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Photoelectron diffraction from random surface alloys: critique of calculational methods

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Abstract

For random single crystal alloys, the lack of periodicity parallel to the surface, which is consequence of the substitutional disorder, complicates the calculation of photoelectron diffraction (PD) patterns. One way to calculate PD spectra from random surface alloys is to evaluate the spectra for each member of the complete ensemble of configurations and then to sum appropriately to generate the PD spectra from the alloy. The number of different configurations is very large, which makes this approach very time consuming computationally. A computationally efficient approximation, which has had success in applications to low energy electron diffraction from random alloys, is the average *t*-matrix approximation (ATA), where the scattering properties are described by an effective *t*-matrix. In this work we compare the ATA with the average over configuration within the context of the cluster-based PD theory and compare the results of both methods with experimental data from a random surface alloy, namely Pd on Cu(1 1 1). The results of this study indicate that the ATA is efficient in extracting structural and concentration information. Cluster details can be obtained from the configuration average method. Furthermore, the ATA is useful in determining the best parameters (energy, angles, etc.) to be used in an experiment.

Keywords: Photoelectron diffraction; Alloys; Surface structure, morphology, roughness, and topography

1. Introduction

In the last few years special attention has been paid to the properties of surface alloys prepared by the controlled deposition of metal on metal surfaces [1–8]. In the surface alloy formation process, the evaporated metal substitutes the substrate metal atoms within a few layers from the surface, yielding a mixed and often ordered array, even between metals which are immiscible in the bulk [2–5]. Fundamental questions which arise naturally regard the relation of the structural and electronic properties of these surface alloys to those of the surfaces of the corresponding bulk alloys, the diffusion of the evaporated metal, and the physical processes responsible for the formation of surface alloys of metals immiscible in the bulk. From the technological point of view, the study of the properties of surface alloys is motivated, for example, by the need to understand the influence of thin intermixed alloy layers on subsequent epitaxial growth and by the use of surface alloys as model substrates to study the effect of alloying on gas adsorption and surface-catalyzed reactions.

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Among all the bimetallic systems, the study of surface alloys obtained by the deposition of palladium on low Miller index surfaces of copper has received considerable attention due to the fact that CuPd alloys are used in industry, for example, for CO and alkene oxidation [9], ethanol decomposition [10] and CO, benzene and toluene hydrogenation [11]. Several experimental studies [12–17] demonstrate the formation of a substitutionally ordered alloy in Pd/Cu(1 0 0) and Pd/Cu(1 1 0), in agreement with theoretical predictions [18,19]. The situation for Pd on Cu(1 1 1) is somewhat different, however. Available experimental results indicate substitutionally disordered superficial alloying, in contrast with theoretical predictions of ordered phases from total energy calculations results [20–22].

Low energy electron diffraction (LEED) [23,24] is one of the few experimental techniques capable of yielding information concerning structure and segregration profiles of substitutionally disordered alloys and it has been successfully applied to the study of surfaces of binary [25–28] and ternary [29] alloys. In order to correctly model the effects of substitutional disorder, LEED theory makes use of such methods as the average *t*-matrix approximation (ATA) [30] and the coherent potential approximation (CPA) [31]. The ATA represents the random alloy local densities of states much more poorly than does the CPA in band structure calculations [32,33]. Crampin and Rous [34], however, demonstrated the validity of using the ATA approximation in LEED by comparing theoretical LEED intensities as functions of primary energy (i.e., LEED profiles) calculated with both the ATA and CPA for $Ni_xPt_{(1-x)}$(1 0 0). They found that the ATA and CPA lead to LEED profiles which are in very close agreement for all of the alloy compositions considered.

