by the change in the angle-bending force constant F_θ in the valence-force potential model; this constant governs the frequency of the transverse-acoustic mode X_3. With reference to the ratios mentioned above, it should be noted that the differences between the dimensionless frequencies Ω_{X_3} conform to a closely similar pattern, the ratio being 8.8 : 1 : 1.7.

ACKNOWLEDGMENT

The authors are indebted to Dr. J. M. Rowe for valuable discussions on the present work.

---

[1] K. B. Tolpygo, Fiz. Tverd. Tela 3, 943 (1961) [Sov. Phys. Solid State 3, 685 (1961)].

[2] W. Cochran, Proc. Roy. Soc. (London) A253, 260 (1959).

[3] T. I. Kucher, Fiz. Tverd. Tela 4, 2385 (1962) [Sov. Phys. Solid State 4, 1747 (1963)].

[4] F. Herman, J. Phys. Chem. Solids Suppl. 8, 405 (1959).

[5] M. Mostoller, J. Phys. Chem. Solids 31, 307 (1970).

[6] R. M. Martin, Phys. Rev. 186, 871 (1969).

[7] H. Y. Fan, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic, New York, 1955), Vol. 1, p. 283.

[8] R. E. Lindquist and A. W. Ewald, Phys. Rev. 135, A191 (1964).

[9] *Physical Properties of Diamond*, edited by R. Berman (Clarendon, Oxford, 1965).

[10] J. L. Warren, J. L. Yarnell, G. Dolling, and R. A. Cowley, Phys. Rev. 158, 805 (1967).

[11] G. Dolling, in *Inelastic Scattering of Neutrons in Solids and Liquids* (IAEA, Vienna, 1963), Vol. II, p. 37.

[12] G. Nilsson and G. Nelin, Phys. Rev. B 3, 364 (1971).

[13] D. L. Price and J. M. Rowe, Solid State Commun. 7, 1433 (1969).

[14] S. Groves and W. Paul, Phys. Rev. Letters 11, 194 (1963).

[15] G. Nelin and G. Nilsson, Phys. Rev. B 5, 3151 (1972).

[16] R. Stedman, Rev. Sci. Instr. 39, 878 (1968).

[17] R. Stedman, L. Almqvist, G. Raunio, and C. Nilsson, Rev. Sci. Instr. 40, 249 (1969).

[18] R. Stedman and G. Nilsson, Rev. Sci. Instr. 39, 637 (1968).

[19] T. R. Hart, R. L. Aggarwal, and B. Lax, Phys. Rev. B 1, 638 (1970).

[20] J. P. Russell, Appl. Phys. Letters 6, 223 (1965).

[21] J. H. Parker, Jr., D. W. Feldman, and M. Ashkin, Phys. Rev. 155, 712 (1967).

[22] M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Oxford U. P., London, 1954).

[23] P. Flubacher, A. J. Leadbetter, and J. A. Morrison, Phil. Mag. 4, 273 (1959).

[24] T. H. K. Barron, W. T. Berg, and J. A. Morrison, Proc. Roy. Soc. (London) A242, 478 (1957).

[25] G. Dolling and R. A. Cowley, Proc. Phys. Soc. (London) 88, 463 (1966).

[26] H. J. McSkimin, J. Appl. Phys. 24, 988 (1953).

[27] D. F. Gibbons, Phys. Rev. 112, 136 (1958).

[28] B. N. Brockhouse and P. K. Iyengar, Phys. Rev. 111, 747 (1958).

[29] We are indebted to Dr. G. Dolling for sending us the actual figures of his calculations.

[30] Z. A. Demidenko, T. I. Kucher, and K. B. Tolpygo, Fiz. Tverd. Tela 3, 2482 (1961) [Sov. Phys. Solid State 3, 1803 (1962)].

[31] B. D. Singh and B. Dayal, Phys. Status Solidi 38, 141 (1970).

[32] A. W. Solbrig, Jr., J. Phys. Chem. Solids 32, 1761 (1971).

