Title
REFLECTIVITY AND BAND STRUCTURES OF CdTe AND HgTe

Author
Chadi, D.J.

Publication Date
1971-12-01

Submitted to Physical Review

LBL-483 c.2
Preprint

REFLECTIVITY AND BAND STRUCTURES OF CdTe AND HgTe

D. J. Chadi, John P. Walter, Marvin L. Cohen,
Y. Petroff and M. Balkanski

December 1971

AEC Contract No. W-7405-eng-48

DISCLAIMER

Reflectivity and Band Structures of CdTe and HgTe

D. J. Chadi, John P. Walter†, and Marvin L. Cohen

Department of Physics, University of California

and

Inorganic Materials Research Division, Lawrence Berkeley Laboratory

Berkeley, California 94720

and

Y. Petroff and M. Balkanski

Laboratoire de Physique des Solides, ~~Faculté des Sciences~~ associé au Centre National de la Recherche Scientifique

Université de Paris VII, France

Abstract

We have measured and calculated the reflectivity spectra of CdTe and HgTe. The measured and calculated reflectivities are compared and prominent features of the reflectivity spectra are identified with critical point transitions in specific regions of the Brillouin zone. The symmetry and contribution to the reflectivity of important critical points are investigated. Empirical pseudopotential calculations of the band structure and the imaginary part of the frequency-dependent dielectric function, with spin-orbit effects included, are also presented.

†Present address: Department of Physics, Brandeis University, Waltham, Massachusetts 02154.

Introduction

The measurement of the optical reflectivity of semiconductors in the visible and ultraviolet has in recent years yielded much information concerning the band structure of both diamond and zincblende type crystals. The similarities in the reflectivity spectra of various semiconductors in this group and calculated band structures and optical constants have been helpful in interpreting the measurements. At present much effort is devoted to fine structure which can be observed when samples are cooled to low temperatures.

We have obtained detailed reflectivity spectra for CdTe and HgTe at 15 and 10°K respectively. The experimental procedures are described in the next section. We have also calculated the energy band structures of these compounds using the empirical pseudopotential method[1,2] as modified by Weisz,[3] and Bloom and Bergstresser[4] to include spin-orbit coupling. In addition we have calculated the imaginary part of the frequency-dependent dielectric function, $\epsilon_2(\omega)$ and the reflectivity, $R(\omega)$. In the energy range considered, almost all the structure in $\epsilon_2(\omega)$ and the reflectivity may be explained by direct electronic transitions at specific regions of the Brillouin zone. We identify structure in $\epsilon_2(\omega)$ and $R(\omega)$ with critical point interband transitions. The symmetry, energy and location in the zone of important critical points are determined and their contributions to $\epsilon_2(\omega)$ and $R(\omega)$ are investigated.

Experiment

The reflectivity measurements are made with a 218 MacPherson monochromator fitted with a special low-temperature reflectometer as described in a previous paper.[5]

The ultraviolet radiation was produced by a hydrogen d.c. glow discharge, through a pyrex capillary, between aluminum-tungsten electrodes. Typical operating conditions were 500 mA and 600V.

The reflectometer was separated from the monochromator by means of a lithium-fluoride window, evacuated by a pressure of about 10^{-9} mm Hg to avoid contamination of the sample surface. The incident and reflected beams were measured by a E. M. I. photo-multiplier coated with sodium salicylate. The optical system (polarizer and mirror) allows measurements on a sample surface as small as 2mm by 4mm. The samples were cleaved outside the reflectometer and transferred immediately to the vacuum chamber.

Method of Calculation

The empirical pseudopotential method is described in detail elsewhere.[1,2,6,7] Spin-orbit coupling is included using the model of Weisz[3] for white tin as modified by Bloom and Bergstresser.[4] The initial form factors for CdTe[2] and HgTe[8] with which the calculations were initially started were slightly modified to improve the agreement between the experimental and theoretical reflectivities. The two spin-orbit variables[7] λ_1 and λ_2 were constrained to have the same ratio as the splittings (of the p-levels) in the free atoms as determined by Herman and Skillman.[9] This left only one adjustable parameter which was varied to give the correct splitting of the valence bands, at Γ for CdTe, and at L for HgTe.

The energy band structures were calculated at 356 points throughout $\frac{1}{48}$ of the Brillouin zone. Lowdin perturbation theory[10] as modified by Brust[11,1] was used. For CdTe, 15 plane waves were treated exactly at Γ while 98

extra plane waves were taken into account through the Löwdin perturbation scheme.[1] The corresponding values at Γ for HgTe are 59 plane waves treated exactly and 54 plane waves treated through perturbation theory. The energy band structure calculated for HgTe, using the form factors derived in this work, is accurate to within 0.1 eV. For CdTe the identification of reflectivity structure with specific interband transitions, as presented in this paper, is unchanged when more plane waves are treated exactly and the form factors are slightly modified.

The scheme for the calculation of $\epsilon_2(\omega)$ and $R(\omega)$ from the band structure is given in references 1 and 6. The lattice constants (adjusted to $0^{\circ}K$) used in these calculations are 6.48 Å for CdTe and 6.45 Å for HgTe.

Results

The electronic band structures of CdTe and HgTe in the principal symmetry directions are shown in Figs. 1 and 2. The imaginary part of the dielectric function $\epsilon_2(\omega)$ for CdTe and HgTe appear in Figs. 3 and 4; the experimental and theoretical reflectivities are shown in Figs. 5 and 6. Important features of the experimental and theoretical reflectivities are compared in Tables I and II. Spin-orbit splittings calculated at symmetry points appear in Table III. Table II compares the form factors derived in this work with those with which the calculations were initially started.

Interpretation of Reflectivity Structure

CdTe. The fundamental gap of 1.59 eV[12] at $\Gamma(4\text{-}5)$, (i.e. between bands 4 and 5), produces the usual M_0 singularity in $\epsilon_2(\omega)$ at the threshold energy of 1.59 eV.

The spin-orbit splitting of the valence bands at Γ is $\Delta_0 = 0.91$ as determined by several independent experiments.[13-15] The value of the spin-orbit parameter[7] was adjusted to reproduce this value.