Over the last years photoelectron diffraction (PD) has evolved into a widely accepted technique for obtaining detailed information about surface structure [35–43]. This local diffraction technique probes short range order around the emitter and a broad variety of surfaces have been studied including metals, semiconductors, oxides, systems exhibiting surface core-level shifts, absorbed atoms and molecules, epitaxial overlayers and atoms at buried interfaces. It appears, however, that no attempt has been made to apply this technique to the study of segregation profiles and structure determinations of random surface alloys. In view of our comments regarding LEED from random surface alloys, it is natural to inquire into the validity of applying such a computationally efficient technique as the ATA to the analysis of PD spectra from random alloys. In this study we implemented the ATA approximation as well as the statistically based average over configurations (AOC) approach within PD theory. Because of the uncertainties regarding the structure of Pd/Cu(1 1 1), we compare the theoretical PD spectra obtained with both approaches with experimental PD spectra from Pd/Cu(1 1 1) collected at the SGM beamline at the Brazilian National Synchrotron Laboratory (LNLS) [22]. The influence of the electron kinetic energy on the concentration and segregation profile determination is also addressed.

2. Theoretical approaches to deal with random systems

The underlying difficulty encountered when one attempts the calculation of PD curves from random surface alloys is the lack of periodicity parallel to the surface resulting from the substitutional disorder. The substitutional disorder breaks the long range order parallel to the surface, which makes it impossible to apply conventional methods based on two dimensional translational invariance to the calculation of PD spectra. The same difficulty appears in LEED theory and is addressed by using either the ATA or the CPA methods [34,44]. These approximations can also be implemented in PD theories in order to model disordered surfaces. Since PD does not involve long-range translational order, cluster-based theories are inherently more suitable for PD modeling. LEED theory, on the other hand, requires the assumption of full translational symmetry parallel to the surface. Because of the nature of the cluster-based PD theories, statistical methods, based on averaging diffraction curves from several random configurations, are also easily implemented. In Sections 2.1 and 2.2, respectively, we

describe the way we used the ATA and the AOC methods.

2.1. Average t-matrix Approximation

In the ATA approximation the substitutional disorder is incorporated indirectly and the random alloy is modeled by an effective ordered system. The atomic scattering properties of the effective ordered system is then described by an effective scattering matrix (t-matrix) calculated by a simple linear combination of the t-matrices of the individual components of the alloy. Restricting ourselves to the case of binary surface alloys composed of atoms A and B, and keeping in mind that the composition may be layer dependent due to segregation processes, the ATA effective t-matrix is given by:

$$t^i_{\mathrm{ATA}} = x_i t_{\mathrm{A}} + (1 - x_i) t_{\mathrm{B}}. \tag{1}$$

x_i is the concentration of element A in the atomic layer i ($i = 1$ being the topmost surface layer) and $t_{\mathrm{A(B)}}$ is the conventional atomic t-matrix for atom type A(B) obtained from the multiple scattering formalism [45]. In terms of the atomic phase-shifts for atom A, $\delta_l(\mathrm{A})$, t_{A} is given by

$$t_{\mathrm{A}} = \mathrm{i}e^{\mathrm{i}\delta_l(\mathrm{A})} \sin \delta_l(\mathrm{A}) \tag{2}$$

with an analogous result for t_{B}.

With this approximation the problem becomes identical to that for a perfect lattice, so that traditional methods used in ordered systems can be applied.

2.2. Average over configurations

In this statistical method, we obtain the PD spectra for a given concentration x of atom type A by summing the PD curves from the complete ensemble N of structural configurations (Fig. 1). It is important to point out that in this approach no average of the individual t-matrices is performed. For the case of the binary surface alloy $\mathrm{A}_x\mathrm{B}_{(1-x)}$, the final PD intensity can be written as:

$$I_{\mathrm{A}}(\theta, \phi, \vec{k}; x) = \frac{\sum_{j=1}^{N} I^j_{\mathrm{A}}(\theta, \phi, \vec{k}; x)}{N}, \tag{3}$$

