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MAGNETOOPTICAL INVESTIGATION OF THE BANDSTRUCTURE OF $Pb_{1-x}Ge_xTe$ AT THE STRUCTURAL PHASE TRANSITION ($O_h \rightarrow C_{3v}$)

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The influence of the structural phase transition in PbGeTe on the electronic bandstructure has been studied by interband-magnetooptical transitions above and below T_c. The observed transition energies are explained by an extended Mitchell and Wallis $\vec{k}\cdot\vec{p}$ scheme taking into account strain and displacement effects.

I. Introduction

$Pb_{1-x}Ge_xTe$ exhibits a structural phase transition from the cubic O_h to a low temperature rhombohedral C_{3v} structure [1]. Apart from changes in lattice dynamics [2,3] this phase transition manifests itself in a modification of the electronic bandstructure: the four equivalent conduction and valenceband valleys at the L-point of the Brillouinzone in the cubic phase are split into three equivalent L-states (triplet) and a T-state (singlet) below the phase transition temperature T_c [4-7]. Below T_c a relative displacement u (order parameter) of the group IV and VI lattice sites along an <111> direction occurs and simultaneously rhombohedral shear and dilatational strains appear.

II. Theory

The bandstructure change due to the O_h-C_{3v} transition is taken into account by considering the strain and displacement effects. For the calculation of the magnetic levels in the cubic phase the Mitchell and Wallis (MW) scheme [8,9] is used. Below T_c the strain-effects cause relatively small shifts of the band-gaps (different at L- and T-points of the BZ) and according to the procedure of Takaoka [6] and Nishikawa [7,1] the effect of the relative displacement u is considered by calculating the matrix elements for $(\nabla V)\vec{u} = u_+(\nabla V)_- + u_-(\nabla V)_+ + u_z(\nabla V)_z$ for the singlet (T) valley ($\vec{u} = u(0,0,1)$, $u_z = u$, $u_\pm = 0$) and the triplet (L) valleys ($u_z = -(u/3)z$, $u_\pm = 2u/3$ $(x \pm iy)$ and taking them into account in the MW scheme by using the MW wavefunctions for the $L_{61} + (\alpha,\beta)$ and $L_{62} - (\alpha,\beta)$ levels. This results in an additional matrix Hamiltonian:

for the singlet:

$$H' = \begin{bmatrix} 0 & 0 & iM_l u & 0 \\ 0 & 0 & 0 & -iM_l u \\ -iM_l u & 0 & 0 & 0 \\ 0 & iM_l u & 0 & 0 \end{bmatrix}$$

and for the triplet:

$$H' = \begin{bmatrix} 0 & 0 & -iM_l u/3 & i2\sqrt{2}M_t u/3 \\ 0 & 0 & i2\sqrt{2}M_t u/3 & iM_l u/3 \\ iM_l u/3 & -i2\sqrt{2}M_t u/3 & 0 & 0 \\ -i2\sqrt{2}M_t u/3 & -iM_l u/3 & 0 & 0 \end{bmatrix}$$

M_l and M_t are the longitudinal and transverse optical deformation potential matrix elements. The effect of the relative displacement u is taken into account only in the two-band CB-VB interaction and its effect on the four distant levels is neglected.

For a magnetic field $\vec{B}||c$, the Landau-states of the singlet (T) are then given by the eigenvalues of:

$$\hat{H} = \begin{pmatrix} -\frac{E_g}{2} - \hbar\omega^+\left(n-\frac{1}{2}+\sigma\right) + \frac{g_i^+\mu_B B}{2} - \frac{\hbar^2 k_B^2}{2m_{\tilde{B}}} & 0 & \left(\frac{E_g}{2m_B}\right)^{1/2}\hbar k_B + iM_i u & [E_g\hbar\tilde{\omega}(n+\sigma)]^{1/2} \\ 0 & -\frac{E_g}{2} - \hbar\omega^+\left(n+\frac{1}{2}+\sigma\right) - \frac{g_i^+\mu_B B}{2} - \frac{\hbar^2 k_B^2}{2m_{\tilde{B}}} & [E_g\hbar\tilde{\omega}(n+\sigma)]^{1/2} & -\left(\frac{E_g}{2m_B}\right)^{1/2}\hbar k_B - iM_i u \\ \left(\frac{E_g}{2m_B}\right)^{1/2}\hbar k_B - iM_i u & [E_g\hbar\tilde{\omega}(n+\sigma)]^{1/2} & \frac{E_g}{2} + \hbar\omega^-\left(n-\frac{1}{2}+\sigma\right) + \frac{g_i^-\mu_B B}{2} + \frac{\hbar^2 k_B^2}{2m_{\tilde{B}}} & 0 \\ [E_g\hbar\tilde{\omega}(n+\sigma)]^{1/2} & -\left(\frac{E_g}{2m_B}\right)^{1/2}\hbar k_B + iM_i u & 0 & \frac{E_g}{2} + \hbar\omega^-\left(n+\frac{1}{2}+\sigma\right) - \frac{g_i^-\mu_B B}{2} + \frac{\hbar^2 k_B^2}{2m_{\tilde{B}}} \end{pmatrix} . \quad (1)$$

