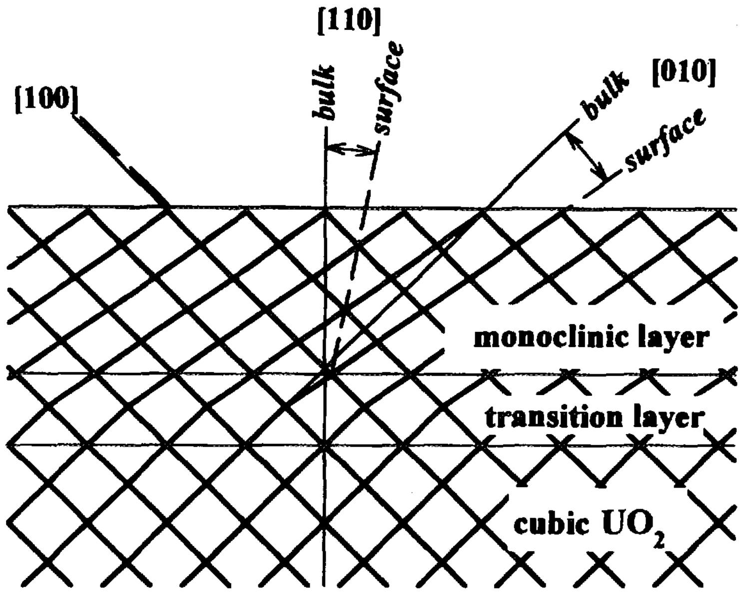

Fig.1 Structural model of the quasi-epitaxial monoclinic surface layer grown on the cubic UO_2 structure.

Channeling experiments performed for four low-index axes combined with XRD measurements enabled us to determine the structure of the formed monoclinic phase as consisting of cells described by: a = 542.8 pm, b = 550.0 pm, c = 546.3 pm, a=b=90.0° and g = 90.75°. The phase belongs to the family of polymorphic structures existing in the $UO_{2.24}$-$UO_{2.50}$ region. It remains unknown whether the obtained a , b and c lengths concern an elementary cell or a sub-cell of a larger structure.

Monte Carlo simulations of ion-channeling in the transformed monoclinic layer linked to the crystal bulk were performed. They enabled us to state that incorporation of additional oxygen atoms into the UO_2 structure results not only in the monoclinic deformation of the elementary cells but also in displacements of uranium and matrix oxygen atoms from their lattice sites. The simulations also showed that uranium atoms were displaced preferentially in one of the crystalline planes.

The work was supported by a Convention - Polish Laboratories the IN2P3 (France).

[1] D.K.Smith, B.E.Scheetz, C.A.F.Anderson and K.L.Smith, Uranium 1 (1982) 79
[2] L.Nowicki, A.Turos, C.Choffel, F.Garrido, L.Thomé, J.Gaca, M.Wójcik and Hj.Matzke, Phys. Rev. B1, in print

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PL9800601

1.16 M-shell ionization of atoms by C, N and O ions

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The existing data K-, L- and M-shell ionization by light ions can be reproduced quite well by theoretical models based on the plane wave Born approximation (PWBA) or the semiclasical approximation (SCA), when the corrections for higher-order effects are included in these approaches.

For heavy ions perturbing stronger the initial electronic state , these theories cannot describe the data so well. In this case, substantial discrepancies were reported mostly for M- and L-shells. We summarize our systematic studies of M-shell ionization in heavy elements (Au, Bi, Th and U) by C, N and O ions [1]. Results for a $O^{q+} \rightarrow$ Au system, for energy range 0.1 - 2 MeV/u (performed in INR Dubna and Erlangen University), are compared with the predictions of the ECPSSR theory discribing both the direct ionization (DI) and the electron capture (EC), and with the SCA calculations for DI, performed in the separated (SCA - SA) and the united (SCA - UA) atoms limit. Two importent effects, the ion charge equilibrium in the target and the multiple ionization, are discussed.

