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Optical Absorption of Se$_x$Te$_{1-x}$ Alloys Between 38 eV and 65 eV

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OPTICAL ABSORPTION OF Se_xTe_{1-x} ALLOYS BETWEEN

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The maxima at the onset of the Se 3d and Te 4d absorption in Se_xTe_{1-x} alloys are investigated. Both shift towards lower energy with increasing content of Te. The shift of the Te 4d peaks is proportional to the Te concentration whereas the shift of the Se 3d peak deviates from the linear behaviour at Te concentrations > 30 %.

I. INTRODUCTION

The properties [1] and the band structure of pure Se [2] and Te [3] are very similar. It seems reasonable, therefore, to assume, that the structure of the valence and conduction bands in Se_xTe_{1-x} alloys continuously changes from the band structure of pure Te to the band structure of pure Se if one increases the concentration x of Se from 0 to 1. This assumption is in general agreement with the results of absorption [4] and reflection measurements [5] on Se_xTe_{1-x} alloys in the region of valence band transitions. These measurements give information on both the valence and the conduction bands and may help to attribute structures in the spectra of the pure substances to interband transitions localized at critical points or certain regions in the Brillouin Zone.

By transitions from the sharp (in comparison to the width of the valence and conduction bands), localized Se 3d and Te 4d states the behaviour of the conduction bands, especially the p-symmetric lower conduction band as a function of the concentration can be investigated separately. The core states don't amalgamate and are affected much less on alloying than the valence and conduction states as has been demonstrated e.g. for solid rare gases [6].

2. EXPERIMENTAL PROCEDURE

The Se 3d and Te 4d absorption of thin layers (500 Å - 1500 Å) of Se_xTe_{1-x} alloys has been determined. The samples have been prepared by flash evaporation ($\sim$1000 Å/min, pressure $\sim$10^{-5} Torr) in order to ensure stoichiometry. The Al substrates were kept at room temperature during evaporation in order to prevent decomposition of the evaporated material. The layers with more than 20 % Se were amorphous. As the Se 3d and Te 4d absorption spectra are almost the same for crystalline and amorphous samples (7,8) no care was taken to get the same modification for all the layers. The measurements were performed by use of the synchrotron radiation of the 7.5 GeV electron synchrotron DESY and a 1 m Rowland grazing incidence spectrometer. Details of the experimental arrangements are described elsewhere (9).

3. RESULTS AND DISCUSSION

The absorption coefficient of Se_xTe_{1-x} alloys in the photon energy region from 38 eV to 65 eV is shown in Fig. 1. Transitions of the 3d electrons to the p-symmetric conduction band give rise to the maximum at 56 eV in the spectrum of pure Se. The spin orbit splitting of the Se 3d levels (1 eV) causes the shoulder at the low energy side of the maximum, whereas the shoulder at the high energy side is explained by a maximum in the density of states of the conduction band (7). Pure Te (8) (x=0) shows a pronounced doublet at 41 eV and 42.4 eV which is due to transitions from the spin orbit split 4d states. In the case of Te no fine structure which is related to the density of states of the conduction band can be detected. Towards higher photon energies the absorption of Te increases strongly. This increase is caused by delayed transitions of the 4d electrons to f-symmetric final states. The weak structure between 47 eV and 50 eV in the case of Te and around 63 eV in the case of Se are due to transitions to higher conduction bands and are not discussed here.

In the absorption spectra of the alloys both the Se 3d and Te 4d absorption show up. Within the accuracy of our measurements ($\pm$20 %) the absolute values of the absorption coefficients of Se_xTe_{1-x} alloys agree with the values calculated as a proportional superposition of the absorption

