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Международная научно-практическая конференция
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Секция 3. Математическое моделирование в фундаментальных и прикладных исследованиях

MODELLING OF FREE POSITRON STATES IN TIHx

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Electron energy structure, positron spectrum and positron characteristics of □-Ti and □-$TiH_{0.125}$ were calculated. Self-consistent calculations of the band structure were performed by the linear muffin-tin orbital method in the atomic sphere approximation. Modelling has been made on low content of hydrogen into □-Ti with expanded close-packed hexagonal cell inclusive 8 titanium atoms. Only one octal pore (1/4; √3/12; c/4) was located with hydrogen and others were filled up empty spheres (zero electron density). Variation of sphere radiuses permitted to consider anisotropy and spherical symmetry of potential. The positron states problem have been solved on basis of two-component density functional theory [1]. Positron potential and positron wave function were calculated on a base of self-consistent electron density. Then positron probability of existence into TiH_x lattice and lifetime were founded.

There are positron characteristics in table 1. Variation of atomic sphere radiuses leaded to charge repartition in cell. The absolute value of free-positron lifetime obtained were in satisfactory agreement with the experimental (150 ps) [2]. But the tendency of increase of the free-positron annihilation mean life with hydrogen atom introduction has not displayed via calculation. The experiment had shown «swelling» of Titanium sample because of hydrogen absorption. So as rough to estimate that the positron characteristics of cubic $TiH_{1.0}$ were calculated. It was shown positron was redistributed significantly in to the hydrogen centers area, free positron life increased, but the charge changed insignificantly in hydrogen sphere.

Table 1. Positron lifetime τ(ps), probability of positron distribution W (%) to atomic spheres (S), electron charge Q (el.) into atomic spheres and probability of electron-positron annihilation ω (%)

	α-Ti	α-$TiH_{0.125}$			α-$TiH_{0.125}$			SIC-$TiH_{1.0}$		
τ(ps)	158.1	154.5			149.8			163.5		
atomic radius (a.u.)	3.0532	$R_{Ti}=R_H=R_E=2.4233$			$R_{Ti}=2.800$ $R_H=R_E=1.867$			$R_{Ti}=R_H=R_E=2.0656$		
atomic sphere	Ti	Ti	H	E	Ti	H	E	Ti	H	E
W (%)	100	32.25	4.90	62.85	59.87	1.93	38.20	10.05	23.72	66.23
ω(%)	100	42.19	5.35	52.46	64.79	2.24	32.97	16.68	27.97	55.35
Q (el/at)	22	20.47	2.48	1.48	21.28	1.35	0.75	19.68	1.64	0.84

REFERENCE

1. E.B. Boronski, R.M. Nieminen. Electron-positron density-functional theory// Phys.Rev.B –1986.– V.**34**.– P.3820.

2. K.P.Arefev, O.V.Boev, O.N.Imas, A.M.Lider, A.S.Surkov, I.P.Chernov Annihilation of positrons in hydrogen-saturated titanium // Physics of the Solid State. – 2003. – Т. 45. – № 1. – P. 1-5.