LEED STUDIES OF SURFACE STRUCTURES
ON AN UNCLEANED (100) FACE OF IRON WHISKERS

M. LÁZNIČKA

Institute of Solid State Physics, Czechosl. Acad. Sci., Prague

The uncleaned (100) surfaces of iron whiskers have been studied by means of LEED. The heating of samples to elevated temperatures was the only treatment used in the experiments. It was shown by means of a simple kinematical theory that the geometric features of diffraction patterns and the relative intensities of diffraction spots can be understood if one supposes periodic ordered displacements of undisturbed areas of the 2D lattice present on the surface under examination.

1. INTRODUCTION

In an examination of surface structures by means of LEED, most investigators carried out their experiments on clean surfaces. This is due to the fact that an interpretation of low-energy diffraction features at the same time is very difficult, since the interaction of low-energy electrons with a solid state is more complicated than that of high-energy electrons and not yet understood in all its details.

An ion bombardment, which undoubtedly changes the properties of the examined surface drastically, is the method that is often used for the cleaning of surfaces. In future, however, it will be important, from the practical point of view, to deal with the surfaces having properties the same or nearly the same as on real surfaces. With regard to this fact, heating to elevated temperatures was the only treatment of our samples in UHV.

2. EXPERIMENTAL

The investigations reported here were performed with Varian LEED apparatus. The iron whiskers were approximately 0.5—1 cm long and 0.2—0.3 mm wide.

The main requirement for the crystal treatment is to heat it in such a way that the small sample should not be stressed. Heating of the sample by means of a direct flow of electric current is possible, of course, but it leads to difficulties. Firstly, fixed contacts cannot be used to prevent the stress of the sample and, secondly, the ends of the sample are cooled down so that the temperature is not the same all over the surface.

In order to avoid these difficulties we used another method, schematically shown in Fig. 1.

Fig. 1. Arrangement for heating of samples. a — el. leads, b — Mo rod, c — insulation, d — Mo cylinder, e — W spiral, f — iron whisker.

*) Cukrovarnická 10, Praha 6, Czechoslovakia.
At the end of the crystal manipulator a Mo rod was placed, the diameter of which was 1 mm, and the iron whisker was spot welded to the end of this rod. The electrons emitted from a W spiral were accelerated towards the Mo rod so that the latter was heated by means of electron bombardment and the iron whisker by heat conduction.

The W spiral was shielded by a Mo cylinder in order to prevent the disturbance of diffraction image observation by light from the W spiral and the contamination of the iron whisker. We can see the shadow of the manipulator, which covers some of the diffraction spots in all of our diffraction patterns.

The temperature of the sample was measured in two different ways. Firstly, a spot pyrometer was used for measuring at higher temperatures and, secondly, a thermocouple which was used only after all the diffraction experiments were finished, because it was then spot welded to the iron whisker, the use of which was excluded from further diffraction experiments. In order to determine the temperatures at different stages of our experiment by means of the thermocouple, all of the experimental conditions were repeated in the same way as in the diffraction measurements. The accuracy of such temperature measurements was undoubtedly not very high and each temperature value must be considered as informative.

The diffraction experiments were not started until a vacuum of the order of $10^{-10}$ Torr had been reached. The intensive background was the first to become visible on the diffraction screen.

Heating of the sample to 500 °C and the following cooling to room temperature leads to the diffraction pattern of Fig. 2 (Appendix I, p. 1314a) taken at 58 eV. The heating was done in steps of about 50 °C and each of them was followed by cooling to room temperature. The diffraction pattern of Fig. 3 (Appendix I, p. 1314a), taken at 59 eV, was observed as soon as a temperature above 550 °C had been reached.

The following steps of heating did not lead to a change in the diffraction pattern until a temperature of 750 °C was reached. The diffraction pattern of Fig. 3 changed at this temperature to the diffraction pattern of Fig. 4 (Appendix I, p. 1314b).

The structure that corresponds to the diffraction pattern of Fig. 4 did not change until a temperature of 850 °C was reached. This was the highest temperature used in our experiments.

We studied the surfaces of approximately 10 different samples and the results were reproducible.

3. DISCUSSION

The diffraction pattern of Fig. 2 has already been observed and the appertaining structure Fe(100) c(2 × 2)* - ? described by Szostak and Molière [1] who took into account, in analogy with Raether [2], the possibility of explaining the diffraction features on the assumption that two-dimensional antiphase areas are present on the examined surface, but they did not deal further with this problem.

The choice of a coordinate system was found to be suitable if it was rotated 45° with respect to the unit vectors of the substrate lattice. In such a way we can formally use the structure c(2 × 2) as a basic structure (1 × 1) and the surface structures, the diffraction patterns of which correspond to Figs. 2 and 3, are then as the examined superstructures of this basic structure.

We choose the basic translations $\mathbf{a}_1$ and $\mathbf{a}_2$ in the directions {11} of the Fe substrate,