[33] H. L. McMurry, A. W. Solbrig, Jr., J. K. Boyter, and C. Noble, J. Phys. Chem. Solids 28, 2359 (1967).

[34] H. B. Rosenstock, Phys. Rev. 129, 1959 (1963).

[35] H. J. McSkimin and W. L. Bond, Phys. Rev. 105, 116 (1957).

[36] C. D. Clark, J. Phys. Chem. Solids 8, 481 (1959).

PHYSICAL REVIEW B VOLUME 6, NUMBER 10 15 NOVEMBER 1972

Reflectivity of $ZnSe_xTe_{1-x}$ Single Crystals

Atsuko Ebina, Mitsuo Yamamoto, and Tadashi Takahashi
Research Institute of Electrical Communication, Tohoku University, Sendai 980, Japan
(Received 28 January 1972)

Reflectivity spectra of $ZnSe_xTe_{1-x}$ single crystals were measured from 2.0 to 6.6 eV through the whole range of mole fraction x at room temperature. The variation of the band gaps such as the E_0, e_1, E_1, and E_2 with x is reported. The E_0, e_1, and E_1 gaps exhibit spin-orbit splitting. The lowest gap E_0 shows a minimum in energy at $x = 0.33$. The minimum value is 2.13 eV.

I. INTRODUCTION

Since an early report by Larach *et al.*[1] on the diffuse reflectance of the microcrystalline powders of the ZnSe-ZnTe system, few papers have reported on the variation of the band gaps with composition. The variation of the lowest band gap with composition in the $ZnSe_xTe_{1-x}$ alloys has been investigated by the crystal color observed under a microscope[2] and by the reflection spectra.[3] Aven *et al.*[4] have reported the crystal growth of $ZnSe_xTe_{1-x}$ using a closed vapor-phase technique in an excess Te atmosphere.

Single crystals of $ZnSe_xTe_{1-x}$ of uniform composition were grown through the whole range of composition by a slightly modified version of the technique reported in Ref. 4 without the addition of extra Te. The present paper describes the reflectivity measurements for the $ZnSe_xTe_{1-x}$ single crystals. The reflectivity spectra reveal well-defined peaks, which are assigned using the assignment of the end-point compounds ZnSe and ZnTe.[5,6] The variation of the band gap with composition is satisfactorily explained by a dielectric method reported recently by Van Vechten and Bergstresser.[7] Present reflectivity measurements of the $ZnSe_xTe_{1-x}$ alloys provide the first report on the reflectivity experiment over the several band gaps for the zinc-blende semiconductor-alloy systems of the popular Zn and Cd chalcogenides, although reflectivity measurements have been reported for the wurtzite II-VI alloy systems.[8,9]

II. EXPERIMENT

Single crystals were grown on a small (110) cleaved plane of ZnSe or ZnTe seed crystal using a modified version of the closed vapor-phase technique reported by Aven *et al.*[4] The single crystals with the grown surfaces (110) and (111) were up to 4×3 mm. The grown crystal can be cleaved along the (110) plane and contains no inclusions of other substances such as Te metal. The details of the crystal growth will be presented elsewhere.

Using an electron-probe x-ray microanalyzer, it was found that the single crystal is homogeneous in composition and the transition region from the seed to the $ZnSe_xTe_{1-x}$ crystal is about 25 μm in thickness. The uniformity in composition of the grown crystal was also estimated from x-ray lattice-constant measurements. On the basis of the well-known Vegard's law, the mole fraction x was determined from the lattice constant.[1] The value of x can be determined with great accuracy, because the difference in lattice constant between ZnSe and ZnTe is large. The lattice constant was determined from high-angle x-ray diffraction measured on the small pieces cut from a crystal. The lattice constant of ZnTe grown by a vapor-phase technique is 6.1033 ± 0.0006 Å, which is in agreement with the reported value 6.1037 Å.[10] The lattice constants measured on the small pieces cut from various sections of a grown crystal are in agreement with each other within ± 0.02%. These results also indicate that the deviation in composition of the grown crystal is within ± 0.2%. The (110) surfaces, grown to a size of 4×3 mm, are optically flat and sufficiently homogeneous and can be used directly for reflectivity measurements.