In experiments using the targets of intermediate thicknesses, 20 - 40 $\mu g/cm^2$, the equilibrium charge state distribution is reached. So essentially, the equilibrium X-ray production and ionization cross sections are measured. Such equilibrium ionization cross sections σ_{eq} are calculated for the equilibrium charge state distribution [2]: $\sigma_{eq} = \Sigma\ F(q)\ \sigma(q) = \sigma_{DI} + \Sigma\ F(q)\ \sigma_{EC}$. Fig. 1 shows theoretical M-shell cross sections for DI and EC for $O^{q+} \rightarrow Au$ calculated according to the ECPSSR theory for 0.1 and 1 MeV/amu vs charge state q for thin target ($< 1\ \mu g/cm^2$). From Fig. 1 we concluded that electron capture contributions for high energies are important. Another important aspect is the multiple ionization effect. In this case the atomic parameters should be known for the multi-vacancy configuration, but practically, only their single-vacancy values are available. To correct this effect the energy shifts of L -X - ray lines can be measured to estimate the probabilities of ionization of M-, N- and O-shells, which in turn allow one to correct approx. the atomic parameters for the multiple ionization effect. In Fig. 2 differences between the L_γ peaks from Au bombarded by O^{q+} and p (3MeV) are shown. The peaks are shifted, independent of the ion energy, of about 100 eV for $L_{\gamma 1,2,3,5}$ ($N_{4,3,2,1} \rightarrow L_{2,1}$), 200 eV for $L_{\gamma 4,4'}$ ($O_{3,2} \rightarrow L_1$) and 320 eV for $L_{\gamma 6}$ ($O_4 \rightarrow L_2$) transisions. Using these results, and relating the observed energy shifts [3] we can estimate the ionization probability. The corrected data for the multiple ionization effects are accurate, within 20-30 %.

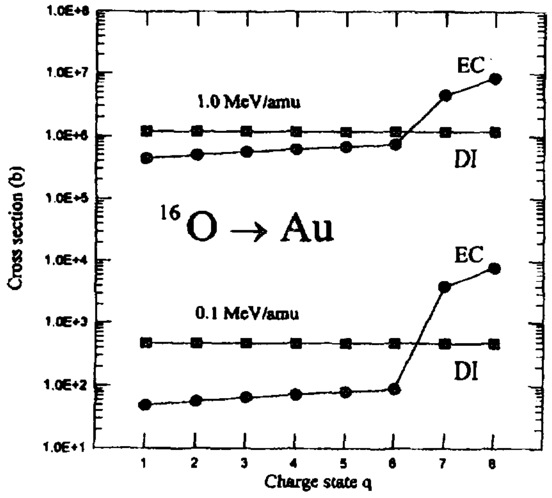

Fig.1

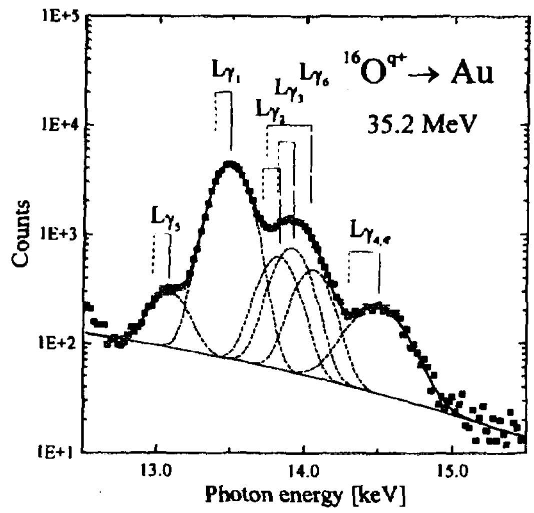

Fig.2

[1] T.Czyżewski, et al., Nucl. Instrum. and Methods, B109/110 (1996) 52
[2] R.K.Gardner, et al., Phys.Rev. A15 (1977) 2202
[3] G.Lapicki, et al., Phys. Rev. A34, (1986) 3813

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