The two peaks at 3.42 and 3.97 eV in the calculated reflectivity are caused by spin-orbit split $\Lambda(4-5)$ and $\Lambda(3-5)$ transitions respectively. These are consistent with the experimental values of 3.46 and 4.03 eV. The spin-orbit splitting of the valence bands at L is $\Delta_1 = L(3-4) = L_{4,5} - L_6 = 0.57$ eV. This agrees very well with the values of 0.57 eV obtained by Cardona and Greenaway[14] at 77°K. The energy of the top valence band at L is - 0.40 eV with respect to the energy at Γ_{8V}.

The calculated $R(\omega)$ rises sharply between 5.02 and 5.07 eV. This is caused by $\Delta(4-5)$ transitions occurring at (0.7,0,0) in the zone. The experimental reflectivity also rises sharply in this energy range and has a peak at 5.18 eV. The calculated reflectivity has a peak at 5.27 eV caused by (4-5) transitions from the critical point (0.9,0.2,0.2) inside the zone.

The calculated $R(\omega)$ has two adjacent peaks at 5.47 and 5.52 eV that correspond to the main peak in the reflectivity data at 5.53 eV. The 5.47 and 5.52 eV peaks are caused mainly by $\Sigma(4-5)$ and $\Delta(3-5)$ transitions respectively. The major contribution to the strength of $\epsilon_2(\omega)$ and $R(\omega)$ comes from the $\Sigma(4-5)$ transitions; $\Delta(3-5)$ transitions account for only 20 percent of the value of $\epsilon_2(\omega)$ at 5.52 eV.

The small shoulder extending from 5.67 to 5.73 eV in the calculated reflectivity is caused by (4-6) transitions from the critical points (0.35, 0.07, 0.07) at 5.63 eV and (0.2, 0, 0) at 5.73 eV.

The two small peaks at 6.07 and 6.17 eV in $R(\omega)$ result from (3-6) transitions near (0.35, 0.07, 0.07) and (0.3, 0, 0) respectively. Γ(4-6) transitions at 6.13 eV make a small contribution to the 6.17 eV peak. The corresponding structure in the experimental $R(\omega)$ is a slight shoulder extending from 5.95 to 6.0 eV. The assignment of 6.13 eV to Γ(4-6) transitions agrees very well with the results of photoemission experiments.[16,17]

The large peak in the calculated reflectivity at 6.67 eV is caused by (4-6) transitions from a large volume of the zone centered at (0.6, 0.5, 0.2). This peak is broadened by L(4-6) transitions at 6.79 eV and Λ(4-6) transitions at 6.89 eV coming from the point (0.36, 0.36, 0.36) in the zone. Transitions at 6.8 to 7.0 eV near the zone edge from W to K make a negligible contribution to this peak contrary to the suggestion of reference 17. The small peak at 7.13 eV in $\epsilon_2(\omega)$ and $R(\omega)$ arises mainly from volume (4-7) transitions near (0.6, 0.3, 0.14); Σ(2-5) transitions also contribute to this peak.

The 7.38 eV peak in the calculated $R(\omega)$ is caused by (3-6) transitions from a large volume centered at (0.6, 0.5, 0.2) with an average transition energy of about 7.36 eV. The experimental peak occurs at 7.44 eV.

The 7.63 eV peak in $\epsilon_2(\omega)$ corresponds to the 7.6 eV peak in the reflectivity data. This peak is caused by (3-7) transitions from a volume near (0.6, 0.2, 0.1) and is not related to the 6.82 eV peak through spin-orbit

splitting of the bands at L as suggested by Cardona and Greenaway.[14] Our result that the 6.8 and 7.6 eV peaks are caused by transitions to different final states are consistent with the photoemission studies of Shay and Spicer.[17]

The over-all agreement between the theoretical and experimental reflectivity data is very good for CdTe. The enhancement of the experimental peaks at L may be caused by excitonic effects. We will discuss this further in the final section of this paper.

HgTe. At the Γ point this compound is a zero-gap semiconductor with the conduction and valence bands degenerate at Γ_8. Away from Γ, we expect the energy of the top valence band to increase slightly, i.e. HgTe is in principle a semimetal. Unlike CdTe and most other zincblende structures, HgTe has an inverted order of bands Γ_6 and Γ_8, as first suggested by Groves and Paul.[18] The spin-orbit splitting of the top valence bands at Γ is about 0.30 V at 1.5°K.[19,20] This agrees very well with the calculated value of 0.30 eV. The calculated spin-orbit splittings $\Delta_0 = \Gamma_{8V} - \Gamma_{7V}$ and $\Delta_1 = L_{4,5V} - L_{6V}$ are 0.94 and 0.62 eV respectively. The splitting of the valence bands at L was fitted to 0.62 eV by adjusting the spin-orbit parameter.[7] The experimental value of 0.64 eV was obtained by Cardona and Greenaway[14] at 77°K.

The peaks occurring at 2.32 and 2.92 eV in the calculated reflectivity are caused by spin-orbit split L(4-5) and L(3-5) transitions at 2.25 and 2.87 eV. These peaks correspond to the experimental peaks at 2.25 and 2.87 eV. The experimental reflectivity has a shoulder starting at 4.18 eV caused by (4-5) transitions extending from 4.0 to 4.2 eV. The matrix element for these transitions has a maximum near 4.03 eV; the theoretical reflectivity does not have conspicuous structure at this energy because of the sharp rise of the reflectivity resulting from other sets of transitions. However, a calculation of the modulated reflectivity, $\frac{1}{R(\omega)} \frac{dR}{d\omega}$ shows that $R(\omega)$ does have a small peak near 4.03 eV.

The calculated reflectivity has a shoulder beginning at 4.47 eV arising from volume (4-5) transitions from a region of the zone centered at (0.8,0.2,0.2) with an average transition energy of 4.42 eV. Transitions from nearly the same region of the zone give rise to the 5.27 eV peak in CdTe and were associated with the critical point (0.9,0.2,0.2). For HgTe the corresponding critical point is at (1,0.2,0.2) and the transition energy is 4.61 eV. These transitions do not give rise to a peak because of the sharp rise of the reflectivity spectra leading to the main peak at 4.87 eV.

The peak at 4.87 eV in the theoretical $R(\omega)$ is caused mainly by Σ(4-5) transitions occurring at points near K. The strength of this peak is increased by X(3-5) transitions at 4.71 eV. The contribution of the Σ(4-5) transitions to this peak is more than four times as large as the contribution of the X(3-5) transitions. The corresponding reflectivity peak is at 4.98 eV.

