PACS number(s): 31.15.Ar, 79.70.+q

A STATISTICAL METHOD OF PROCESSING THE IMAGE FROM THE FIELD ION MICROSCOPE

A. Tomaszewska, Z. Stępień, P. Sawicki

Institute of Physics, The Jan Dlugosz University, Al. Armii Krajowej 13/15, 42 – 201 Częstochowa, Poland

Interpretation of images obtained by field ion microscopy (FIM), that are due to imaging the surfaces such as those of disordered solid solutions, often faces with difficulties. Their main reason is the topological disorder of the surface on the atomic scale. This paper presents a method of elaboration of FIM image, which consists in statistical analysis of the distribution of distances between neighboring points of the FIM image which gives a pattern of array of the most protruding atoms of the hemispherical surface of the micromonocrystal that is the ending of the field emitter tip. The method has been employed to elaborate the patterns of FIM imaging a palladium surface after hydrogen adsorption in the high electric field.

Key words: hydrogen, palladium, field ion microscopy.

More and more interest in materials that have a disordered structure is notably stimulated by their importance in technology. During research into such materials the problem of stating their structure often appears. Field ion microscopy (FIM) [1] is one of the techniques that enable to examine on the atomic scale the surface of disordered layers of solid. Structural information on the surface under investigation, bt the FIM technique, is obtained from analysis of relative positions as well as the intensities and shape of bright image spots on the screen of the microscope that compose the pattern of the arrangement of surface atoms of the rougly hemispherical microcrystal. FIM patterns of the disordered surface display an irregular arrangement of the atoms, where the sets of concentric rings of net plane edges typical of perfect lattices are lacking.

From the point of view of chemical bonding the most essential is short range order which, for the three- dimensional space, can be characterized by giving the number of nearest neighbors. Generalization of the notion of coordination number, onto a sequence of numbers specifying the numbers of neighbors in successive layers surrounding a given atom, leads to a definition of the radial function (RDF). The RDF is useful in structure research and is commonly applied to characterize structure of amorphous bodies. It can be obtained, via Fourier transform, from the diffraction experiments. In the case of the surface the function is modified and is called the pair correlation function (PCF). A modification of the latter is the distribution function for angles between the directions to nearest neighbors (ADF). These both functions were applied to interpret FIM patterns from imaging the surface of metallic glasses [2, 3], which yielded information on the symmetry of the surface structures of metallic glass 'molecules'. Due to certain ambiguities in interpretation the method is not widely used for analysis of FIM

patterns of disordered surfaces. In many instances we deal with observations of the effect of the effect of gas atoms on a crystal surface that was cleaned by thermal treatment. The FIM pattern of such a surface reveals some elements of symmetry, however, these are strongly deformed by the presence of the thermic disorder. In this case much information seems to be available by analyzing the nearest-neighbor distance distribution.

If we consider the positions of atoms lying on an ideal crystal plane of high symmetry of an fcc crystal, such as in Fig. 1, then it can be easy seen there are several typical interatomic distances present.
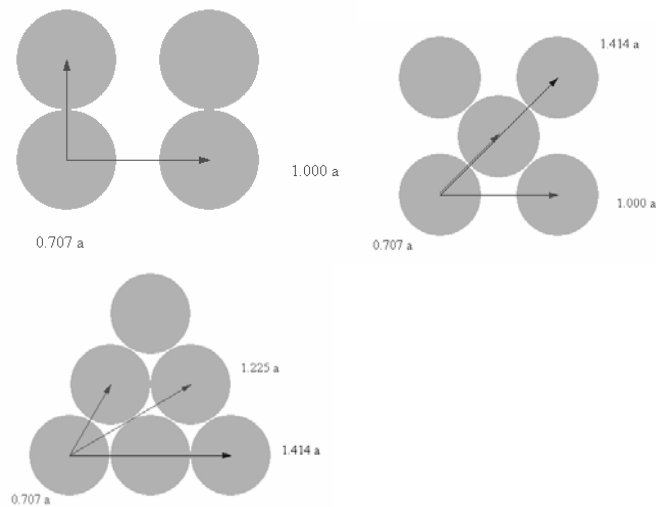

Fig. 1. The high symmetry plane o fan fcc metal: (110), (100) and (111) with a corresponding typical interatomic distances

Expressed in a unit of the lattice parameter a the first four can be written as $a/\sqrt{2}$, a, $a\sqrt{2}/\sqrt{3}$, and $a\sqrt{2}$. Thus, the theoretical distance distribution function (DDF) for an atomically perfect surface is given by a discrete sequence of values characteristic of a given crystallographic plane. Any change in surface structure, for instance a one upon the process of rearrangement or chemisorption, should result in recording a new DDF that is characteristic of this process.