The reflectivity measurements were made on the as-grown or the cleaved (110) surfaces using a conventional Hitachi–Perkin–Elmer grating monochromator from 2.0 to 6.6 eV at room temperature. Measurements for as-grown and cleaved surfaces are in agreement with each other within the experimental error. Because of the small size of the reflecting plane, only relative reflectivity was measured except in the case of ZnSe and ZnTe, for which the absolute reflectivity was measured. The measured absolute reflectivity is in satisfactory agreement with previous work.[11–13] These results indicate that the reflectivity measurements for the $ZnSe_xTe_{1-x}$ crystals are reliable enough for the analysis of the peak positions. The reflectivity measurements were thoroughly made several times over the whole spectrum, and it was found that the energy positions of the structures in the spectra are satisfactorily reproducible.

III. RESULTS

The spectra of $ZnSe_xTe_{1-x}$ are shown in Fig. 1. All of the peak positions indicated by arrows in the figure are quite reproducible to within a few hundredths of an eV. As can be seen in Fig. 1, the spectra for both $x = 0$ (ZnTe) and $x = 1$ (ZnSe) reveal more and generally better-defined structures than reported in any previous work.[11–14] The weak peaks at 4.32 and 4.85 eV for ZnTe and the very weak peak at about 4.3 eV for ZnSe were observed for the first time. The crystal of ZnTe was grown by a vapor-phase technique of Piper and Polich,[15] and its color is more pure than that of melt-grown

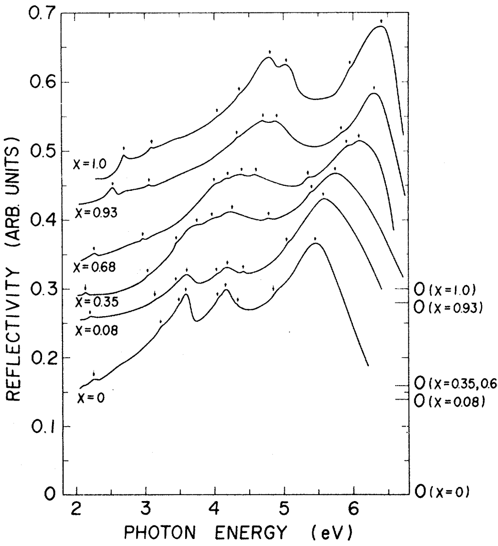

FIG. 1. Reflectivity spectra of $ZnSe_xTe_{1-x}$ for $x = 0$, 0.08, 0.35, 0.68, 0.93, and 1.0 at room temperature. Arrows in the figure indicate the energy positions of the structures in the spectra.

crystals. This crystal shows the very steep absorption rise at the fundamental absorption edge. The cleaved surface used for measurements is as large as 10×5 mm. The lattice constant of vapor-phase-grown ZnTe is in agreement with the reported value, as mentioned in Sec. II, while that of the melt-grown crystal shows slight deviation in lattice constant. These results as well as the clear pattern of x-ray diffraction of the vapor-phase-grown ZnTe crystal indicate that the vapor-phase-grown crystal is free of crystallographic strains. The ZnSe crystal was also grown by a vapor-phase technique and as a purer color than melt-grown crystals. The cleaved-surface size of ZnSe was sufficient for measurements of the absolute reflectivity, although its size was about one-half of that of the ZnTe crystal. Thus, the crystals of ZnTe and ZnSe are seemingly of good quality, and free of impurities and crystallographic strains. The better-refined structures for ZnSe and ZnTe than reported in previous work may be mainly related to the high quality of the cleaved surface and to the large surface size, and partly related to the measurement technique.