The peak at 5.02 eV in the calculated reflectivity is caused by (4-6) transitions from a large volume of the zone near Γ and around Δ. The Γ(4-6) transitions at 4.92 eV and the critical point transitions at 5.00 and 5.02 eV from (0.14,0,0) and (0.14,0.07,0.07) contribute to this peak. The reflectivity decreases very slowly between 5.07 and 5.17 eV because of (4-6) transitions. The X(4-6) transitions at 5.09 eV and (4-6) transitions from a group of points near Δ give rise to a local maximum at 5.12 eV in the matrix element for (4-6) transitions. This is in addition to the larger maximum occurring at 5.02 eV.

The experimental reflectivity has two small peaks at 5.45 and 5.62 eV. The 5.45 eV peak is, most probably, caused by X(3-6) transitions at 5.43 eV and Γ(4-7) transitions at 5.44 eV. The contributions of the X(3-6) transitions is about 3 times as large as the contributions of the Γ(4-7) transitions. The matrix element for both sets of transitions has a maximum at 5.47 eV, but any associated reflectivity structure seems to have been absorbed in the broad peak centered at 5.57 eV. This 5.57 eV peak is caused by (3-6) critical point transitions at 5.52 eV from (0.2,0,0) and at 5.57 eV from (0.15,0.07,0.07).

The large and broad peak in the reflectivity data at 6.53 eV is caused by volume (4-6) transitions from a region of the zone centered at (0.6,0.5,0.3); L(4-6) transitions at 6.49 eV also contribute to this peak. The theoretical reflectivity peak occurs at 6.63 eV and is in fairly good agreement with the experimental value. Cardona and Greenaway[14] assign the 6.53 eV peak to L(4-6) transitions.

The peak at 7.07 eV in the calculated $R(\omega)$ arises from (3-6) transitions from a region of the zone centered at (0.6,0.5,0.3). The magnitude of this peak is much smaller than the corresponding spin-orbit split volume (4-6) transitions at 6.63 eV. The experimental reflectivity, however, does not show a corresponding peak. There is also no contribution to this peak from L(3-6) transitions at 7.10 eV even though this peak is close in energy.

The peak at 7.57 eV in the calculated reflectivity is caused by volume (4-7) transitions at an average energy of 7.47 eV from a region of the zone centered at (0.6,0.4,0.1). In addition L(3-7) transitions at 7.36 eV

also contribute to this peak. The L(3-7) transitions contribute 30 percent of the value of the $\epsilon_2(\omega)$ peak at 7.38 eV. The spin-orbit split L(4-7) transitions at 6.75 eV have weak matrix elements and do not give rise to any peaks. The peak at 7.88 eV in $R(\omega)$ is caused by volume (3-7) transitions from a region of the zone centered at (0.6, 0.3, 0.1). The experimental reflectivity peak corresponding to the 7.57 and 7.88 eV peaks in the theoretical reflectivity is the broad peak at 7.6 eV.

The peaks at 8.17 eV in $\epsilon_2(\omega)$ and 8.32 eV in $R(\omega)$ are caused by volume (3-7) transitions from a region of the zone centered at (0.6, 0.3, 0.1). The spin-orbit split (3-7) transitions from this region contribute both to the 7.88 and 8.32 eV peaks.

Scouler and Wright[21] assign their 7.5 and 8.25 eV peaks to spin-orbit split L(3,4-6) transitions and deduce a Δ_1 value of 0.75 eV. This value for Δ_1 seems to be too large compared to the value of 0.62 eV obtained from the spin-orbit split L(4-5) and L(3-5) transitions at 2.25 and 2.87 eV. The value of Δ_1 obtained from L(4-6), L(3-6) transitions in our case is 0.61 eV, close to the value of 0.62 obtained from L(4-5), L(3-5) transitions.

Discussion of Results

The enhancement of some experimental peaks relative to the theoretical peaks, particularly near the first Λ and L transitions, are probably caused by excitons. The effect of the Coulomb interaction between electrons and holes on the four different types of critical points has been investigated by several authors.[22-27] The effect of such interactions on an M_1 type critical point occurring at L or "L-like" points where $m_1 = m_2 > 0$ and for the case $|m_3| \gg m_1$ with m_1, m_2, m_3 being the principal effective

masses has been calculated by Kane.[27] His calculations indicate that the most characteristic feature of an M_1 critical point, with electron-hole Coulomb interactions taken into account, is the sharp dropoff in $\epsilon_2(\omega)$ and $R(\omega)$ near the critical point. This is particularly evident in the case of CdTe where the reflectivity drops sharply at 3.46 and 4.03 eV. According to Kane's calculations the small structure in the measured reflectivity at 3.60 and 4.20 eV actually correspond to the M_1 critical point transitions near L. The prominent peaks at 3.46 and 4.03 eV are to be associated with the electron-hole bound state. The binding energy of the exciton is given by the energy difference between the M_1 structure at 3.60 eV and the main peak at 3.46 eV and is about 0.14 eV. In HgTe the binding energy of the exciton has been assumed to be small[28] (about 0.04 eV). If this is the case, the corresponding M_1 structure is not expected to be resolvable experimentally.

In many cases our resolution was not sufficient to discuss all the calculated critical points. Tables I and II contain only prominent critical points.

Table Captions

Table I — CdTe. Theoretical and experimental reflectivity structure at 15°K and their identification. The symmetry, location in the zone and the transition energy at the critical points are given.

Table II — HgTe. Theoretical and experimental reflectivity structure at 10°K and their identification. The symmetry, location in the zone, and the transition energy at the critical points are given.

Table III — Calculated spin-orbit splittings for CdTe and HgTe.

Table IV — Comparison of the CdTe and HgTe form factors (in Ry) obtained in the present work (on top) with those of Refs. 2, 8.

