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Plastic bending of $Cd_xHg_{1-x}Te$

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Preliminary results are reported of three-point plastic bending tests on $Cd_xHg_{1-x}Te$ single crystal samples, for an x value of about 0.2, conducted in air at strain rates of the order of 10^{-5} sec^{-1}, and at temperatures in the range 303 K (30° C) to 363 K (90° C) (in the region of $0.35T_m^0$, where T_m^0 is the absolute melting point). Single crystal samples were cut from polycrystalline ingots, and the orientation, although measured in each case, was not consistent from sample to sample, being determined by the available grain shape. The stress–strain curves resemble those found for Group IV and III–V semiconductors. They display a yield drop, followed by a region of zero work hardening. All tests were stopped in this region, and in no case did the overall glide strain exceed 3%. The upper and lower yield stresses (outer fibre glide stress values) varied from 16 MN m^{-2} and 10 MN m^{-2}, respectively, at 363 K (90° C) to 24 MN m^{-2} and 17 MN m^{-2}, respectively, at 303 K (30° C).

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1. Introduction

$Cd_xHg_{1-x}Te$ for $x \simeq 0.2$ is important as a material for infra-red detectors, operating in the 8–14 μm wavelength range at 77 K (− 196° C). It is a solid solution, lying in the quasi-binary section between CdTe and HgTe, and crystallizes in the sphalerite structure. The Group II atoms lie on an fcc sublattice, with the origin at the point 0,0,0, and the Group VI atoms lie on a second fcc sublattice, displaced from the first by $(\frac{1}{4}\,\frac{1}{4}\,\frac{1}{4})$. The lack of inversion symmetry in this structure leads to polarity effects, and, in particular, to the fact that positive and negative edge components of perfect dislocations have different types of atoms at the edge of their extra half-planes [1]. There is considerable evidence for dislocation dissociation in materials with the sphalerite structure (reviewed in [2]) but the basic concept of the nonequivalence of opposite sign edge components still applies to the partial dislocations.

The usual technique used for the crystal growth of $Cd_xHg_{1-x}Te$ is the Bridgman method [3]. The large segregation coefficient in the quasi-binary (T–x) section of the phase diagram leads to a considerable longitudinal compositional gradient in the ingot. Grain diameters rarely exceed 1 cm, and the crystals have a dislocation density of between 10^6 cm^{-2} and 10^7 cm^{-2}, most of these lying in sub-grain boundaries.

Very little work has been reported on the dislocation behaviour or the mechanical properties of $Cd_xHg_{1-x}Te$. Several workers have studied microhardness (e.g. [4], [5]). Brown and Willoughby [6] have shown that the slip planes are $\{1\,1\,1\}$, by etching dislocations generated around microhardness identations, and these results have been shown to be reproducible using a similar method [7]. Regarding the macroscopic mechanical properties, Baranskii *et al.* [8] reported plastic flow in $Cd_xHg_{1-x}Te$ at temperatures as low as 77 K (− 196° C) under uniaxial compression at an unspecified strain rate, while the present author, also using uniaxial compression, demonstrated that $Cd_{0.2}Hg_{0.8}Te$ exhibits plastic flow at room temperature, 293 K, (20° C) and at strain rates up to 6×10^{-2} sec^{-1} [7].

In view of the importance of this material, and the relative lack of information on its basic mechanical properties, the present work was undertaken to obtain values of yield stress and other

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fundamental mechanical property data, under controlled and monitored conditions of strain rate, temperature and sample orientation.

2. Experimental methods

$Cd_xHg_{1-x}Te$ was obtained in the form of slices, 0.3–0.5 mm thick, having compositions in the range $0.21 < x < 0.23$, which had been cut from Bridgman-grown ingots, perpendicular to the freeze direction. This minimizes compositional variations within a slice. The ingots were polycrystalline with a grain diameter not exceeding 1 cm, so that each slice contained sections of a number of grains.

This available material was very appropriate for the preparation of test-pieces for plastic bending. Cutting damage was removed by polishing each specimen on a pad soaked in 2 vol% Br_2/methanol. Each slice was then etched for 30–45 seconds in a solution containing 12 cm^3 nitric acid, 5 cm^3 hydrochloric acid, 1 cm^3 acetic acid (glacial), 18 cm^3 distilled water and 0.02 cm^3 bromine. This etchant was developed for use on HgTe by Polisar *et al.* [9], and henceforth is referred to as "Polisar etch 2". It was successfully used on $Cd_xHg_{1-x}Te$ by Brown and Willoughby [6], to display the presence of dislocations, a result confirmed in a separate study by the present author [7]. However, it has not been established that this etchant produces a 1:1 correspondence of etch-pits with dislocations.