Figure 2 shows the variation of peak positions as a function of x. In the case of $x = 0.48$, only crystals of small size with rough surfaces were grown. The reflectivity spectrum of this material was so broad at the photon energies between 3 and 5 eV that it did not show any discernible structure; the structure being seen only for the photon energy lower than 3 eV and higher than 5 eV. The peak positions at low photon energies are reproducible, while those at high photon energies were not. Roughness of the reflecting plane is probably responsible for the unreliable results. Thus, in this case, only two peaks at low photon energies are presented in Fig. 2. The tentative assignments of the peaks are also shown in this figure, where generally used notations defined by Cardona *et al.*[11, 14] are employed except for the two curves from the top for which the notations used by Walter *et al.*[6] are employed. These peak positions are summarized in Table I. Two values 6.30 and 6.20 eV for $x \approx 1$ in the table correspond to the weak shoulders on the low-energy side of the main peak. These values had larger uncertainty than the others.

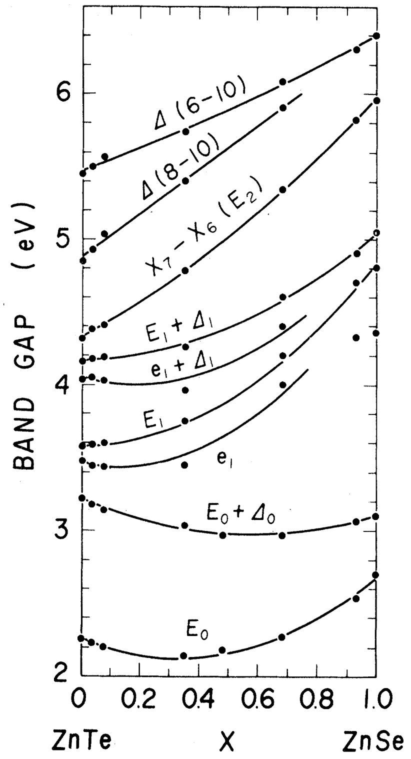

FIG. 2. Variation of the peak positions in the reflectivity spectra as a function of x for $ZnSe_xTe_{1-x}$. The tentative assignments of the band gaps are also shown.

Figure 3 shows the variation of the lowest band gap E_0 with x, along with the results of Larach *et al.*[1] and of Shiozawa and Jost.[2] The least-squares fit to an expression quadratic in x, which is usually assumed, gave $E_0 = 2.26 - 0.82x + 1.23x^2$ eV. This fit shows the minimum value of 2.13 eV at $x = 0.33$. Figure 4 shows the spin-orbit splittings Δ_0 and Δ_1 as a function of x. Both Δ_0 and Δ_1 are seemingly nonlinear but quadratic in x with a bowing parameter (a measure of the deviation from linearity)[7] of the negative sign. Quadratic least-squares fits to Δ_0 and Δ_1 are shown as the solid lines in the figure. These nonlinear relations are rather unusual. Niculescu[16] has reported that for ZnTe-HgTe system, Δ_1 shows the nonlinear variation with composition having a bowing parameter of the positive sign. For the GaAs-GaP system[17] and the GaAs-InAs system[18] the nonlinear variation of Δ_1 with composition has also been reported. It is noted that while the present results indicating the nonlinear variation are of interest, they must be considered to be tentative, because the experimental uncertainty in the determination of the gap energy from reflectivity measurements is not as small as the case of the electroreflectance or thermoreflectance measurements. The quadratic least-squares fits to the E_0, $E_0+\Delta_0$, E_1, and $E_1+\Delta_1$ gaps give Δ_0 (ZnSe) = 0.42 eV, Δ_0 (ZnTe) = 0.95 eV, Δ_1 (ZnSe) = 0.20 eV, and Δ_1 (ZnTe) = 0.59 eV. These values are in good agreement with the previously measured values,[5, 19, 20] and the calculated values[21] reported recently.

