IDENTIFICATION OF DEEP STATES FROM AU/PT/IR/OS IMPURITIES IN SILICON USING RADIOACTIVE TRANSMUTATION

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Defect spectroscopic investigations on silicon samples implanted with various radioactive Hg isotopes which decay fully or partly through the series Au/Pt/Ir/Os/Re/W are reported. For each individual element well documented defect parameters are confirmed. In all cases the recoil by the transmutation of the nuclei is much smaller than displacement energies. Thus the daughter elements should be in the same configuration as the Au/Pt - atoms have been in-diffused. We find two more Au related acceptor-like defect levels, two Pt acceptors but no evidence for the elsewhere reported Pt- donor level. The deep Au donor level at E_V+374(3)meV is observed in all cases and its concentration correlates with the population of Au atoms in the samples

1 Introduction

After some decades of intensive investigations of deep level centres from 5d transition elements in silicon some controversies are still under discussion. Because most of these elements are ionised and favour interstitial positions, they show a strong tendency to form defect complexes. These elements will complex readily with fast-diffusing species in the crystal (such as H, Li, Fe, Cu, etc.)

On the other hand, the solubility and a corresponding electrical activation of these elements are very low. So experiments with an adequate purity standard can

be achieved only by ion implantation in materials with high purification, perfection, and a controlled background of residual contaminants. Defect spectroscopic methods on radioactive atoms are straightforward means of correlating deep levels to impurities by comparing time dependent spectra with the half-lifes of incorporated unstable elements /1/.

2 Experimental

Phosphorus-doped n-type, float zone refined and dislocation-free silicon crystals with a nominal free carrier density of (3-5)x10^{13} cm^{-3} were implanted with different radioactive Hg isotopes using the facilities of ISOLDE at CERN.

Spallation reactions on a lead target by GeV proton bombardment result in a variety of unstable isotopes having somewhat lighter masses. From all of the produced isotopes mercury can be easiest vaporized and ionized. After acceleration and mass separation Hg beams from mass 182 to 199 are available. Depending on to the Hg isotope yield, implantation times from minutes up to one hour give fluxes of ~ 10^{12} cm^{-2} ;which are suitable limits for radiation safety considerations. X-ray spectroscopy measurements after implantation as well as after annealing give the amount, purity and loss of implanted unstable elements.

The annealing and in-diffusion have been carried out in quartz ampoules under He atmosphere (0.5atm) at temperatures in the range of 900°C - 1050°C for 10min, finished by dropping the ampoules into water. Schottky contacts for the electrical measurements were prepared by standard technology.

3 Results

Two Pt-related electron traps (at E_c-153(2)meV and E_c-281(2)meV in case of ^{191}Hg or E_c-248(2)meV for ^{193}Hg/stable Pt, respectively) are found to show concentration changes which correspond to the Pt population changes for both ^{193}Au→^{193}Pt and ^{191}Pt→ ^{191}Ir. Clear identifications have also been obtained for two Ir-related electron traps at E_c-605(2)meV and E_c-305(2)meV by their growth and decay for ^{191}Pt→ ^{191}Ir and ^{189}Ir→ ^{189}Os, respectively. A single Os-related level at E_c-0.268(1)meV is detected by its appearance in the $^{183/186/188}$Hg decay series. Table 1 gives a summery of all detected and so far identified deep levels. Note, that in all experiments on n-type silicon only the Au donor in the lower part of band gap appears. We have examined these results in the light of the lines observed in PL studies of Pt doped n-Si /2/, and it is observed that the DLTS measurements show good agreement with the PL data. The sharp lines observed in low temperature PL data are due to localised transitions at deep centres. The DLTS data indicate the presence of acceptor-like defects, occupied by electrons in n-type material and thus negatively charged. The envisaged PL mechanism is that free holes generated by

the optical excitation source are trapped at the negatively charged defect sites. This generates a neutral excited state of the defect and a radiative transition occurs, leaving the defect in a neutral charge state. This is effectively an electron transition to the valence band. The energy of the emitted photon will be lower than the band-gap energy by an amount equal to the energy of the electron trap state (plus the hole binding energy which is generally around 50meV for effective-mass type states /3/). Comparing the DLTS energies for the electron traps with the PL line energies we have been able to associate some of the DLTS features with PL lines. To compare optical (PL) and thermal (DLTS) determined energies one has to extract Gibb's free energy of the transition from the thermal measurements. Taking into account all these corrections it appears that the most likely correspondence between the PL and DLTS data are that the E8 level corresponds to the 777meV center and the E12 level to the 884meV center /2/. Our results show trends in the energy level positions which are in agreement with theoretical predictions for electron states of 5d transition metal impurities in silicon /4/. Two additional significant results have been obtained. Firstly, a dominant mid-gap level, widely believed to occur for Au occupying a distorted 'substitutional' lattice site in silicon, was not observed under our conditions. Thus the occurence of such a characteristic level due to Au alone must be questioned. We have observed several Au-related levels for which the concentrations are strongly dependent on the annealing temperature, and the involvement of additional impurities is likely to be a factor in determining which levels are involved. A second significant result is the observation of a distinct Au- and Pt-related defects which could not be formed by doping with stable atoms.