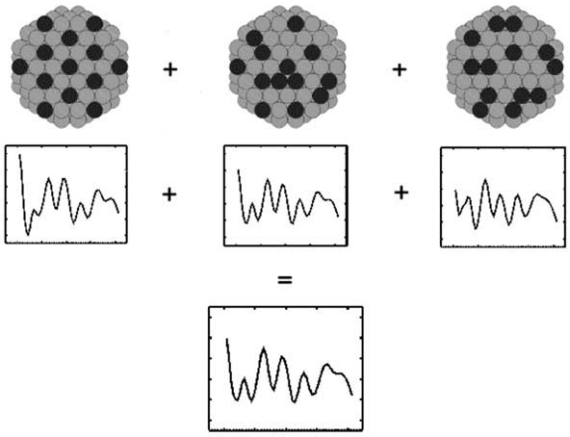

Fig. 1. Schematic view of the AOC method. The final PD curve $I_{\mathrm{A}}(\theta, \phi, \vec{k}; x)$ is obtained by averaging the PD curves $I^j_{\mathrm{A}}(\theta, \phi, \vec{k}; x)$ from different structural configurations.

where $I^j_{\mathrm{A}}(\theta, \phi, \vec{k}; x)$ is the energy and angular resolved photoemission intensity from atom A evaluated using the structural configuration j, $\vec{k}$ is the final electron wave-vector (related to the final kinetic energy), θ and ϕ are the polar and azimuthal angles of photoelectron emission. It would be more appropriate to include interference between the scattering amplitudes from different configurations. The phases of the scattering amplitudes from the different configurations should be randomly related, however, so that the configuration averaging should make the interference terms minimal and we expect Eq. (3) to be a good approximation in case of core-level photoemission.

Since N should be made as large as possible in order to correctly model the disorder of the system, this approach is very time consuming from the computational point of view. However, this method has the advantage of being able to identify the neighbors of the photo-emitting atom, which yields information, such as that regarding clustering of the deposited atoms, not obtainable from the ATA.

3. Implementation and comparison with experimental data

In order to produce PD spectra from random surface alloys using the two approaches described

in Section 2, we modified the MSCD PD program package developed by Cheng and Van Hove [46]. We modeled diffusion of the deposited metal into the bulk by allowing the surface layers to have different concentrations. In all the calculations we used a cluster of 165 atoms with radius of 9.0 Å and depth of 10 Å (five layers) as defined in Ref. [46]. The scattering phase shifts and the radial matrix elements for Pd and Cu were evaluated assuming the muffin-tin model for the crystal potential. The experimental PD spectra with which we compare the theoretical results correspond to Pd 3d emission from sub-monolayers of Pd on Cu(1 1 1) collected at room temperature, after annealing at 600 K, using linearly polarized light at the Brazilian National Synchrotron Light Laboratory (LNLS) [22]. The experimental data presented here are raw data, without any kind of smoothing or mirror-folding operation. The level of agreement between experiment-theory was quantified by the R factor defined as:

$$R_{\mathrm{A}} = \sum_i \frac{(\chi_{\mathrm{c}}^i - \chi_{\mathrm{e}}^i)^2}{(\chi_{\mathrm{c}}^i)^2 + (\chi_{\mathrm{e}}^i)^2}. \tag{4}$$

From the definition, it is clear that the smaller the R-factor, the better the agreement with experiment. The quantities χ_{c}^i and χ_{e}^i are calculated and experimental χ curves defined as:

$$\chi(\theta, \phi, \vec{k}) = \frac{I(\theta, \phi, \vec{k}) - I_0(\theta, \phi, \vec{k})}{I_0(\theta, \phi, \vec{k})}, \tag{5}$$

where $I(\theta, \phi, \vec{k})$ is the photoemission intensity and $I_0(\theta, \phi, \vec{k})$ is the free atom cross-section [46]. The summation in Eq. (4) is over the angles and energies in the data base.

The first question we address here concerns the applicability of the ATA to calculation of PD spectra. To this end, we compare PD spectra generated from both the ATA and the AOC method for a wide range of parameters. The comparison is exemplified in Fig. 2, where we compare ATA and AOC PD spectra for Pd 3d photoemission for a polar angle, $\theta = 55°$ (with respect to the surface normal) and electron kinetic energy of 460 eV (i.e., $h\nu = 800$ eV) as a function of azimuthal angle. The theoretical spectrum using