Van Vechten and Bergstresser[7] have recently treated the band gaps as a function of composition for alloy systems of the IV, III-V, and II-VI semiconductors by both a dielectric and an empirical

TABLE I. Peak positions in the reflectivity spectra and the spin-orbit splittings Δ_0 and Δ_1 for $ZnSe_xTe_{1-x}$.

Tentative assignment		Peak positions (in eV)						
$x=$	0	0.03	0.08	0.35	0.48	0.68	0.93	1.0
E_0	2.26	2.23	2.20	2.14	2.18	2.27	2.54	2.70
$E_0+\Delta_0$	3.22	3.18	3.14	3.03	2.97	2.97	3.06	3.10
e_1	3.48	3.45	3.44	3.45		4.00		
$e_1+\Delta_1$	4.04	4.05	4.03	3.96		4.40		
E_1	3.58	3.59	3.60	3.75		4.20	4.70	4.80
$E_1+\Delta_1$	4.16	4.18	4.19	4.26		4.60	4.90	5.04
E_2	4.32	4.38	4.41	4.78		5.34	5.82	5.95
Δ(8-10)	4.85	4.93	5.04	5.40		5.90	≈6.20	≈6.30
Δ(6-10)	5.45	5.50	5.57	5.74		6.08	6.30	6.40
Δ_0	0.96	0.95	0.94	0.89		0.70	0.52	0.40
Δ_1	0.57	0.60	0.59	0.51		0.40	0.20	0.24

pseudopotential method. These authors have indicated that the dielectric method gives good agreement with experiment. Thus, we analyze the present results using this method. Figure 5 shows the deviation from linearity in the variation of the E_0 and E_1 gap with x, where the spin-orbit splitting is eliminated by the addition of $\frac{1}{3}\Delta_0$ and $\frac{1}{2}\Delta_1$ to the measured E_0 and E_1 gap, respectively. The calculated curves for E_0 and E_1 using the bowing parameters $c_0=1.10$ and $c_1=1.13$, respectively, are also shown. The value c_0 is given in Ref. 7, and c_1 is estimated from the parameters given in Ref. 7. The least-squares fit to experimental values gave $c_0=1.04$ and $c_1=0.96$. The agreement between experiment and the dielectric method is satisfactory.

IV. DISCUSSION

The assignments of the reflectivity structures of $ZnSe_xTe_{1-x}$ are made on the basis of the early reflectance data and its assignment given by Cardona and co-workers[5, 11, 12, 14] and of the recent reflectance data and the theoretical calculations including the spin-orbit interaction given by Walter, Cohen, Petroff, and Balkanski[6] (hereafter referred to as WCPB) for the end-point compounds ZnSe and ZnTe.

The assignments of the E_0, e_1, and E_1 gaps including the spin-orbit splitting component of these gaps are made on the basis of the assignments for ZnSe and ZnTe given by Cardona and co-workers.[5, 11, 12, 14] For these gaps, the assignments by WCPB, based on theoretical calculations, are the same as those by Cardona and co-workers.

For the three upper curves in Fig. 2, the assignments are made in terms of the assignments of WCPB given for ZnSe and ZnTe. The third curve from the top in this figure is probably attributed to X_7-X_8 transitions, which corresponds to the E_2 gap of Cardona's notation. The theoretical calculations of WCPB have shown that X_7-X_8 transitions cause the reflectivity structure at 4.65 and 5.97 eV for ZnTe and ZnSe, respectively. The present experiments for ZnSe gave the peak at 5.95 eV, in agreement with the theoretically calculated value

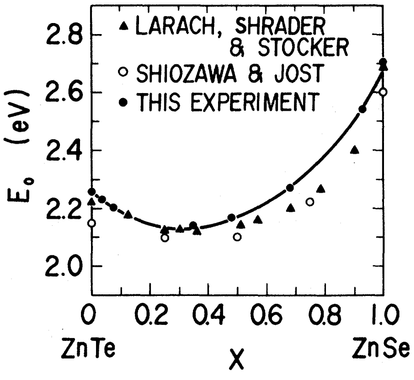

FIG. 3. Lowest band gap E_0 of $ZnSe_xTe_{1-x}$ as a function of x at room temperature. The least-squares fit to an expression quadratic in x gives $E_0=2.26-0.82x+1.23x^2$ eV, which is presented as the solid line. This fit shows the minimum gap of 2.13 eV at $x=0.33$. Previously reported values are also shown (see Refs. 1 and 2).