Table I

Reflectivity Structure		Associated Critical Points (CdTe)		
Theory	Exper.	Location in Zone	Sym	c_p energy
1.59 eV	1.59 eV	Γ(4-5) (0,0,0)	M_0	1.59 eV
3.42	3.46	Λ(4-5) (0.43,0.43,0.43)	M_1	3.39
3.97	4.03	Λ(3-5) (0.43,0.43,0.43)	M_1	3.95
5.02	-	Volume near Δ(4-5) (0.7,0,0)	-	5.05
5.27	5.18	(4-5) (0.9,0.2,0.2)	M_1	5.27
5.47	5.53	Σ(4-5) (0.7,0.7,0)	M_2	5.42
5.52		Δ(3-5) (0.7,0,0)	M_1	5.51
5.67	5.68	(4-6) (0.35,0.07,0.07)	-	5.63
		Δ(4-6) (0.2, 0,0)	-	5.73
6.07	5.95	(3-6) (0.35,0.07,0.07)	-	6.07
6.17		Δ(3-6) (0.3,0,0)	M_1	6.14
6.67	6.82	Volume (4-6) (0.6,0.5,0.2)	-	6.62
7.13	-	Volume (4-7) (0.6,0.3,0.14)	-	7.10
7.38	7.44	Volume (3-6) (0.6,0.5,0.2)	-	7.36
-	7.6	Volume (3-7) (0.6,0.2,0.1)	-	7.6

Table II

Reflectivity Structure		Associated Critical Points (HgTe)		
Theory	Exper.	Location in Zone	Sym	c_p energy
0 eV	0 eV	Γ(4-5) (0,0,0)	M_0	0 eV
2.32	2.25	L(4-5) (0.5,0.5,0.5)	M_1	2.25
2.92	2.87	L(3-5) (0.5,0.5,0.5)	M_1	2.87
4.03	4.18	Volume near Δ(4-5) (0.6,0,0)	-	4.03
4.47	-	Volume (4-5) (0.8,0.2,0.2)	-	4.42
-	-	X(3-5) (1,0,0)	M_1	4.71
4.87	4.98	K(4-5) (0.75,0.75,0)	M_2	4.82
5.02	5.10	Δ(4-6) (0.14,0,0)	-	5.00
		(4-6) (0.14,0.07,0.07)	M_2	5.02
-	5.45	X(3-6) (1,0,0)	M_1	5.43
		Γ(4-7) (0,0,0)	-	5.44
5.57	5.62	Δ(3-6) (0.2,0,0)	M_1	5.52
		(3-6) (0.15,0.07,0.07)	-	5.57
6.63	6.53	Volume(4-6) (0.6,0.5,0.3)	-	6.53
7.07	-	Volume(3-6) (0.6,0.5,0.3)	-	7.02
7.57	7.6	Volume(4-7) (0.6,0.4,0.1)	-	7.47
7.88		Volume(3-7): $[6\text{-}13]^+$ (0.6,0.3,0.1)		7.75
8.32	8.3	Volume(3-7): $[5\text{-}14]^+$ (0.6,0.3,0.1)	-	8.2

$^+$In this notation the bands are numbered consecutively with the doubly degenerate top valence bands at Γ and L numbered 7 and 8.

Table III Calculated spin-orbit splittings for CdTe and HgTe

	CdTe	HgTe
$\Gamma_{8V} - \Gamma_{7V}$	0.91	0.94
$\Gamma_{8C} - \Gamma_{6V}$	-	0.30
$L_{4,5V} - L_{6V}$	0.57	0.62
$X_{7V} - X_{6V}$	0.46	0.35
$\Gamma_{8C} - \Gamma_{7C}$	0.13	0.51
$L_{4,5C} - L_{6C}$	0.06	0.26

Table IV

	$V^S(3)$	$V^S(8)$	$V^S(11)$	$V^A(3)$	$V^A(4)$	$V^A(11)$	$V^A(12)$	spin-orbit parameter
CdTe	-0.200	-0.012	0.027	0.168	0.075	0.028	0	0.0014
	-0.20	0.00	0.04	0.15	0.09	0.04	0	--
HgTe	-0.262	-0.035	0.05	0.10	0.042	0.02	0.019	0.0028
	-0.23	-0.025	0.03	0.095	0.08	0.03	0.03	--

References

1. M. L. Cohen and V. Heine, Solid State Physics 24, 37 (1970).
2. M. L. Cohen and T. K. Bergstresser, Phys. Rev. 141, 789 (1966).
3. G. Weisz, Phys. Rev. 149, 504 (1966).
4. S. Bloom and T. K. Bergstresser, Solid State Comm. 6, 465 (1968).
5. Y. Petroff, R. Pinchaux, J. Dagneaux, and M. Balkanski, Rev. Phys. Appl. Nov. 1970, p. 727.
6. J. P. Walter and M. L. Cohen, Phys. Rev. 183, 763 (1969).
7. J. P. Walter, M. L. Cohen, Y. Petroff and M. Balkanski, Phys. Rev. 1, 2661 (1970).
8. S. Bloom and T. K. Bergstresser, Phys. Status Solidi 42, 191 (1970).
9. F. Herman and S. Skillman, Atomic Structure, Prentice-Hall, New Jersey 1966.
10. P. Löwdin, J. Chem. Phys. 19, 1396 (1951).
11. D. Brust, Phys. Rev. 134, A1337 (1964).
12. D. G. Thomas. J. Appl. Phys. Suppl. 32, 2298 (1961).
13. M. Cardona, K. L. Shaklee, and F. H. Pollak, Phys. Rev. 154, 696 (1967).
14. M. Cardona and D. L. Greenaway, Phys. Rev. 131, 98 (1963).
15. D. T. F. Marple and H. Ehrenreich, Phys. Rev. Letters 8, 87 (1962).
16. J. L. Shay, W. E. Spicer and F. Herman, Phys. Rev. Letters 18, 649 (1967).

17. J. L. Shay and W. E. Spicer, Phys. Rev. 161, 799 (1967).

18. S. Groves and W. Paul, Conf. Int. Phys. Semicond., Paris, 1964, p. 41.

19. S. H. Groves, R. N. Brown and C. R. Pidgeon, Phys. Rev. 161, 779 (1967).

20. C. R. Pidgeon and S. H. Groves, Proceedings of the 1967 International Conference on Physics of II-VI Semiconductors, D. G. Thomas ed., Benjamin, N. Y. 1967.