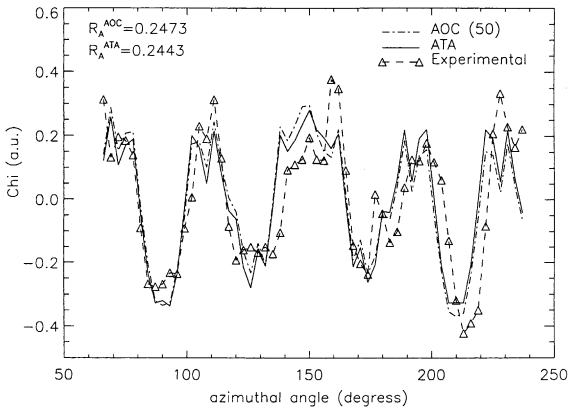

Fig. 2. Experimental (dash line + symbols) and theoretical azimuthal scans for $\theta = 55°$ using Pd 3d emission obtained using both the ATA (solid lines) and AOC (dash-dotted lines). The theoretical curve using the AOC method was generated by averaging over 50 different structural configurations.

the AOC method was calculated by averaging over 50 different randomly generated structural configurations (which seems to be sufficient to represent the complete configuration ensemble). The theoretical spectra were calculated assuming a Pd concentration of 10% in the first two surface layers with atomic positions corresponding to those of pure Cu(1 1 1). The very good agreement exhibited in Fig. 2 between the results from the two calculational schemes is typical of that resulting from all our calculations. Since the ATA and the AOC produce basically the same spectra and the ATA is much more computationally efficient than the AOC, all the theoretical PD spectra we present in this paper from this point on are evaluated with the ATA with the same structural parameters as for pure Cu(1 1 1).

Given the good agreement between the two calculational schemes, it is natural to inquire into their agreement with experiment. In Fig. 2, we also present an experimental azimuthal scan with the same parameters as those used in the calculations. We collected the experimental data after deposition of 0.3 ML (monolayer, ML) of Pd over Cu(1 1 1). The degree of agreement between theory and experiment is reflected in the relatively low R-factor values: $R_{\mathrm{A}} = 0.2473$ for the AOC and $R_{\mathrm{A}} = 0.2443$ for the ATA.

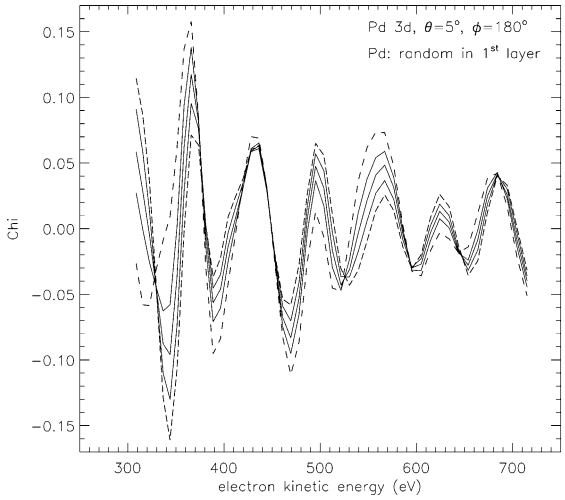

Fig. 3. Typical ATA theoretical energy scan profiles as a function of Pd concentration in the first surface layer. The thick dash-dotted and dash correspond respectively to 10% and 100% of Pd. Similar dependence is also observed in angular scans.

In order to extract information regarding concentrations from experimental data, it is necessary to evaluate the sensitivity of the theoretical spectra to concentration. In Fig. 3 we present theoretical energy scan profiles for several different concentrations of Pd randomly substituted in the first surface layer. The thick dash-dotted and dash lines correspond respectively to 10% and 100% of Pd in the topmost layer. The spectra for the intermediate Pd concentrations (30%, 50% and 70%) are indicated in the figure. Even though it is clear that the spectra are, in general, sensitive to the concentration, we observe that, for certain values of the energy, the influence of concentration is very small (as, for example, in the region around 450 eV). We verified that the phase shifts of the dominant scattering channels for Cu and Pd as a function of energy are not similar in this energy range. Obviously, analyses of experimental azimuthal scans of random surface alloys measured at energies where the spectra are insensitive to concentration could prove to be relatively useless in concentration determinations. It seems clear, therefore, that studies such as those presented in Fig. 3 should be performed in order to indicate the most favorable experimental energies for the measurements. The same type of dependence on the concentration was also observed in both azimuthal and polar scans.

