Lithium - gold - related complexes in p-type crystalline silicon

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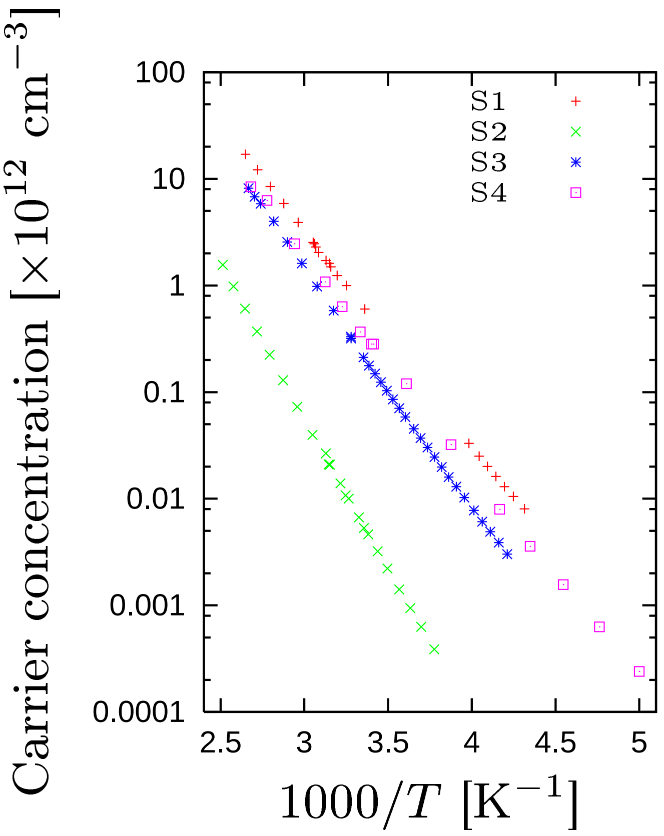
Substitutional gold is known to introduce two energy levels in the band gap of silicon [1, 2]

- a deep acceptor level at $E_{\mathrm{c}} - 0.56$ eV
- a deep donor level at $E_{\mathrm{v}} + 0.34$ eV.

We observe two energy levels introduced by lithium diffusion of Au-doped silicon,

- acceptor at $E_{\mathrm{c}} - 0.41$ eV in n-type Si:Au [3]
- level at $E_{\mathrm{v}} + 0.41$ eV in p-type Si:Au

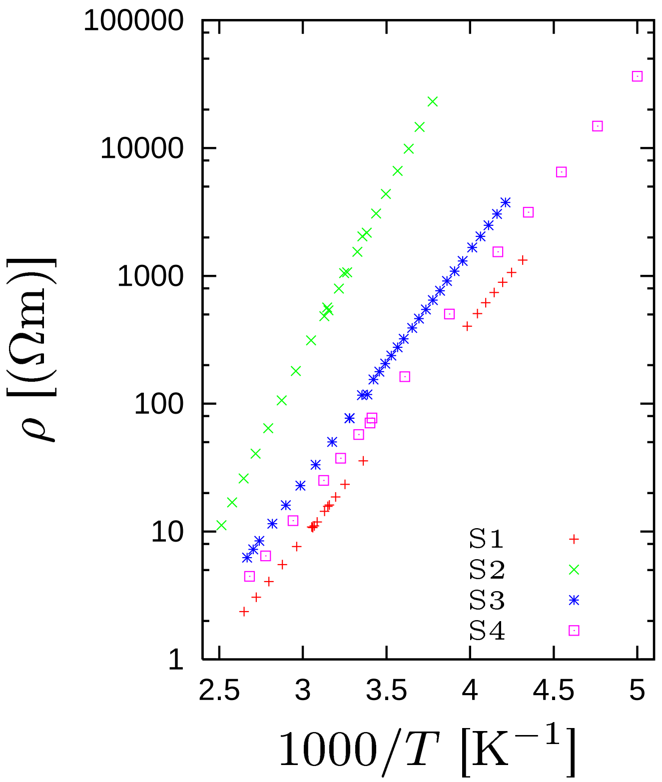
We discuss the identity of these levels in comparison with theoretical predictions for the interaction between hydrogen and the energy levels of substitutional Au in silicon.



S1 - S4 were Au diffused at 1179 °C for 4 h

		ΔE [eV]	Type
S1		0.36	p
S2	Li 300 °C 20 min baked 300 °C 10 h	0.52	n
S3	Li 300 °C 20 min baked 300 °C 5 h baked 100 °C 12h, 200 °C 30 min	0.41	p
S4	Li 300 °C 20 min baked 300 °C 4 h baked 100 °C 10 h, 205 °C 30 min	0.35	p

A hitherto unknown level at $E_\mathrm{v} + 0.41$ eV appears in Au-Li co-doped samples after baking at relatively low temperatures (100 - 200 °C).



