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EXTENDED X-RAY BREMSSTRAHLUNG ISOCHROMAT FINE STRUCTURE OF PALLADIUM ANALYSED BY USING THE EXAFS METHOD

E. Sobczak and S. Mobilio[x]

Institute of Physics, Polish Academy of Sciences,
PL-02668 Warszawa, Al. Lotnikow 32/46, Poland

[x]INFN, Laboratori Nazionali di Frascati,
I-00044 Frascati, Italy

ABSTRACT

The extended fine structure of the x-ray bremsstrahlung isochromat (EXBIFS) of palladium measured at the photon energy of 5415 eV has been compared to the extended x-ray absorption fine structure (EXAFS) at the K edge of Pd by using Fourier analysis.

The extended fine structure of the x-ray bremsstrahlung isochromat (EXBIFS) of palladium [1] measured at the photon energy of 5415 eV shows a close similarity to the extended x-ray absorption fine structure (EXAFS) at the K edge of Pd, because the bremsstrahlung transition is localized to the core region and the probability of bremsstrahlung transitions to the final states of p-symmetry dominates over those to the d, f, and g states [2, 3, 4].

One can expect some differences between EXBIFS and EXAFS, namely in the phase shift due to another potential of the central atom and in the amplitude of oscillations according to the bigger damping in EXAFS due to a core-hole lifetime. Recently the EXBIFS of some 3d transition metals (Co, Ni, Cu) has been studied by using standard EXAFS methods and compared with the K-shell EXAFS's [5]. It was found that the EXBIFS phase for the 1st shell oscillations was the same in the case of Ni and slightly different from that of K EXAFS in the case of Co and Cu. The nearest-neighbour distance obtained from EXBIFS by using the EXAFS experimental phases was smaller than crystallographic data by 1.6 % and 3% for Co and Cu respectively. The 1st shell amplitude of the EXBIFS uncorrected for electron energy losses was found to be in the range 50%-65% of that one for EXAFS.

The energy width of the Pd K core level equal to 6.8 eV is much bigger than 1.4 eV of the Cu K level. The result of a small mean free path λ_h (a few Å) passed by the Pd K

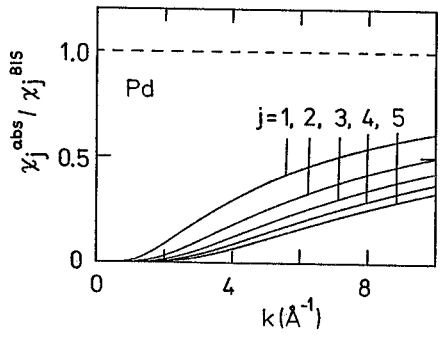

Fig. 1.

The BIS spectrum (uncorrected) of the Pd metallic foil measured at the photon energy of 5415 eV by means of an x-ray vacuum spectrometer [1] is shown in Fig. 2a. The K-shell absorption spectrum of Pd measured at the room temperature at the PULS laboratory by using synchrotron radiation from the storage ring ADONE is shown in Fig. 2b after correction for Victoreen's curve. The zero energy in BIS spectrum was chosen 6.5 eV below the Fermi level. In the case of the Pd K edge the Fermi level is not precisely determined due to a big broadening of the threshold. We tried to move the zero energy point of the Pd K absorption spectrum to the same feature like in BIS. The function $\mu_o(k)$ was found by fitting a polynomial of the third degree to each spectrum in Fig. 2 in the range used then for the Fourier transform.

photoelectron during the Pd K core hole lifetime can be described like the damping factor $\exp(-2R_j/\lambda_h)$ which lowers the amplitude of oscillations from the jth shell. Fig. 1 shows that, in the case of equal temperatures, the Pd K EXAFS amplitude for the jth shell oscillations should be smaller than that of the Pd EXBIFS (corrected for electron energy losses) by factor $\exp(-2R_j/\lambda_h)$.

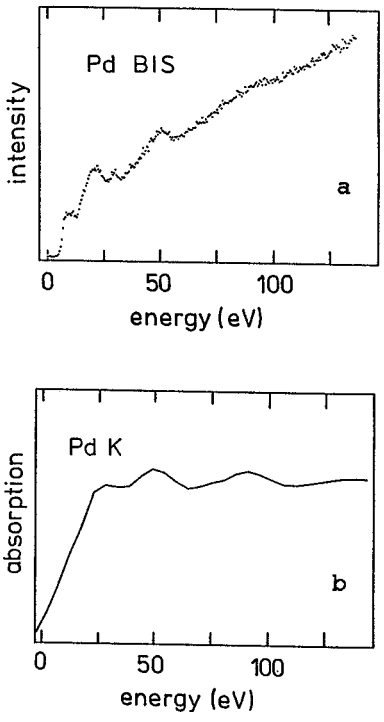

Fig. 2 a, b.