In order to further study the limitations of the theoretical analysis in the determination of the layer dependent concentration of the deposited metal, we applied the analysis to theoretical PD spectra for the Pd/Cu(1 1 1) system. We generated scanned-energy and azimuthal scanned-angle spectra using the ATA approximation assuming a Pd concentration of 50% in the first two surface layers for four different polar angles ($\theta = 5°$, 30°, 55° and 80°). The scanned-energy spectra covered the electron kinetic energy range $\Delta E_K = 95$–750 eV with a fixed value of the azimuthal angle of $\phi = 0$. The azimuthal angle scans covered the range from $\phi = 0°$ up to $\phi = 120°$ for five different electron kinetic energy, $E_K = 64$, 142, 250, 366 and 444 eV. For each of the five kinetic energies, the theoretically generated data were compared with simulations using different values of the Pd concentration in the first (x_1^{Pd}) and second (x_2^{Pd}) layers. In Fig. 4, we present the R-factor contour plots for each of the theoretically generated data sets as functions of x_1^{Pd} and x_2^{Pd}. All the R-factors were calculated from Eq. (4). In the plots, the same shade of grey represents the same value of the R-factor, and the darker shades correspond to lower values of the R-factor. From the contour plots of the angular scanned data, it is clear the sharpness of the R-factor minimum is sensitive to the value of the kinetic energy.

A clearer understanding of the contour plots is provided in Fig. 5 which shows orthogonal projections of the parameter space defined by the Pd concentrations, chosen to pass through the minima in the contour plots. Fig. 5a shows the variation of the R-factor respect to x_1^{Pd}, keeping x_2^{Pd} fixed at 50%, and Fig. 5b shows R-factor as a function of x_2^{Pd} while keeping x_1^{Pd} fixed at 50%. Considering the angle scanned data first, it is clear that the uncertainties in the determination of the concentration become larger when the electron kinetic energy is increased. The scanned-energy result just reflects the behavior embodied in the azimuthal angle scanned data: its minimum is sharper than that for $E_K = 142$ eV and less sharp than that for $E_K = 64$ eV. Had we begun the scanned-energy range at a higher kinetic energy

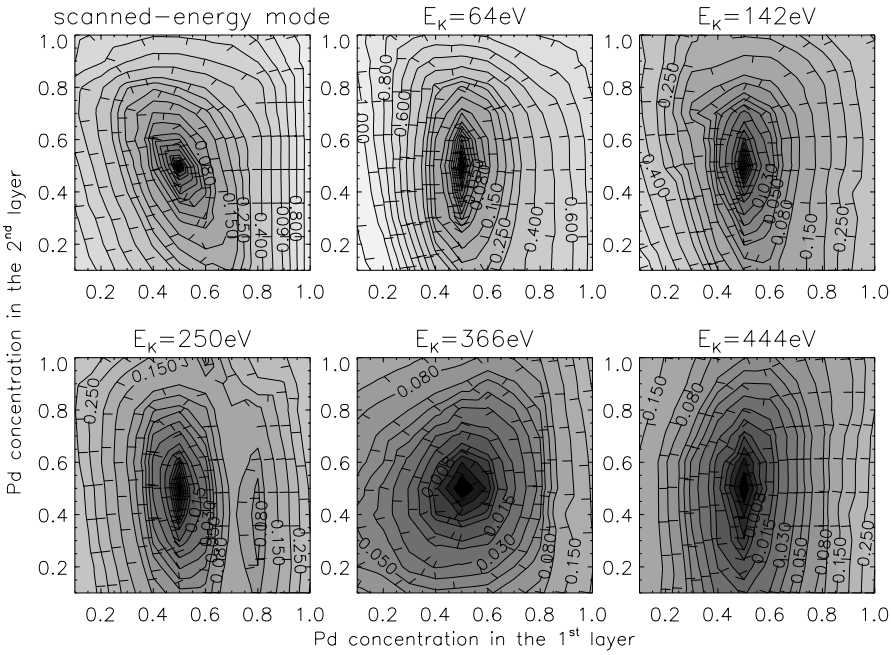

Fig. 4. Contour plots of R_A as a function of Pd concentration on the first two surface layers for both scanned-energy and scanned-angle (at different kinetic energies) modes.

