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ANOMALOUS BEHAVIOR OF SHALLOW DONOR GROUND STATE LEVELS IN Ge UNDER PRESSURE

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The crossing between absolute (L_1) and secondary (Δ_1) minima which occurs in Ge under the application of a hydrostatic pressure has been found to evidence the strong multi-valley interactions responsible of an anomalous pressure dependence of the A_1 level. Two alternative experimental investigations are suggested to evidence these expectations.

WE PRESENT in this paper a detailed analysis of the ground state levels of shallow donors in Ge when pluri-minima effects are considered. The valley-orbit and subsidiary minima interactions have been here accounted for the first time in the configuration of the conduction band structure of Ge which, under hydrostatic pressure, assumes the typical features of the GeSi alloys.[1] Our results evidence important effects when the four L_1 minima and the six Δ_1 minima (Si-like) lie at about the same energy a configuration in which the multi-valley interactions play a dominant role. The non crossing rule (among states of the same symmetry) is here clearly evidenced and an anomalous pressure dependence of the binding energy of the A_1 level is predicted for the first time. These results could suggest new experimental investigations to evidence the strong interactions arising from pluri-minima configurations, here theoretically predicted.

At atmospheric pressure in Ge the shallow donors ground states is split into two levels of degenerancies 1 and 3 whose symmetries are A_1 and T_1 respectively, and for the Si-like minima into three levels of degeneracies 1, 2 and 3 whose symmetries are A_1, E and T_1 respectively. All these levels are here computed taking into account the valley-orbit[2,3] and subsidiary minima[4] interactions. Central cell corrections[5] were not included, since the exact location in energy of the A_1 level[2] is not the aim of the present study.

Following[6] the complete formal treatment of Bassani, Iadonisi and Preziosi[7] we have started with the conduction band structure of Ge at atmospheric pressure and separated the k-space in the extended zone scheme into ten subzones Ω ($i \equiv 1, 10$). Every subzone contains a minimum located at $\underline{k}_{0i}$, four for the absolute L_1 minima, and six for the Δ_1 subsidiary minima (Si-like),[8] which are about 0.18 eV above, located at $k_0 = 2\pi/a_0(0.82, 0{,}00)$, being a_0 the lattice parameter. The eigenvalues E of the impurity states are so obtained from the solution of the secular determinant[7]

$$\mathrm{Det}\,|\,(E_i^0 - E)\,\delta_{ij} + U_{ij}(1-\delta_{ij})\,| = 0 \qquad (1)$$

where U_{ij} is defined by:

$$U_{ij} = \int_{\Omega_i} \mathrm{d}\underline{k} \int_{\Omega_j} \mathrm{d}\underline{k}'\; \phi_i^{0*}(\underline{k})\, U_{ij}(\underline{k}, \underline{k}')\, \phi_j^0(\underline{k}') \qquad (2)$$

being $U_{ij}(\underline{k}, \underline{k}')$ the Bloch matrix elements connecting states of different subzones through the impurity potential $U(r) = -e^2/r\epsilon$. $\phi_i^0(\underline{k})$ and E_i^0 are the eigenfunction and eigenvalue respectively of the zero order solution for the ground state calculated for each minimum i (considered as independent) in the EMA.[9] The q-dependence of the

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