabes-Retchkiman and J.A. Venables, *Surface Sci.* 105 (1981) 536.
- [19] H. Shiba, *J. Phys. Soc. Japan* 48 (1980) 211.
- [20] J. Villain, *Phys. Rev. Letters* 41 (1978) 36.
- [21] J. Villain, *Surface Sci.* 97 (1980) 219.
- [22] M.A. Van Hove, R.J. Koestner, P.C. Stair, J.P. Biberian, L.L. Kesmodel, I. Bartos and G.A. Somorjai, *Surface Sci.* 103 (1981) 218.