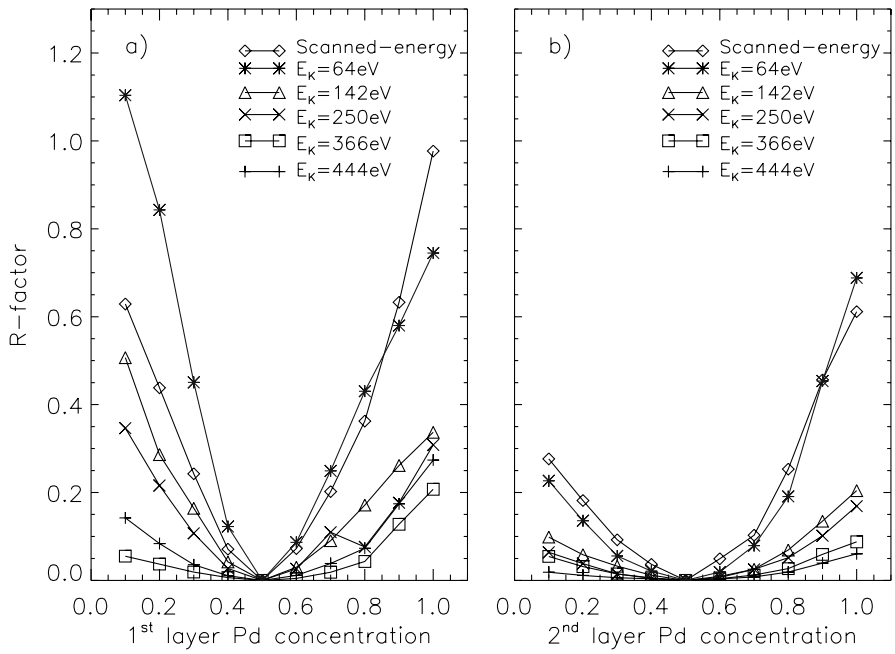

Fig. 5. (a) R-factor as a function of x_1^{Pd} for $x_2^{Pd} = 50\%$, (b) R-factor as a function of x_2^{Pd} for $x_1^{Pd} = 50\%$. The vertical scales in both plots are the same.

than 95 eV, its minimum would have been broader and the concentration determination less certain. Therefore, in order to be able to obtain the concentration of the deposited metal in these random surface alloys, experiments should be performed either in the scanned-energy mode, starting at low kinetic energies, or in the scanned-angle mode with low electron kinetic energy.

Finally, in Fig. 6, we present theoretical and experimental Pd 3d emission patterns in the polar angle range $15° \leqslant \theta \leqslant 55°$. In the figure, the kinetic energy of the photoelectrons is 360 eV ($h\nu = 700$ eV) and the experimental pattern was collected after deposition of about 1 ML of Pd. The Pd 3d intensity was transformed into a linear grey scale while angles are projected using the following transformation: $x = \theta \cos\phi$ and $y = \theta \sin\phi$. The center of each plot represents normal emission. The upper left theoretical pattern corresponds to Pd randomly substituted on the first layer only and is clearly different from the experimental pattern (lower right). Allowing diffusion of Pd atoms into the second layer is enough to reproduce the strong diffraction peaks at about $\theta = 35°$ (upper right pattern). The lower left pattern corresponds to allowing diffusion of Pd to the third layer. This

