

THE $TiL\alpha$ AND $OK\alpha$ EMISSION SPECTRA NARROWING PECULIARITIES IN CONSEQUENCE OF TiO_2 POWDERS WITH RUTILE AND ANATASE STRUCTURE NANODISPERSION

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Introduction

The $TiL\alpha$ and $OK\alpha$ emission bands of TiO_2 (with average nanoparticles size of 10 and 107nm) and coarse powder with rutile and anatase structure were investigated in equal experimental conditions by means of the ultrasoft X-ray spectroscopy.

Results and discussion

The $TiL\alpha$ и $OK\alpha$ bands narrowing as in [1-3] increase when nanoparticles size decrease. The lowenergy subbands in $OK\alpha$ – bands structure practically disappear. It occurs owing to $O2p$ -states displacement to lowenergy part after Ti-O bonds braking that confirmed by relative peak intensity increase of $OK\alpha$ normalized on inner $TiLl$ – line.

The $TiL\alpha$ -полос narrowing was observed in lowenergy part of spectrum as a result of splitting of $Tisd$ –hybrid states equipped in covalent constituent Ti-O bonds.

Conclusions

It was shown that the narrowing appears owing to localization of the $O2p$ -energy levels of the O^{2-} anions thicken with electrons equipped in covalent constituent. Then it was shown that ratio $n(OK\alpha)/n(TiL\alpha)=Q(Op)/Q(Tisd)$, where n – is bands relative narrowing, Q – is partial density of valence electrons near titanium and oxygen.

It was revealed that $Tisd$ and Op -states energy redistribution under rutile and anatase powders nanodispersion are close owing to similar nearest environment of Ti and O atoms in that phases.

The present work was supported by STCU (grant 3101).

Literature

1. Zhurakovsky E.A, Zaulychny Ya. V. at all Osobennosti elektronogo stroenija ultradispersnyh poroshkov cubicheskogo nitride bora. // Poroshkovaja metallurgija. -1991. - №1. - C. 72-76.
2. Zaulychny Ya.V. Rengenospectralnoe issledovanie elektronij struktury I himicheskij svyazi v ultradispersnyh poroshkah I poluchennyh iz nih kristallicheskih materialah. I. Nitrid titana. II. Carbid titana. // Poroshkovaja metallurgija.-1999. - №7/8, №9/10. - C.75-85, C.75-84.
3. Zaulychny Ya.V. Osoblyvosti elektronij struktury metastabilnyh ultradyspersnyh system ta oderzhnyh z nyh materialiv. // Fizyka i himija tverdogo tila, t.3, №3, C.312-314 (2002).

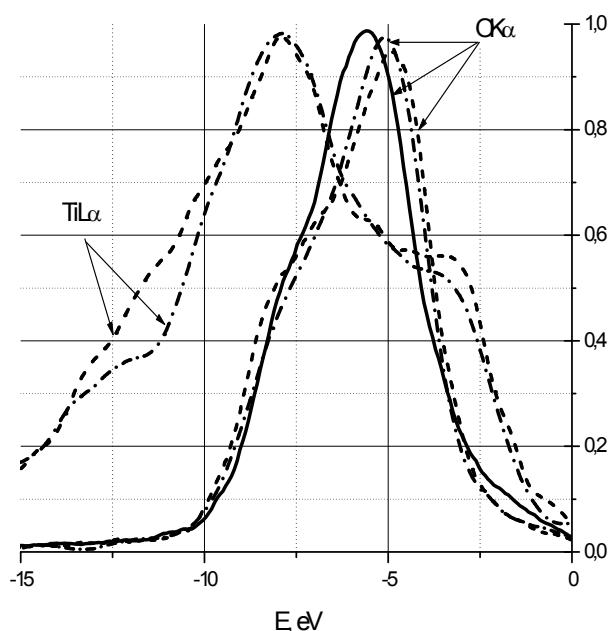


Fig. 1. $TiL\alpha$ and $OK\alpha$ – bands of TiO_2 with rutile structure: (- - -) – coarse powder, (- . -) – $d=107$ nm, (_ . _) – $d=10$ nm