21. W. J. Scouler and G. B. Wright, Phys. Rev. 133, A736 (1964).

22. B. Velicky and J. Sak, Phys. Status Solidi 16, 147 (1966).

23. J. C. Phillips, Phys. Rev. 136, A1705 (1964).

24. C. B. Duke and B. Segall, Phys. Rev. Letters 17, 19 (1966).

25. Y. Toyozawa, et al., J. Phys. Soc. Japan 21, 133 (1966).

26. J. Hermanson, Phys. Rev. 166, 893 (1968).

27. E. O. Kane, Phys. Rev. 180, 852 (1969).

28. Y. Petroff and M. Balkanski, Phys. Rev. B 3, 3299 (1971).

Figure Captions

Figure 1 Electronic band structure of CdTe in the principle symmetry directions.

Figure 2 Electronic band structure of HgTe in the principle symmetry directions.

Figure 3 Imaginary part of the dielectric function, $\epsilon_2(\omega)$ of CdTe.

Figure 4 Imaginary part of the dielectric function, $\epsilon_2(\omega)$ of HgTe.

Figure 5 Experimental and theoretical reflectivity spectra of CdTe.

Figure 6 Experimental and theoretical reflectivity spectra of HgTe.

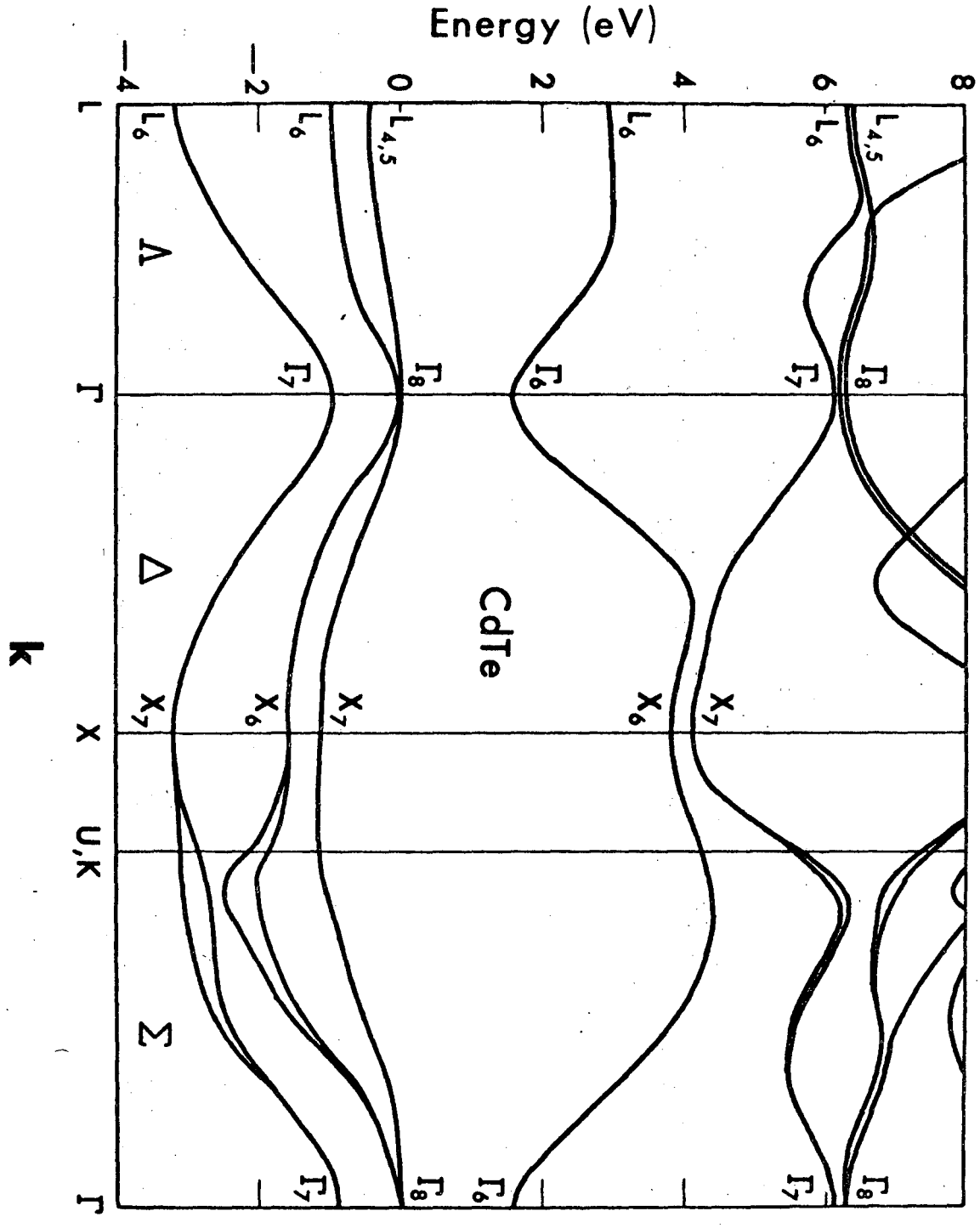
Energy (eV)
−4
−2
0
2
4
6
8
L
Γ
X
U,K
Γ
k
Δ
Δ
Σ
CdTe
L_6
$L_{4,5}$
Γ_7
Γ_8
Γ_6
X_7
X_6