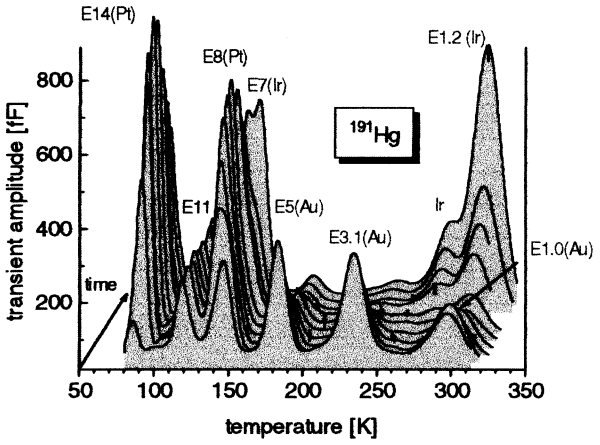

Figure1 : Evolution of deep level density detected by DLTS. (n-type Si doped with ^{191}Hg ; $e_n = 500s^{-1}$; see Tab. 1)

4 References

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/2/	E.Alves et al	ICDS '97, to be published
/3/	S.M.Kogan and T.M.Lifshits	phys. stat. sol.(a),**39**,11(1977)
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isotope mass			^{183}Hg	^{186}Hg	^{188}Hg	^{189}Hg	^{191}Hg	^{193}Hg	Au	Pt	Ag
decay serie			Hg,Au,Pt → Ir(0.9h) → Os(9.9h) → Re(71d) → **W**	Hg(2m) → Au(10m) → Pt(2h) → Ir(16h) → **Os**	Hg(3m) → Au(9m) → Pt(10d) → Ir(41.5h) → **Os**	Hg(7m) → Au(30m) → Pt(11h) → Ir(13.1d) → **Os**	Hg(50m) → Au(3h) → Pt(2.9d) → **Ir**	Hg (11h) → Au (17h) → **Pt** (50y)	stable		
sample / preparation			FZ-refined, dislocation free n-type silicon (n= 5e13cm^{-3}); implantation: 60keV, 2e 12 cm^{-2} ; ann 900°C, 10 min, sealed ampoules (0.5 atm. He), quenched,								
not.	E_c -E_t [eV]	ident.									
EB00/ EB01	0.541(5) 0.582(5)	**W**	296K(*)								
E1.0	0.592(5)	**Au**					300K	300K			
E1.2	0.605(2)	**Ir**				300K(*)	300K(*)				
E1.?	0.576	**Pt?**						285K			
E2.1	0.539(3)	**Ir**					276K(*)				
E3	?	**Pt**		236K(*)							
E3.1	0.432(2)	**Au**					234K(*)	234K(*)	234K		
E3.2	?	**Ir**					240K(*)				
E4.0	0.488(7)	**stable**			226K				226K		225K
E4.1	0.508(7)	**Os**				220K(*)					
E4.3	?	**Rh**	226K(*)								
E5	0.385(1)	**Au**					184K(*)	184K(*)	184K		
E6	0.345(8)	**stable**				163K		163K	164K	164K	164K
E6.2	0.322(1)	**Rh**	155K(*)								
E7	0.305(2)	**Ir**				147K(*)	147K(*)	147K(*)			
EB10	0.278(2)	**W**	184K(*)								
E8	0.281(1)	**Pt**					138K(*)				
E8.1	0.268(1)	**Os**	141K(*)	141K(*)	142K(*)						
E9	0.248(1)	**Pt**						131K(*)		131K	
E11	0.218(2)	**stable**			120K		120K	120K	118K		119K
E12	0.198(1)	**Ir?**		100K(*)		100K					
E12.1	?	**Rh**	100K(*)								
E12.2	?	**W**	97K(*)								
E13	0.165(1)	**Pt**						89K(*)			
E14	0.151(1)	**Pt**					89K(*)			89K	
H1	0.374(2)	**Au**					209K(*)	210K(*)	210K		

Tabel 1: Summary of detected deep level centres from 5d TM in silicon. (given are the temperatures of peak maxima for an emission rate of 500s^{-1}; levels marked by (*) are clearly identified by their time evolution)