Fig. 1

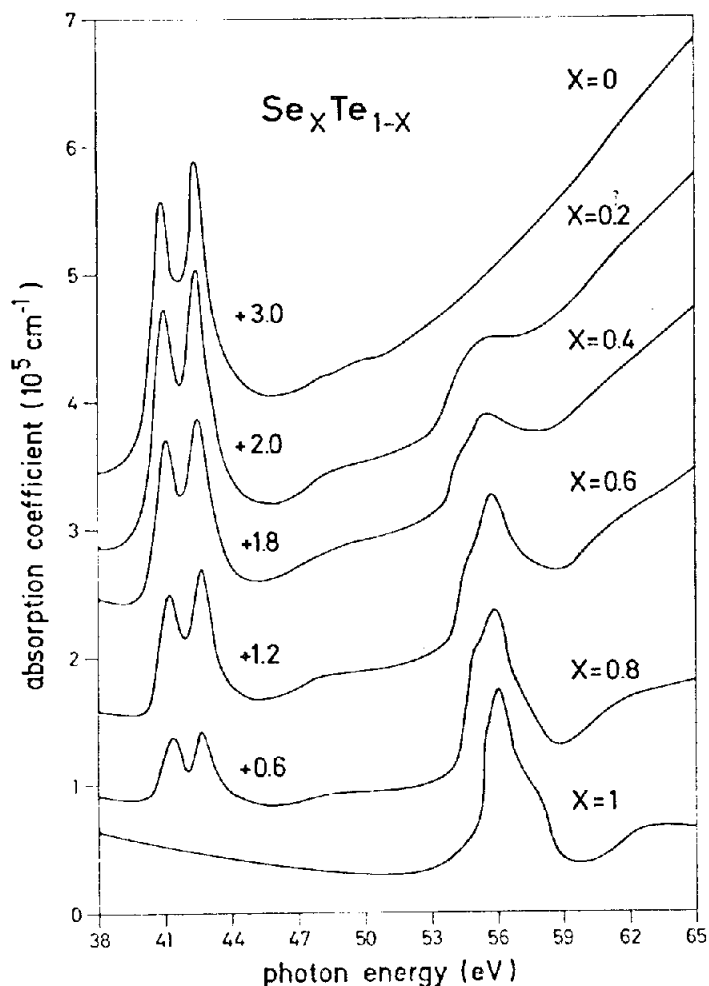Absorption coeffi-
cient of Se_xTe_{1-x}
alloys between 38 eV
and 65 eV. The shift
of the curves for
different alloys with
respect to the ab-
sorption scale is
given by the number
(in 10^{-5} cm^{-1}) beside
the Te 4d doublet

coefficient of the pure substances. Both the Se 3d and the Te 4d peaks shift to lower energy when the Te content is increased. This can be seen in detail in Fig. 2 where the difference in energy position of the maxima in pure Se and in the alloys is drawn as a function of the Te concentration. The position of the Te 4d absorption in pure Se was obtained by linear extrapolation. The shift of the Te doublet is proportional to the concentration of Te, the spin orbit splitting remains constant. In order to determine the position of the Se 3d maximum the background due to the Te d-f absorption has been subtracted. At low concentrations of Te the Se 3d maximum also shifts linearly, the slope being about the same as for the Te 4d maxima. However, at higher amounts of Te the shift
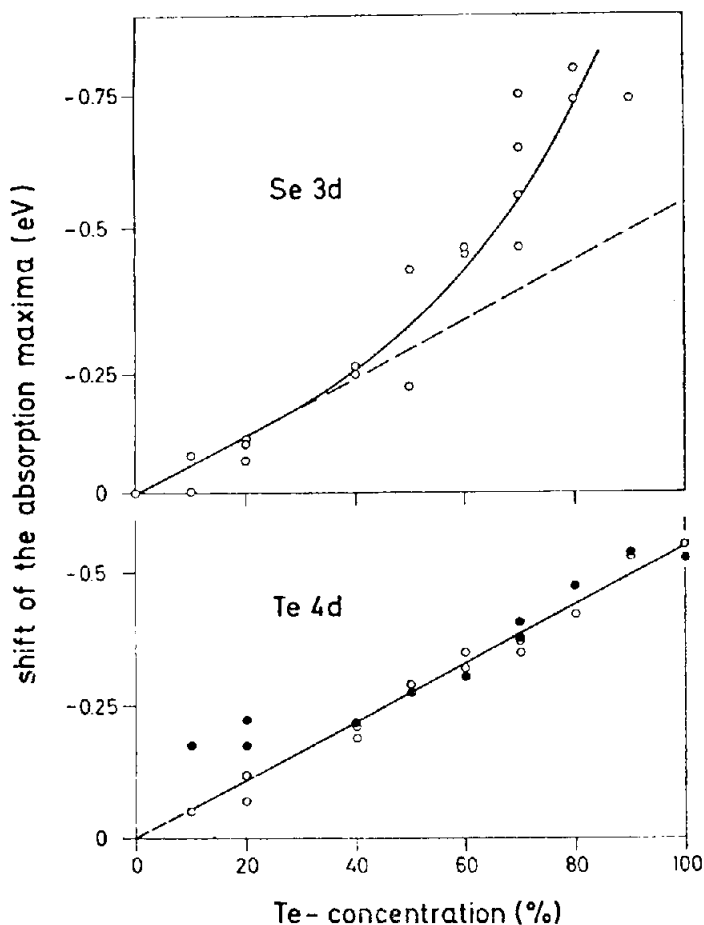
Fig. 2
Energy shift of the
Se 3d and the Te 4d
maxima (open circles
low energy component,
full circles high
energy component of
the doublet) as a
function of the Te
concentration

of the Se 3d maximum shows a marked deviation from the linear behaviour.