Figure 1

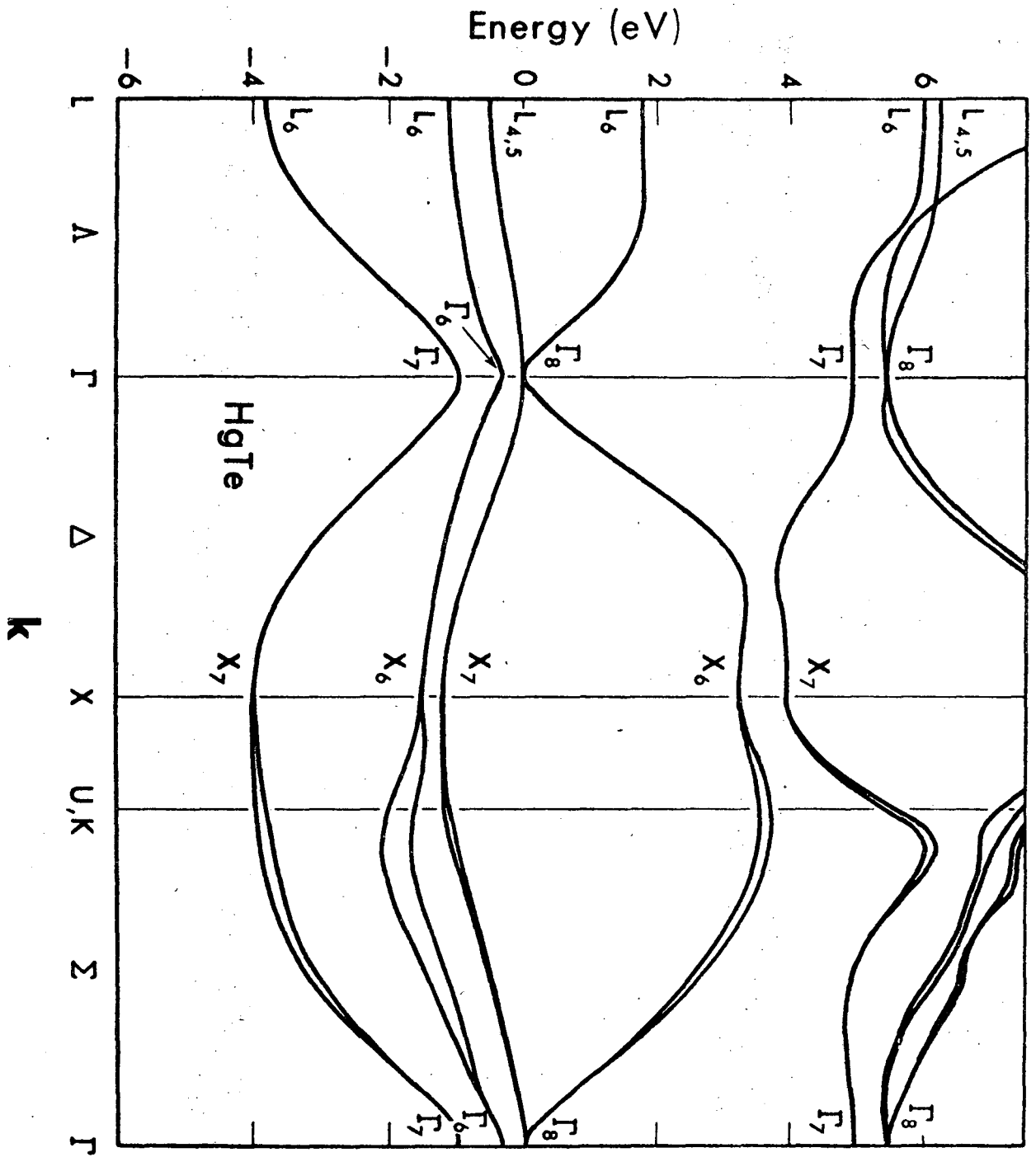

Figure 2

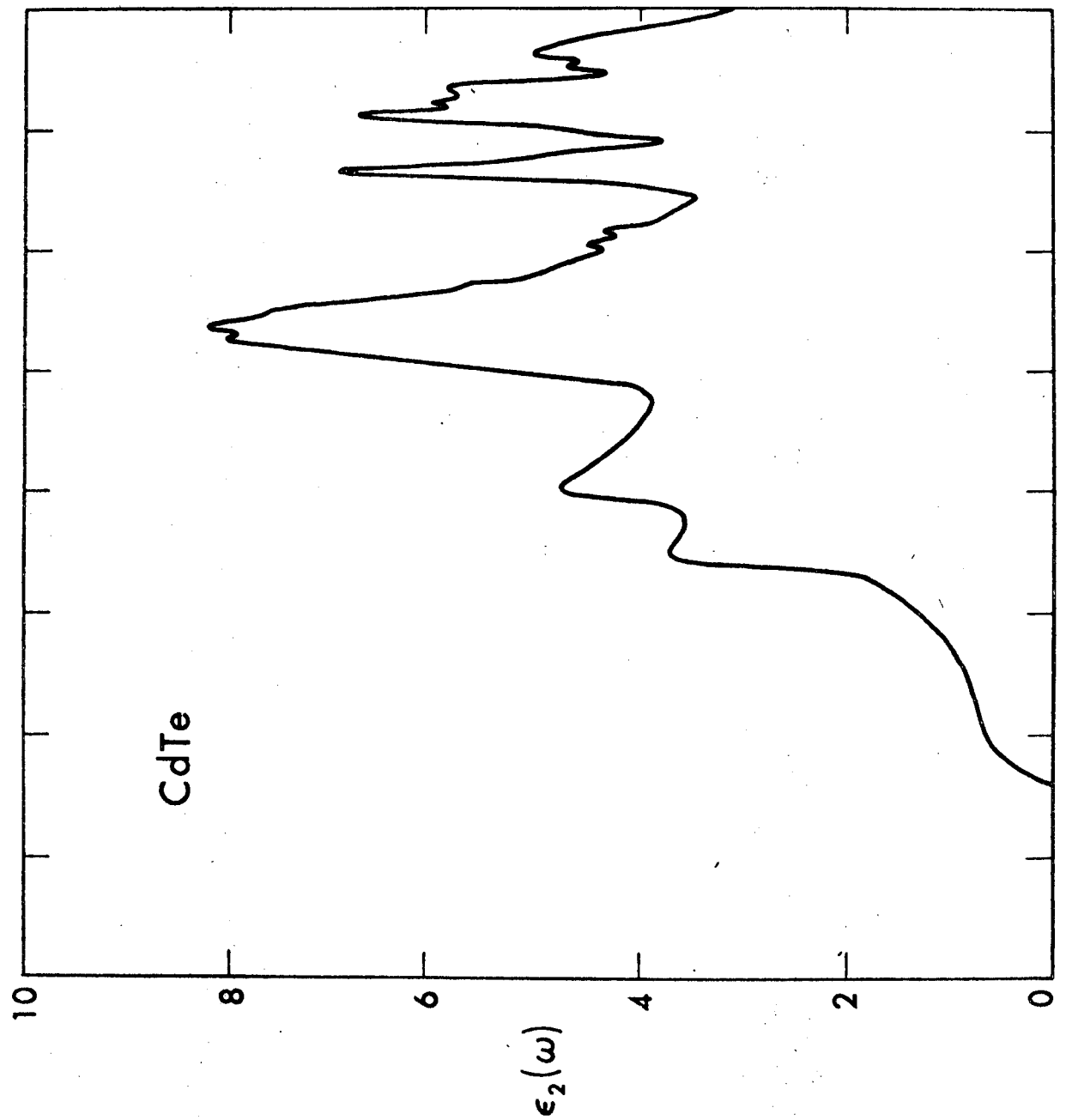

Figure 3

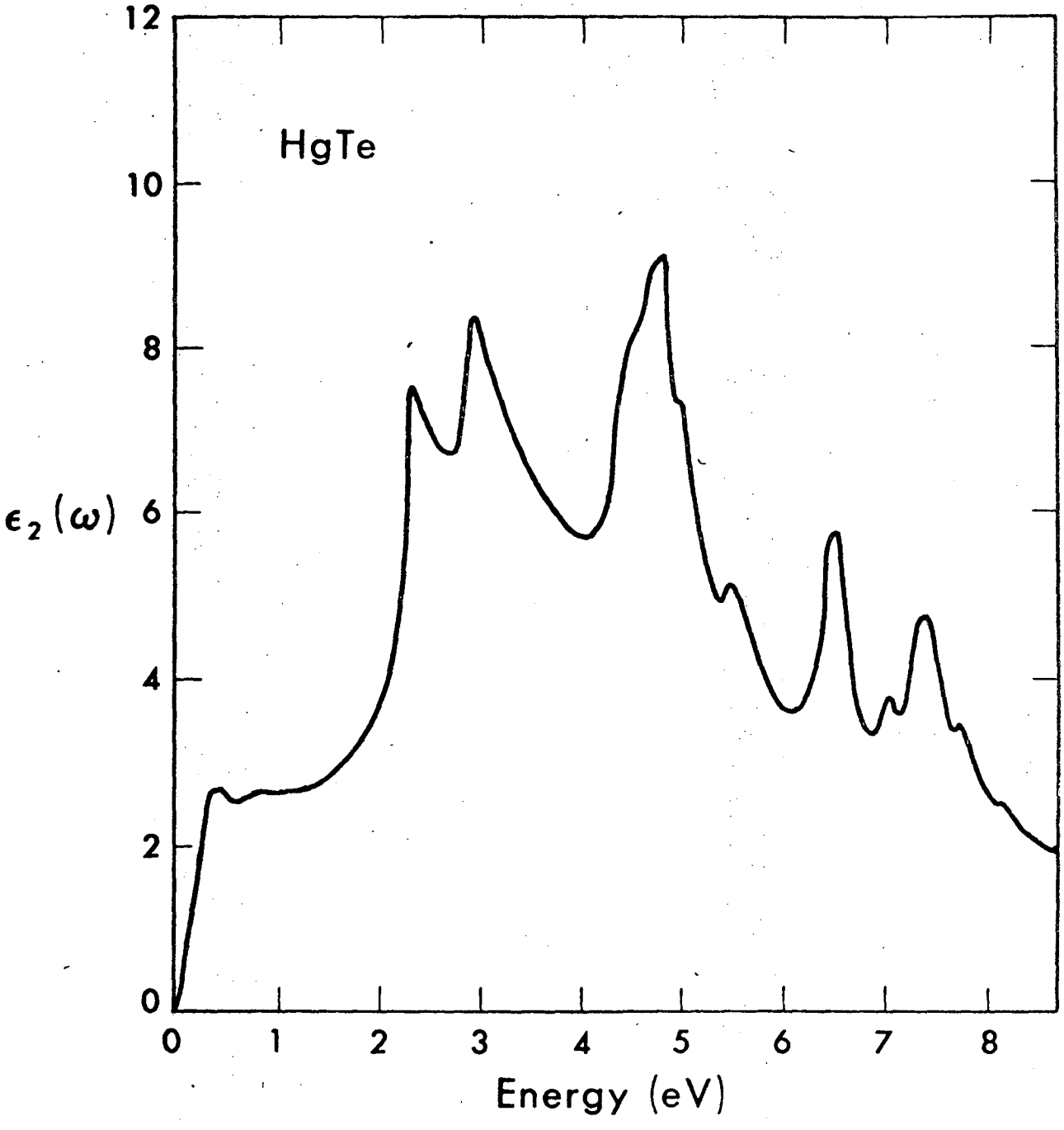

Figure 4