The Fourier transform (FT) of the EXBIFS and K-EXAFS of Pd calculated in the k range from 3.3 to 6.0 $Å^{-1}$ is presented in Fig. 3. The 1st shell peak in FT of EXBIFS is shifted by 0.1 Å to lower R values in comparison to the K EXAFS. The lowering of the next neighbour peak occurs in the

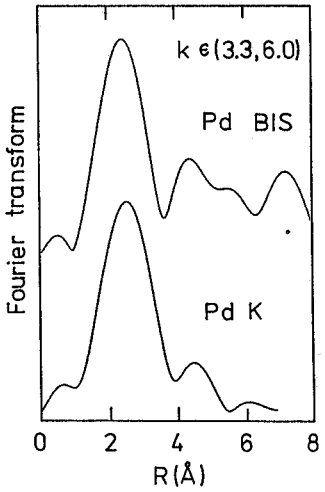

Fig. 3.

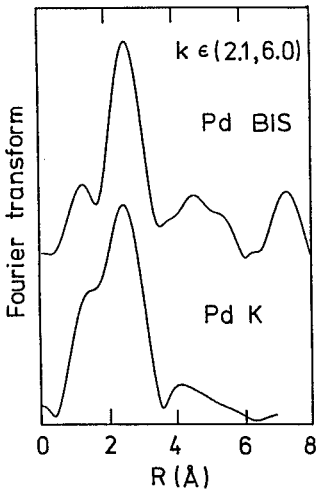

Fig. 4.

FT of Pd K EXAFS is due to the Pd K core-hole lifetime. It is not a case in the FT of EXBIFS. The FT calculated for lower value k_{min} shows a splitting of the main peak (Fig. 4) due to a Ramsawer-Townsend effect.

By using the Fourier backtransform of the 1st shell peak, the phase and amplitude of EXBIFS versus momentum k were studied and compared with EXAFS. In Fig. 5 there are shown the real part and modulus (scaled by k) of the Fourier backtransforms of the 1st shell peaks from the Fig. 3. The EXBIFS amplitude of the 1st shell peak strongly decreases with momentum k due to the high temperature during

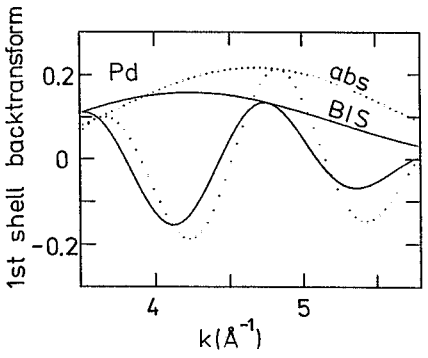

Fig. 5.

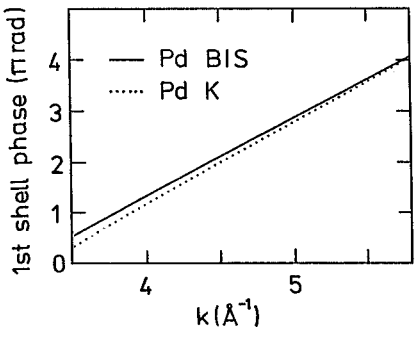

Fig. 6.

measurement, however for k < 3.9 $Å^{-1}$ it becomes bigger than that of the K EXAFS. The difference between the EXBIFS and EXAFS phases decreases linearly with momentum k in the k range studied (Fig. 6).

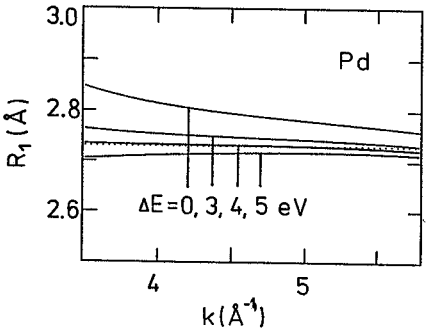

Fig. 7.

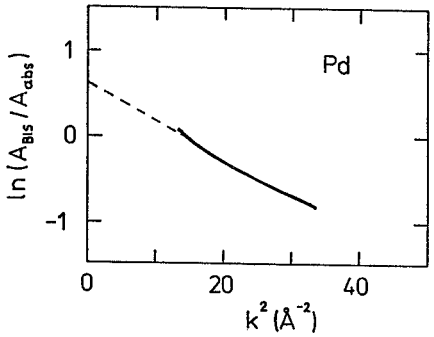

Fig. 8.

Assuming the EXAFS data as the "model system" with the value R_1=2.751Å, we have obtained the value R_1=2.729 Å (i. e. smaller by 0.8%) from the EXBIFS data treated as the "unknown system", while the value E_o of EXBIFS had been shifted by ΔE = 4 eV (dotted line in Fig. 7).

By extrapolating $\ln(A_{BIS}/A_{abs})$ to k^2=0 in Fig. 8 we have obtained that the EXBIFS amplitude is bigger than EXAFS by the factor 1.9, which is smaller (due to nonprimary contribution to the BIS intensity from inelastically scattered electrons) than the factor 2.9 estimated from the K core-hole lifetime of palladium .

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