Since the lowest Landau-state of the CB and the highest of the VB are determined in their magnetic field dependence only by the remote band contributions, these two Landau-states do not reflect the influence of u. For the triplet state a complication arises due to the fact that the Landau-states are coupled (n : no good quantum number) and no longer a 4x4 scheme leads to the magnetic quantum states. By solving a 12x12 matrix approximate solutions for the first three Landau levels in CB and VB were obtained.

III. Experimental

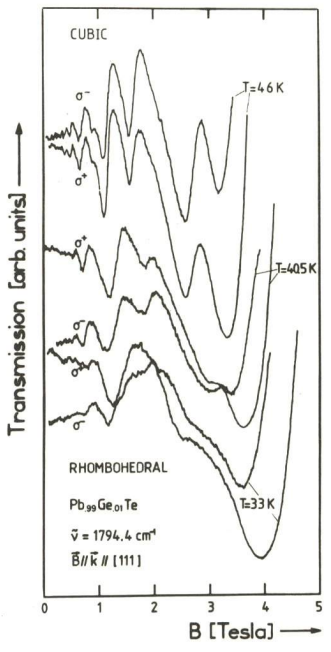

Fig. 1 Transmission vs B for $T>T_C$ and $T<T_C$ of $Pb_{1-x}Ge_xTe$ for $\vec{B}||$ surface normal (cubic [111])

Epitaxially grown n- and p-type $Pb_{1-x}Ge_xTe$ films (D = 5...20 μm) were produced by the hot-wall technique on {111} BaF_2 substrates. Interband magnetooptical transmission experiments (σ_+,σ_-) were performed with CO-laser lines (189 to 246.6 meV), in magnetic fields up to 6.5 T in Faraday configuration $\vec{B}||\vec{k}||$ surface normal ([111]). For samples with Ge-compositions between 0.6 % and 1.33 % and carrier-concentrations between 7×10^{16} and 3×10^{17} cm^{-3} the transition temperature varied between 10 and 45 K. Figure (1) shows typical experimental transmission data as a function of B for various temperatures. Above T_C (42K) the shift of the equivalent transmission extrema is determined by $E_g(T)$. In addition the splitting between σ_+ and σ_- transitions is small and comparable to PbTe. Below T_C the transitions exhibit a clear splitting between the two circular polarisations.

In Fig. (2) the apparent temperature dependence of several magnetooptical transitions indicated by their resonance field B is plotted. A typical bend occurs near T_C which clearly distinguishes a region of a rather rapid change of B with T from a nearly constant transition energy region, which reflects the temperature dependence of the energy gaps at L-and T-point near T_C.

A similar behaviour was found in optical absorption measurements [3,4].

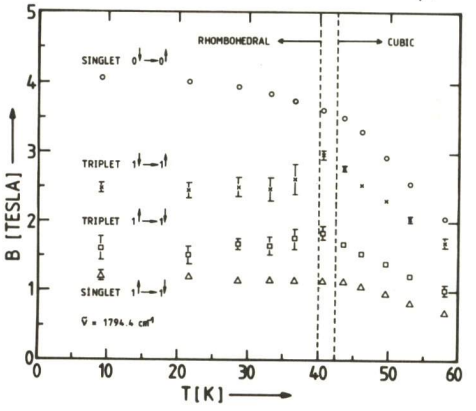

Fig. 2 Resonance B-positions for several transitions for $T > < T_c$

IV. Discussion

The comparison of the experimental and calculated transmission data for the cubic phase is based on the 4x4 scheme, using the selection rules $\Delta n=0$ and $\Delta\sigma=\pm1$ for RCP, LCP radiation in Faraday configuration. In Fig. (3) this comparison is shown for n-PbGeTe (1%) and a temperature of 53 K. Transitions between the Landau ladders of the valleys oriented $\| \vec{B}$ and within the Landau ladder system of the valleys oriented oblique to $\vec{B}$ are observed.