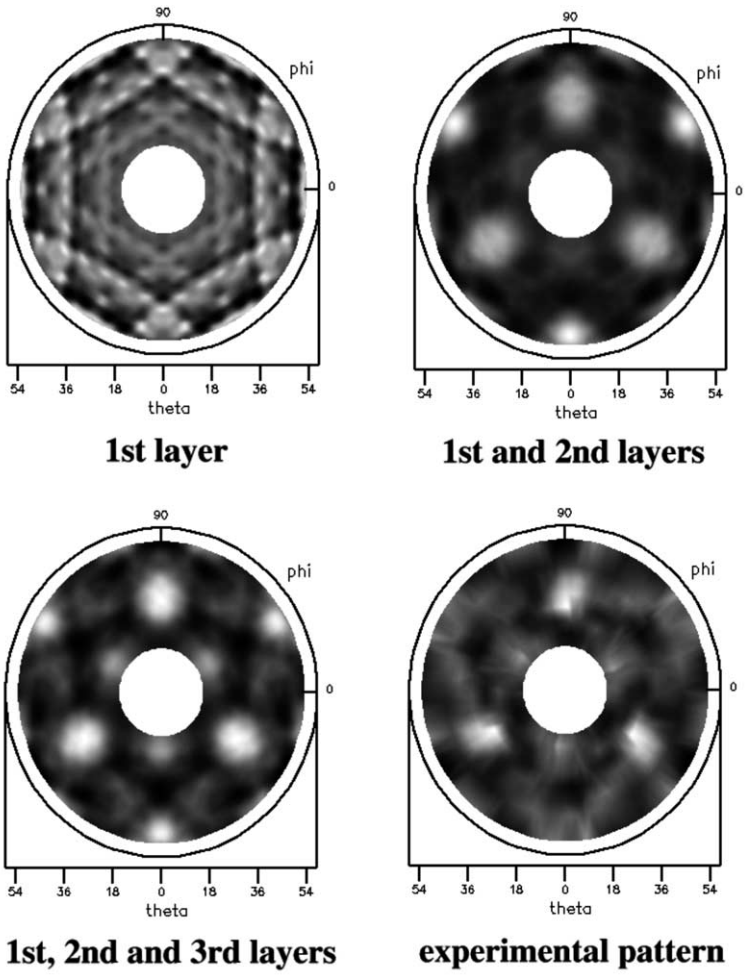

Fig. 6. Theoretical and experimental Pd 3d emission patterns in the polar angle range of $15° \leqslant \theta \leqslant 55°$. The kinetic energy of the photoelectrons is 360 eV ($h\nu = 700$ eV) and the experimental pattern was collected after deposition of about 1 ML of Pd. The center of each plot represents normal emission.

clearly improves the agreement between theory–experiment since the diffraction peaks at about $\theta = 20°$ are now well defined. It is well know that PD is a powerful tool for studying surface diffusion and this result is confirmed here for the case of random surface alloys. We analyse the experimental results in more detail elsewhere [22].

One last point that deserve discussion concerns the ability of the AOC to identify the sites occupied by the deposited metals. Although it is clear that the ATA is much more efficient computationally than the AOC, since it involves only one calculation instead of 50 or 100, it has a drawback: in the ATA approximation, the randomness of the system is replaced by a periodic effective medium, so that no conclusion can be reached regarding the environment of the deposited metal atoms. The ATA, therefore, does not provide information about, for example, whether the deposited atoms prefer to cluster or whether they prefer to stay far from each other. It is in connection with this point that the AOC method becomes important, at least for the case of Pd on Cu(1 1 1). Preliminary results show that AOC theoretical PD simulations using random clusters with Pd atoms in nearest-neighbor sites corresponded to rather high values of the *R*-factor. When the occupation of nearest-neighbor sites by Pd atoms was not allowed, lower values of the *R*-factor were obtained. The results for the case of Pd/Cu(1 1 1), therefore, suggest that the Pd atoms cluster minimally. In a more general sense, it appears that a reasonable strategy to follow is to use the ATA approximation to obtain the structural and non-structural (such as concentration, Debye temperature) parameters of the system and then to use the AOC to obtain information about the surrounding of the deposited atoms.

4. Conclusions

We have shown that both ATA and the average of configurations approach reproduce experimental PD spectra from random surface alloys. In addition, the AOC was able to give useful information about the occupation of nearest-neighbor or next-nearest-neighbor in the alloy. We also showed that the determination of the surface alloy concentration and segregation profile is quite sensitive to the electron kinetic energy. These results allowed us to formulate recommendations of experimental procedures for maximizing the structural and concentration information derivable from PD from such alloys.

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