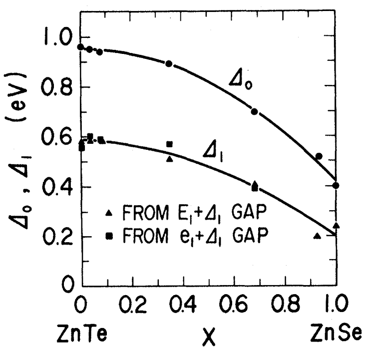

FIG. 4. Variation of the spin-orbit splittings Δ_0 and Δ_1 as a function of x for $ZnSe_xTe_{1-x}$. The solid lines are the least-squares fits to an expression quadratic in x.

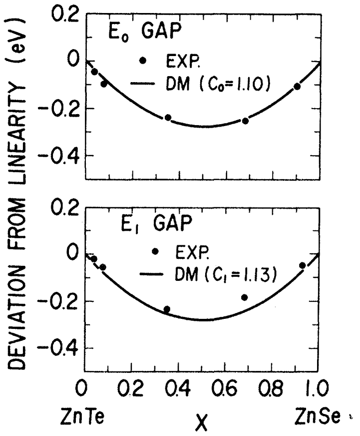

FIG. 5. Deviation from linearity of the band gaps E_0 and E_1 without spin-orbit splitting for $ZnSe_xTe_{1-x}$. The solid lines for the E_0 and E_1 gaps are calculated using the dielectric method with the bowing parameters $c_0=1.10$ and $c_1=1.13$.

of WCPB. The measured peak position of 4.32 eV of ZnTe is lower than the calculated position of 4.65 eV. Taking into account of the slope in the variation of the measured 4.32-eV peak with x for $x\approx 0$, this peak may be related to the 5.95-eV peak of ZnSe. These results suggest that the 4.32-eV peak of ZnTe is caused by X_7-X_6 transitions. The first curve from the top in Fig. 2, which corresponds to the main peak in the reflectivity spectrum, is attributed to K(7-10), Δ(6-10), and Σ(7-10) transitions for ZnTe and to Δ(6-10), Δ(8-10), Σ(7-9), and Σ(8-10) transitions for ZnSe. The calculations by WCPB have indicated that these transitions are responsible for the peak at 5.45 eV for ZnTe and at 6.47 eV for ZnSe. These transitions are referred to as Δ(6-10) transitions in Fig. 2. The second curve from the top in Fig. 2 is attributed to Δ(8-10) transitions, which produce the reflectivity peak at 4.95 eV for ZnTe and at 6.20 eV for ZnSe on the basis of the calculations of WCPB. Thus, the assignments of Δ(6-10), Δ(8-10), and X_7-X_6 transitions derived from the calculations of WCPB may explain quite satisfactorily the measured structures in the reflectivity spectra of the $ZnSe_xTe_{1-x}$ alloys.

On the other hand, according to the early assignments of Cardona and co-workers[5, 11, 12, 14] for ZnTe and ZnSe, there is no reasonable assignment for the third curve from the top in Fig. 2, as far as the direct transitions are concerned. In view of the dielectric method,[22] which employs the assignments of Cardona and co-worker, this curve may be assigned to the indirect $\Gamma \to X$ transitions. The first curve from the top may be assigned to the E_2 gap (X_7-X_6 transitions), on the basis of the assignment of the 6.7-eV peak of ZnSe by Cardona and co-workers. The second curve may be assigned to the E_0' gap on the basis of the E_0'-gap assignment of Cardona and co-workers for ZnTe. Thus, the assignments based on the early report for ZnTe and ZnSe by Cardona and co-workers cannot be ruled out completely.