- Lithium co-doping of the gold doped silicon samples increases their resistivity. The resistivity decreases again with baking of the co-doped samples.

- The Li-doping of p-type Si is found to shift the Fermi level position between the deep donor level to the deep acceptor level as expected, thus confirming their presence in the samples.

Gold-hydrogen co-doped silicon

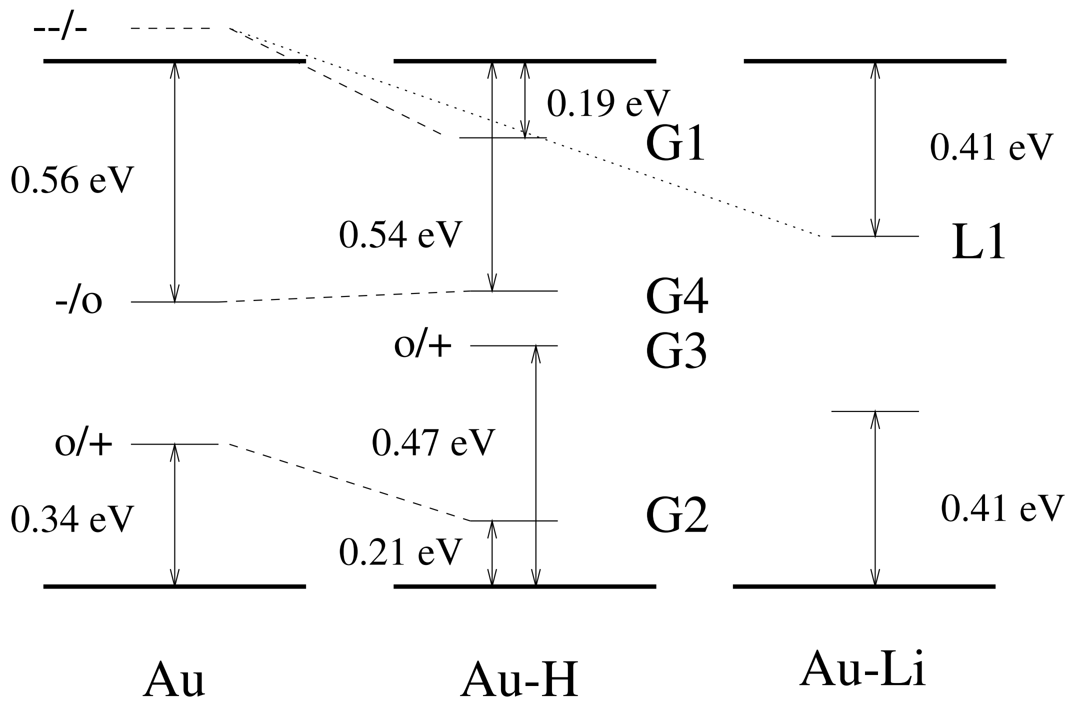
			Ref.
G1	$E_c - 0.19$ eV (in n-type samples)	Au-H_1	[4, 5, 6]
G2	$E_v + 0.21$ eV (in p-type samples)	Au-H_1	[4, 5, 6]
G3	$E_v - 0.47$ eV	Au-H_2	[4, 7]
G4	$E_c - 0.54$ eV	Au-H_1	[4, 8]

The three levels in gold-lithium co-doped samples

- L1 at $E_c - 0.41$ eV
  (observed in n-type samples)
- the new level at $E_v + 0.41$ eV
  (observed in p-type samples)
- the level at $E_c - 0.52$ eV

could well correspond to the levels G1, G2, and G4.

Discussion



- The L1 level is then possibly due to a downward shift of the $\mathrm{Au}^{--/-}$ level and thus in the Au-Li_1 configuration.
- The new level at $E_\mathrm{v} + 0.41$ eV could correspond to the G2 level which is in the Au-Li_1 configuration. However, we cannot exclude the possibility that the $E_\mathrm{v} + 0.41$ eV level corresponds to the G3 level and thus the Au-Li_2 configuration.

Summary

At least five complexes of gold and lithium have been reported in silicon by different researchers:

- An electrically inactive complex and an electron trap at $E_c - 0.41$ eV deduced from DLTS measurements [3]
- Two centres, an orthorhombic Au-Li pair and a trigonal $Au\text{-}Li_3$ complex, observed by EPR and ENDOR [9].
- A new level at $E_v + 0.41$ eV.

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