Simplified energy band schemes of pure Se and Te are given in Fig. 3. It has already been pointed out that the broad maxima at the onset of the Se 3d and Te 4d absorption show almost no fine structure that can be attributed to the density of the conduction states [7,8]. Therefore, it is not necessary to give all the details of calculated band structures. The energy of the top of the valence band with respect to the vacuum level has been taken from photoemission data [10], the value for the band gaps from Ref. [1,11]. By adjusting the calculated density of conduction states to the absorption spectrum of Te one finds that the Te 4d maximum coincides approximately with the middle of the lower conduction band [8]. In the case of Se the transitions from the two spin orbit
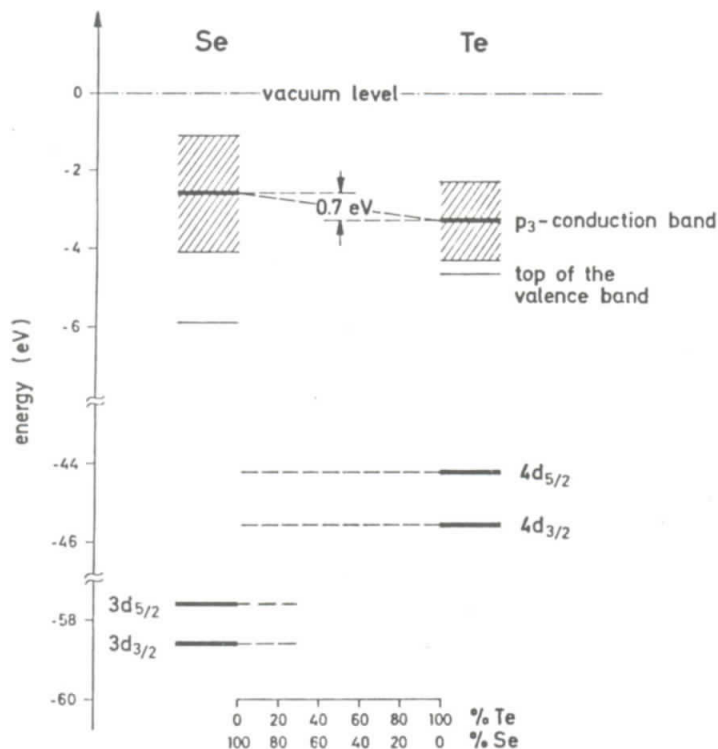
Fig. 3

Energy scheme of Se and Te. The shift of the energy levels on alloying is indicated by the dashed lines. The widths of the conduction bands have been taken from Ref. (3,10)

split $3d_{5/2}$ and $3d_{3/2}$ levels overlap appreciably. By separating both contributions one can show that the main part of the absorption stems from transitions of the $3d_{5/2}$ electrons to states in the middle of the lower conduction band. Superimposed is the absorption due to transitions of the $3d_{3/2}$ electrons to a density of states maximum at the lower edge of the conduction band (7). In Fig. 3 the distance between the core levels and the middle of the conduction bands corresponds to the experimentally determined photon energies.

The simplest explanation for the shift of the Te 4d maxima is a linear shift of the middle of the conduction band from its position in pure Se to the position in pure Te. The resulting shift of 0.7 eV as indicated in Fig. 3 is in reasonable agreement with the experimentally determined value of 0.5 eV. A linear shift is also supported by the nearly linear dependence of the lattice constant on concentration (12) and by the linear shift of reflectivity maxima in the fundamental ab-

sorption region over a broad range of concentrations (5).

The model also explains the linear shift of the Se 3d maxima at low Te concentrations. The deviation from the linear shift at high Te concentrations, however, cannot be understood in terms of this simple model. There are a number of possible explanations, e.g., a shift of the Se 3d core levels, or interaction of the final states with the underlying continuum due to Te d-f transitions. However, the different behaviour of the Te 4d and Se 3d absorption is still an open question.

REFERENCES

(1) P. Grosse, Springer Tracts in Modern Physics (ed. G. Höhler) Springer-Verlag Berlin, Heidelberg, New York 48 (1969)

(2) R. Sandrock, Phys.Rev. 169, 642 (1968)

(3) K. Maschke, phys.stat.sol. (b) 47, 511 (1971)

(4) E. Sutter, phys.stat.sol. 33, 749 (1969)

(5) J. Stuke und H. Keller, phys.stat.sol. 7, 189 (1964)

(6) R. Haensel, N. Kosuch, U. Nielsen, U. Rössler, and B. Sonntag, to be published

(7) M. Cardona, W. Gudat, B. Sonntag, and P.Y. Yu, Proc. X Int. Conf. Phys. Semicond., Cambridge, Mass. (1970)

(8) B. Sonntag, T. Tuomi, and G. Zimmerer, to be published

(9) P. Rabe, B. Sonntag, T. Sagawa, and R. Haensel, phys.stat.sol. (b) 50, 559 (1972)

(10) L.D. Laude, B. Fitton, and M. Anderegg, Phys.Rev.Lett. 26, 637 (1971), L.D. Laude, B. Fitton, B. Kramer, and K. Maschke, Phys.Rev. Lett. 27, 1053 (1971)

(11) W. Beyer, H. Mell, and J. Stuke, phys.stat.sol. (b) 45, 153 (1971)

(12) E. Grison, J.Chem.Phys. 19, 1109 (1951)