The question whether DDF is changed by certain process was examined for the case of hydrogen interaction with a palladium surface in the high electric field [4]. An FIM pattern of the clean surface of the palladium field emitter is shown in Fig. 2.

Fig. 2. FIM pattern of the clean palladium surface

Due to the preannealing of the field emitter at a temperature of 1000 K, a considerable thermic disorder is evident on the surface. DDF as measured from this record is shown in Fig. 3.
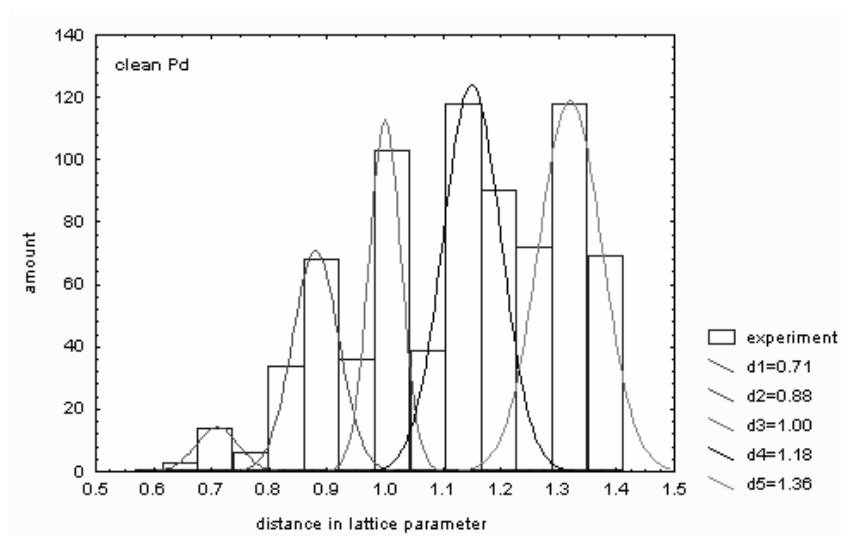

Fig. 3. The theoretical distance distribution function (DDF) for a clean palladium surface

Since the distances collected are burdened with the measurement error, the measured function ρ is a convolution of the (discrete) theoretical function and the measurement uncertainty function. Hence, Gaussian distributions were fitted to the experimental curve to attain the best fit factor. This procedure resulted in obtaining five Gaussians with a fit factor of R=0,9999. The curves are also shown in t he figure. Comparison of the experimental distribution to the theoretical one shows the following distances occurring on the surface, in units of lattice parameter, $0,71 \pm 0,04$, $0,88 \pm 0,04$, $1,00 \pm 0,03$, $1,18 \pm 0,06$ and $1,36 \pm 0,06$. The values obtained are characteristic of the planes (100), (110) and (111). An exception is a distance of 0.88 which does not occur in the fcc structure. Since in the case of palladium a stable surface reconstruction does not appear [5], this effect may be due to the roughening process which leads to the formation of rcp (random close packed) structure [6]. The filling factor for rcp structure is 0,637, which in comparison to the 0,7405 for fcc gives filling density of 86% that for fcc lattice. This means that the spacing between some nearest neighbors would be slightly in excess

of that for fcc structure and lie in the range $\left(a/\sqrt{2}, a\right)$.

Fig. 4 shows a FIM pattern of the palladium surface after the hydrogen adsorption process in the high electric field.
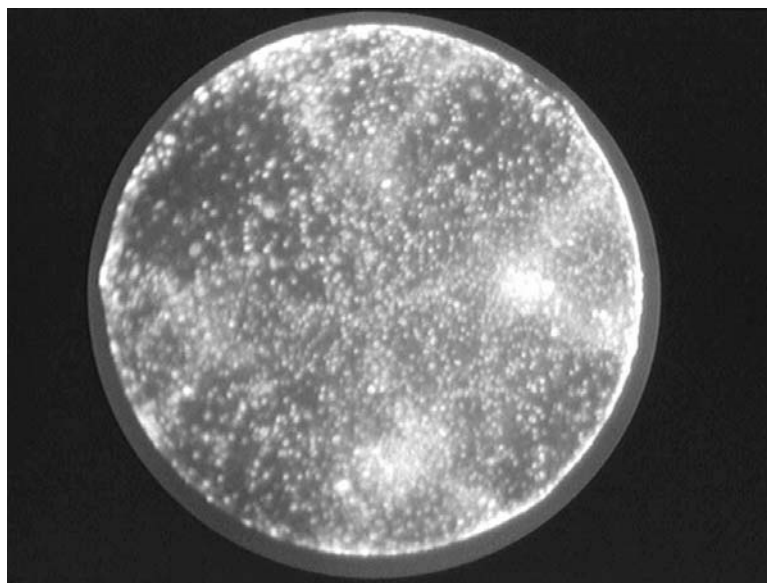