In conclusion, the assignments of the band gaps based on the calculations of WCPB may explain the measured peaks in the reflectivity spectra of $ZnSe_xTe_{1-x}$. The structure at about 4.3 eV for the materials with $x\approx 1$ was not assigned. Although this structure is very weak, its energy position is reproducible. If indirect transitions are involved besides the direct transitions, this structure may be attributed to $\Gamma \to L$ transitions (or $\Gamma \to \Lambda$ transitions).[22]

The structures in the reflectivity spectra of $ZnSe_xTe_{1-x}$ are less sharp compared to those of the end-point compounds. The increase of x from zero to as small as 0.08 does broaden the structure remarkably, as can be seen in Fig. 1. Similar behavior was observed for the decrease of x from one to 0.93. The greater the deviation of x from zero or one, the more the peaks broaden, while line profiles of x-ray diffraction pattern show no significant change with x. This broadening effect on the reflectivity spectra cannot be attributed to impurities. Since the absorption cutoff at the fundamental absorption edge in $ZnSe_xTe_{1-x}$ is as sharp as in ZnTe. Therefore, this effect may be due to the difference in the form factor between Te and Se, i.e., to the aperiodicity in the crystal potential of the $ZnSe_xTe_{1-x}$ alloys.[7] It may be difficult to estimate the aperiodicity using x-ray-diffraction profiles.

---

[1] S. Larach, R. E. Shrader, and D. F. Stocker, Phys. Rev. 108, 587 (1957).

[2] L. R. Shiozawa and J. M. Jost, Aeronautical Research Laboratory USAF, Contract No. AF33 (667)-7399, final report, 1965 (unpublished).

[3] R. E. Halsted, D. T. F. Marple, and M. Aven, Electron Div., Electrochem. Soc. 14, 6 (1965).

[4] M. Aven, R. S. Hall, and J. S. Prener, J. Electrochem. Soc. 115, 846 (1968).

[5] M. Cardona, in *Proceedings of the Seventh International Conference on the Physics of Semiconductors, Paris*, 1964 (Dunod, Paris, 1964), p. 181.

[6] J. P. Walter, M. L. Cohen, Y. Petroff, and M. Balkanski, Phys. Rev. B 1, 2661 (1970).

[7] J. A. Van Vechten and T. K. Bergstresser, Phys. Rev. B 1, 3351 (1970).

[8] R. E. Drews, E. A. Davis, and A. G. Leiga, Phys. Rev. Letters 18, 1194 (1967).

[9] R. L. Hengehold and C. R. Fraime, Phys. Rev. 174, 808 (1968).

[10] W. L. Roth, in *Physics and Chemistry of* II-VI *Compounds*, edited by M. Aven and J. S. Prener (North-Holland, Amsterdam, 1967), p. 127.

[11] M. Cardona and D. L. Greenway, Phys. Rev. 131, 98 (1963).

[12] M. Cardona, J. Appl. Phys. 34, 813 (1963).

[13] M. Balkanski and Y. Petroff, in Ref. 5, p. 254.

[14] F. H. Pollak, in *Proceedings of the International Conference on II-VI Semiconducting Compounds, Providence*, 1967, edited by D. G. Thomas (Benjamin, New York, 1968), p. 552.

[15] W. W. Piper and S. J. Polich, J. Appl. Phys. 32, 1278 (1968).

[16] D. Niculescu, J. Phys. C 1, 804 (1968).

[17] A. G. Thompson, M. Cardona, K. L. Shaklee, and J. C. Woolley, Phys. Rev. 146, 601 (1966).

[18] A. G. Thompson and J. C. Woolley, Can. J. Phys. 45, 2597 (1967).

[19] M. Cardona, K. L. Shaklee, and F. H. Pollak, Phys. Rev. 154, 696 (1967).