Below T_c a relative shift of the singlet (T) and triplet (L) states arises, which is of the order of some meV for Ge contents of 1%. In the CB and the VB the T-states are shifted upwards relative to the L-states. Therefore transitions between triplet states may be blocked, depending on the position of the Fermi-energy. An additional complication arises from the existence of domains with c-axis not only $\|$ to the surface normal but also inclined to it [2,5] (c' $\|$ <$\bar{1}$11>).

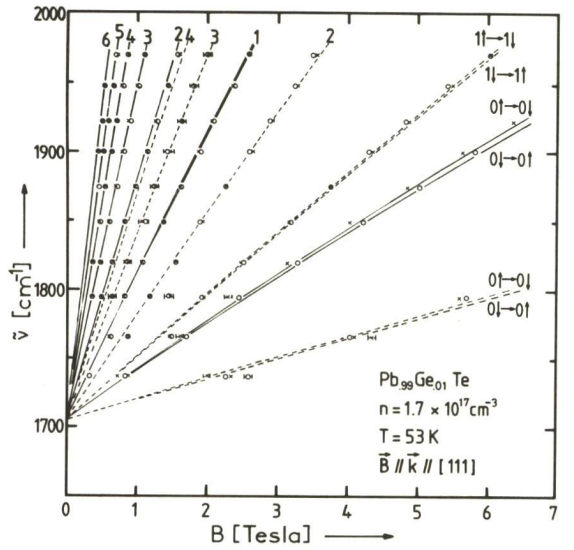

Fig. 3 Interbandtransitions in cubic PbGeTe. (——): within the [111] valley, (---): within the <$\bar{1}$11> valleys; o:σ_+; x :σ_-; experimental data

Below T_c, the Landau-states are qualitatively different from the ones in the cubic phase, and up- and down-states (with respect to $\pm M_{1u}$) occur.

In Fig. (4) experimental data for $T < T_c$ are compared with calculated transition energies for singlet states, oblique singlet states (in c'-domains), triplet states in c- and c'-domains. A short-coming of the present fit is the assumption that u influences only the twoband interaction, which leads to an artifact in the 0 CB and VB Landau states, which are not bent by the M_{1u} terms. For the triplet states the interband transitions occur not at $k_z=0$ but at finite k (depending on M_{1u}). The parameters used are shown in Table I (MW notation [9]). Despite the obvious simplifications, this model describes also observed intraband transitions.

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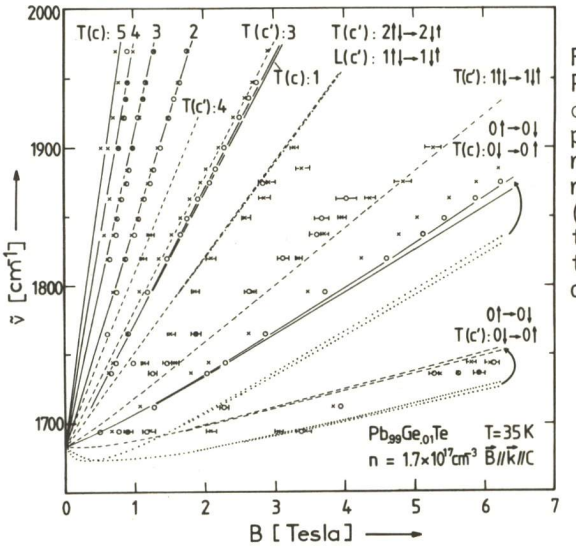

Fig. 4 Interband transitions in $Pb_{1-x}Ge_xTe$ below T_c for σ_+(o) and σ_-(x) involving singlet (T) and triplet (L) states of the c (|| surface normal) and the c' (oblique to surface normal)-domains: Calculated data: (——), (---) (-.-.) for singlet- and triplet states. $0\downarrow,\uparrow \rightarrow 0\uparrow,\downarrow$ transitions were corrected for the influence of $\vec{u}$ on $0\downarrow$ CB-and VB-Landau states

Table I Band parameters of $Pb_{1-x}Ge_xTe$ (x = 0.01)

	two band	far band parameters
$T > T_c$ (T=53 K)	E_g=0.2114 eV $2P_\perp^2/m_0$=5.52 eV $P_\perp^2/P_{\|\|}^2$=14.4	m_t^+/m_0=-0.073, m_t^-/m_0=0.077, m_l^+/m_t^+=11.2 m_l^-/m_t^-=8.7; g_l^+=1.1, g_l^-=-2.8 g_l^-/g_t^-=2.95, g_l^+/g_t^+=3.35
$T < T_c$ (T=35 K)	E_g=0.204 eV (T) $2P_\perp^2/m_0$=5.5 eV $P_\perp^2/P_{\|\|}^2$=14.4 $M_l u = M_t u$=0.022 eV	as above

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