Fig. 4. FIM pattern of the palladium surface after the hydrogen adsorption

The imaging was made under the same experimental conditions as that of Fig. 2. It should be noted here that FIM imaging does not display hydrogen species on FIM images [7]. The distance distribution function which was obtained for the palladium surface after field adsorption of hydrogen is shown in Fig. 5.
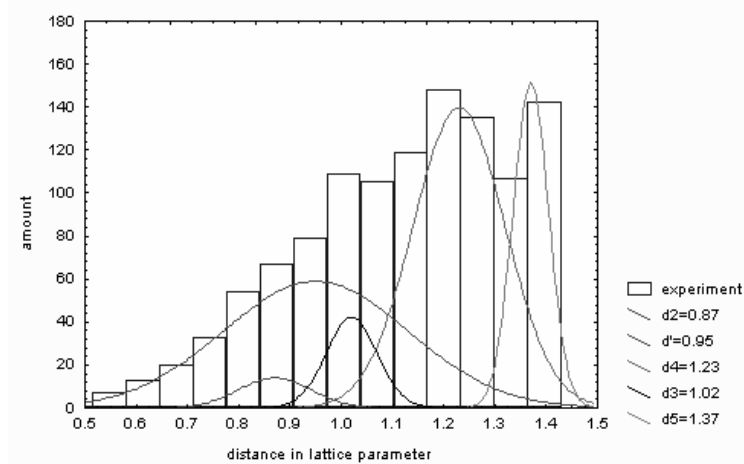
Fig. 5.   The theoretical distance distribution function (DDF) for a palladium surface after field adsorption of hydrogen

The Gaussians' fitting procedure, with a fit factor of R=0,9987 gives the following values of characteristic distances: $0,87 \pm 0,07$, $0,95 \pm 0,18$, $1,02 \pm 0,05$, $1,23 \pm 0,09$ and $1,37 \pm 0,04$. It is clearly seen that the palladium surface has drastically changed. Apart from the broadening of previous peaks and the decay of a peak corresponding to $a/\sqrt{2}$ distance, a broad peak with a maximum of 0,95 has appeared. This peak reflects the formation of palladium- hydrogen surface compounds, which is responsible for the occurrence of the interatomic distances ranging between 0,75 a and about 1,13 a on the palladium surface. Such a considerable difference in distance distribution between the non-adsorbed and adsorbed states indicates a great sensitivity of the DDF shape with respect to the surface structure of the specimen under investigation. This permits to believe that the method can be useful in study of similar adsorption systems by the FIM techniques.

––––––––––––––––––

1. *Müller E.W., Tsong T.T.* Field Ion Microscopy, Principles and Applications, Elsevier, New York. 1969.
2. *Jacobaeus P., Madsen J.U., Kragh F.* R.M.J. Cotterill, Phil. Mag. 1980. Vol. 41. P. 11–20.
3. *Kanitkar M.M., Shukla V.N., Kanitkar P.L., Joag D.S.* Solid St. Comm. 1984. Vol. 50. P. 817–819.
4. *Stępień Z.M., Tsong T.T.* Surf. Sci. 1988. Vol. 409. P. 57.
5. *Christmann K.* Prog. Surf. Sci. 1995. Vol. 48. P. 15–26.
6. *Bernal J.D.* Nature. 1960. Vol. 185. P. 68.
7. *Tsong T.T.* Atom-probe Field Ion Microscopy, Cambridge University Press, Cambridge, 1990.

СТАТИСТИЧНИЙ МЕТОД ОБРОБКИ ЗОБРАЖЕНЬ, ОТРИМАНИХ ЗА ДОПОМОГОЮ ПОЛЬОВОГО ІОННОГО МІКРОСКОПА

А. Томашевська, З. Стенпіень, П. Савіцкі

Інститут фізики, університет імені Яна Длугоша
вул. Армії Крайовей 13/15, 42-201 Ченстохова, Республіка Польща

Інтерпретація зображень, отриманих за допомогою польового іонного мікроскопа, таких, наприклад, як зображення поверхні невпорядкованих твердих розчинів, часто є досить проблематичною. Основна проблема полягає в топологічному розвпорядкуванні поверхні на атомарному рівні. У статті проаналізовано внесок відстаней між сусідніми пікселями зображення, що дає змогу створити модель для групи найвипукліших атомів напівсферичної поверхні мікрокристала, який розміщений на межі поля емітера. Метод було застосовано для обробки зображень поверхні паладію після адсорбції водню в сильному електричному полі.

Ключові слова: водень, паладій, польовий іонний мікроскоп.