[20] E. Matatagui, A. G. Thompson, and M. Cardona, Phys. Rev. 176, 950 (1968).

[21] G. G. Wepfer, T. C. Collins, and R. N. Euwema, Phys. Rev. B 4, 1296 (1971).

[22] J. A. Van Vechten, Phys. Rev. 187, 1007 (1969).

PHYSICAL REVIEW B VOLUME 6, NUMBER 10 15 NOVEMBER 1972

Thermal Conductivity of II-VI Compounds and Phonon Scattering by Fe^{2+} Impurities

Glen A. Slack

General Electric Research and Development Center, Schenectady, New York 12301

(Received 22 June 1972)

The thermal conductivities κ of over twenty different single crystals of synthetic ZnO, ZnS, ZnSe, ZnTe, CdTe, and of natural, cubic ZnS have been measured from temperatures of 3 to 300 K. The results for the undoped crystals above 30 K can be scaled using the parameter $\overline{M}\delta\Theta^3$, where $\overline{M}$, δ, and Θ are the average mass, interatomic spacing, and Debye temperature, respectively. A comparison of these results with those in the literature for BeO, CdS, CdSe, HgSe, HgTe, Si, Ge, GaAs, and InSb show that the same scaling parameter applies for most of them. The compounds HgSe and HgTe exhibit anomalously low κ values. Crystals doped with Fe^{2+} show a resonant-type one-phonon scattering from the five low-lying energy levels of this $3d^6$ ion. Group theory shows that the strongest scattering occurs for phonons of energy 2Δ, where Δ is the interlevel spacing of the Fe^{2+} ion.

I. INTRODUCTION

The present work is a review of the thermal conductivity of undoped II-VI compounds with new data on ZnO, ZnS, ZnSe, ZnTe, and CdTe. With this knowledge of the behavior of pure crystals, the extra phonon scattering produced by Fe^{2+}-ion impurities in ZnS and CdTe has been studied.

A. Pure Crystals

The II-VI compound with the highest thermal conductivity κ is BeO. Results for BeO have recently been published,[1] and will not be reviewed here. Some comments on the κ of BeS have also been made.[1] Nothing is known about the κ of BeSe or BeTe. The κ of ceramic samples of ZnO[2,3] has been published, as well as a measurement[4] of the anisotropy of its κ. In addition there are some unpublished results of Martin and Wolf[5] and Pohl.[6] Pohl's results are reported here. There is one report[7] in the literature for a single crystal of ZnS, as well as two[8,9] for ZnSe. The κ of ZnTe has been reported[10–12] several times. For the Cd compounds there exists a lot of work[13–18] on CdS, and some work[19,20] on CdSe. The work on CdTe has been reviewed,[21] but a number of papers[9,13,21–26] on CdTe were not included in that review. Of these references, three (Refs. 13, 25, and 26) give κ values in reasonable agreement with Slack and Galginaitis.[21]

Numerous measurements of κ have been made for the compounds HgSe[10,11,20,27–32] and HgTe.[10–12,20,33–36] These κ results are more complicated because there is an electronic as well as a lattice contribution to κ at 300 K. Both HgSe and HgTe are classed as semimetals instead of semiconductors.

Note that the compounds CdO, HgO, and HgS have been omitted because they do not possess the adamantine (diamondlike) crystal structure.

B. Crystal Doped with Fe^{2+}

Previous measurements[21,37–47] have shown that substitutional Fe ions can drastically lower the thermal conductivity of crystals of Ge,[37] $ZnSO_4 \cdot 7H_2O$,[38] CdTe,[21,42] $MgCr_2O_4$,[39] $MgAl_2O_4$,[40,41] ZnS,[42] $KZnF_3$,[43] and MgO.[44–47] In these crystals the Fe^{2+} ions have either tetrahedral[21,39–42] or nearly octahedral[38,43–47] coordination with their nearest neighbors. The interaction of the phonons with the Fe^{2+} ions appears to be strong for