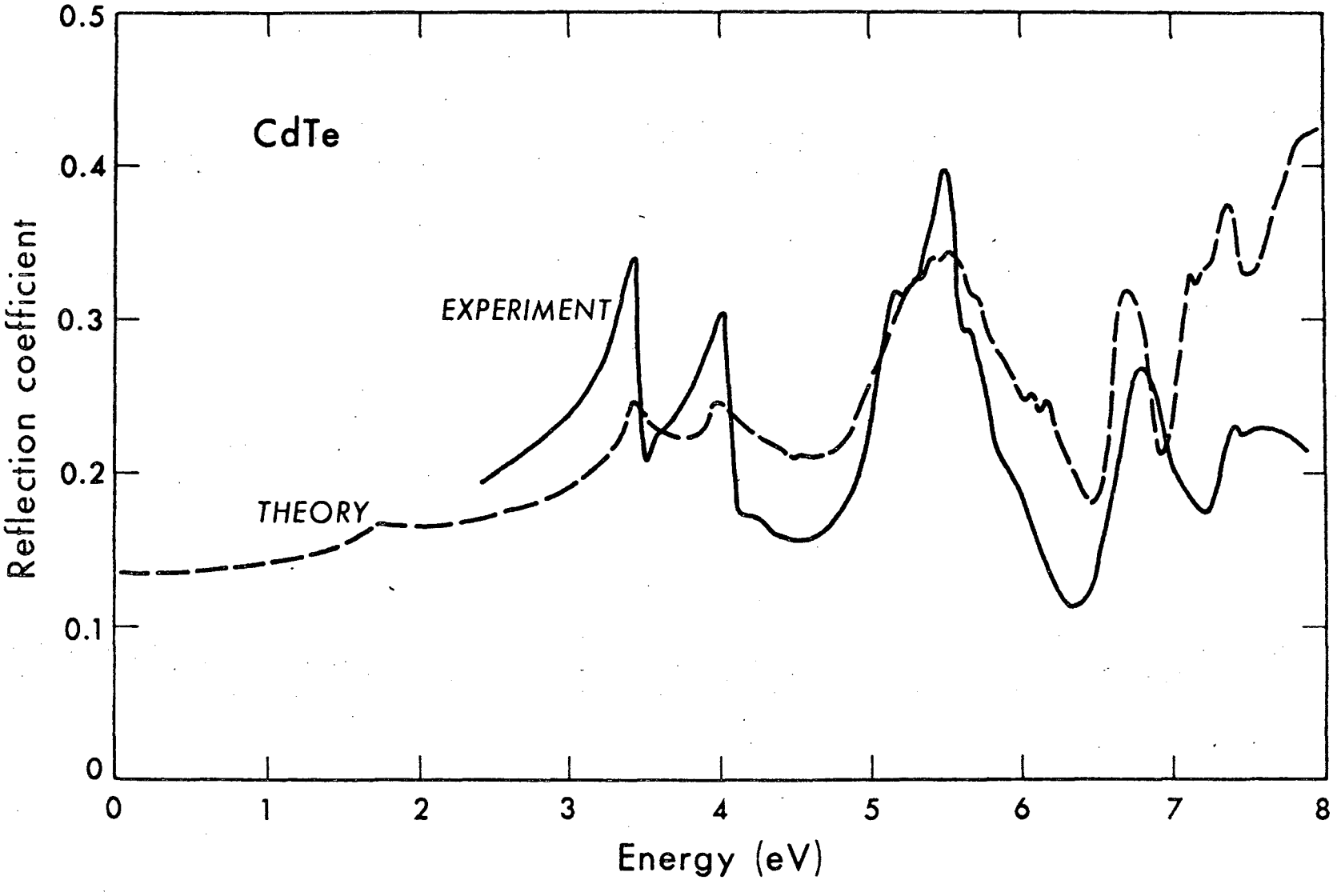
CdTe
EXPERIMENT
THEORY
Reflection coefficient
Energy (eV)
0.5
0.4
0.3
0.2
0.1
0
0
1
2
3
4
5
6
7
8

Figure 5

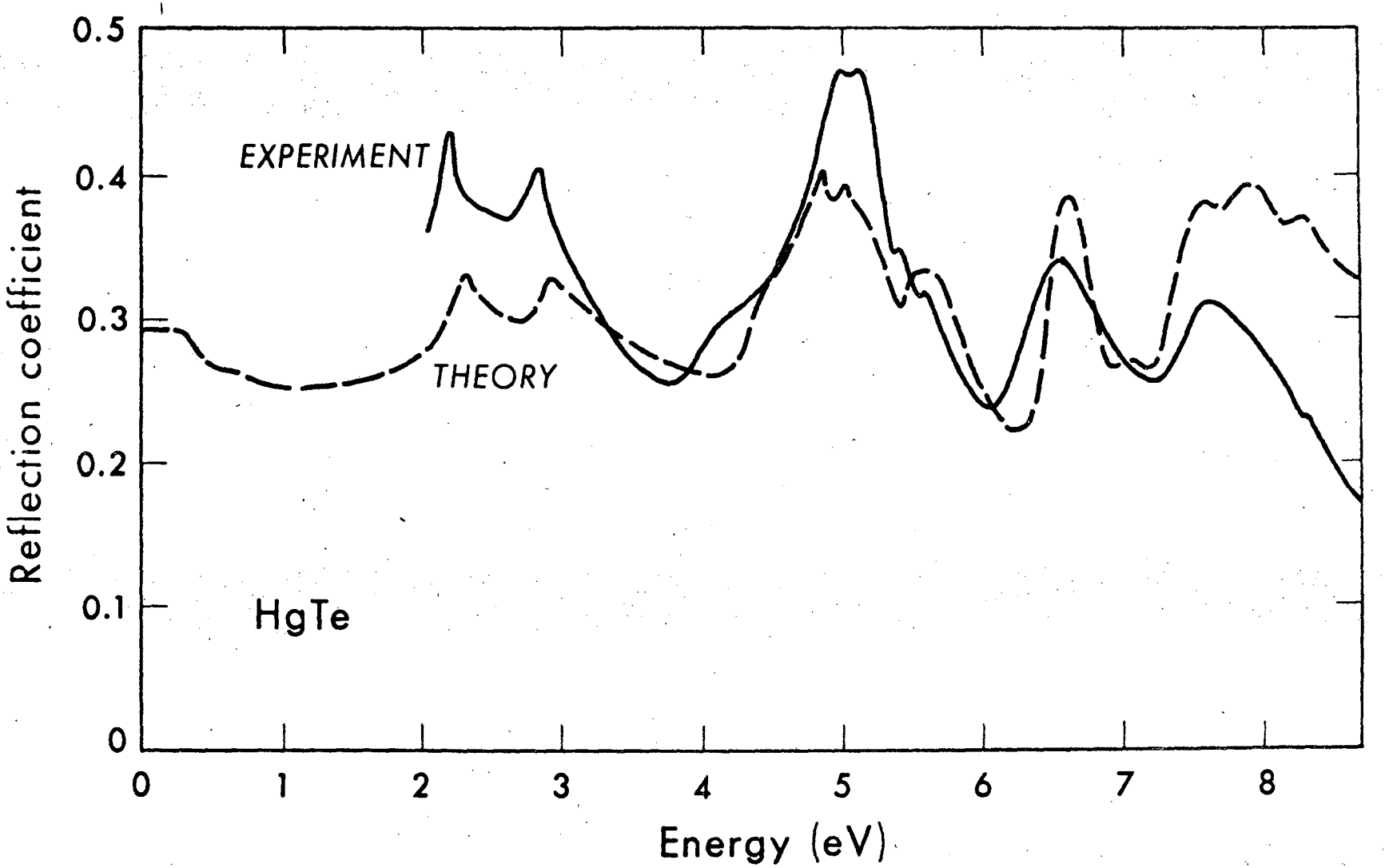
0.5
0.4
0.3
0.2
0.1
0
Reflection coefficient
EXPERIMENT
THEORY
HgTe
0
1
2
3
4
5
6
7
8
Energy (eV)

Figure 6

TECHNICAL INFORMATION DIVISION
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720