In the present work Polisar etch 2 revealed the major grain boundaries, sub-grain boundaries and individual dislocation etch-pits on the slices. Typical etch-pit densities within the major grains were 10^6 to 10^7 cm^{-2}, of which, most lay in the sub-grain boundaries. The density of pits in these boundaries was too high to be determined accurately, so that variations in overall dislocation density between samples cannot be ruled out, with possible consequences for the mechanical properties.

A back-reflection Laue X-ray photograph was taken of the largest single grain in each slice, and bars, of rectangular cross-section, were cut from these grains, any growth twins being avoided. Fig. 1 shows the sample geometry. Because of the need to obtain the longest possible sample from each grain, the orientations of the vectors **a** and **b** were necessarily not consistent, being dominated by the available grain shape. The distribution of the orientations of **a** and **b** are plotted on a stereographic projection in Fig. 2. Orientations 1 and 2 are more likely to favour slip on a single system than 3 and 4, although etching after bending showed that two systems were activated in all samples.

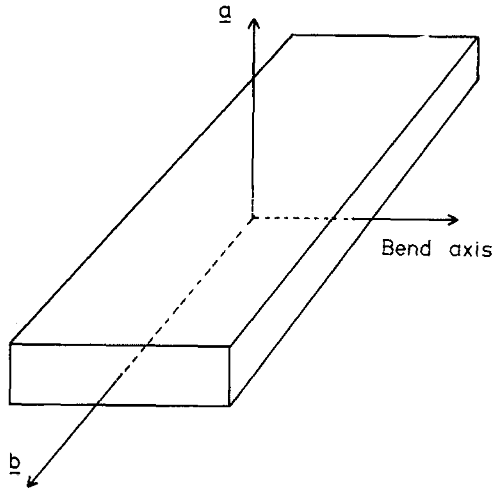

Figure 1 Geometry of the test-pieces.

The cut edges were polished using a pad soaked in 2 vol% Br_2/methanol to remove work damage. The finished test-pieces were too small for practical four-point testing, so the three-point technique was adopted. During all polishing and etching procedures, specimens were appropriately masked with a chemically-resistant lacquer to preserve their rectangular cross-section. This lacquer was

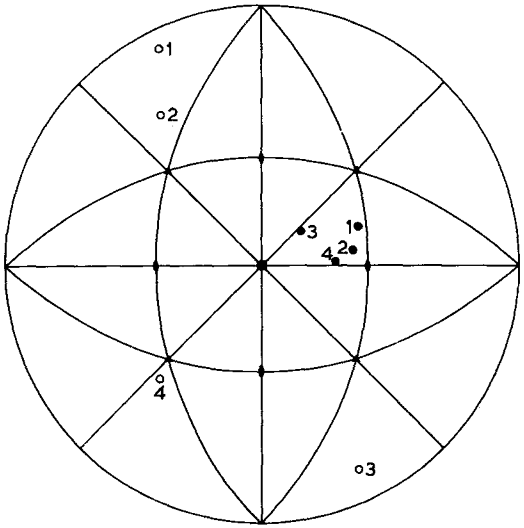

Figure 2 Stereographic projection showing the distribution of the orientations of vectors a (open circles) and b (closed circles) (see Fig. 1).

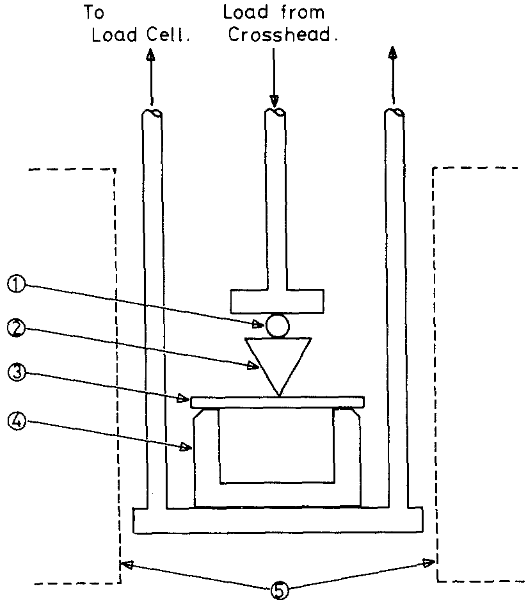

Figure 3 Diagram of the bend-testing apparatus showing: (1) Ball bearing, (2) upper knife edge, (3) test-piece, (4) lower knife edges and (5) resistance furnace.

removed with acetone prior to testing, and a final brief polish in 2 vol % Br_2/methanol removed previous etch-pits and any oxide film.

Fig. 3 shows the bend-testing apparatus. The upper knife-edge runs freely on two guides, and the load is applied via a ball-bearing. The bend-jig is contained in the compression cage of a model TM-M-L Instron machine, and a resistance furnace is positioned around the whole cage. This provides uniform heating of the sample, and also excludes light. (Photoplastic effects have been observed in the related compound, CdTe [10]). All tests were conducted in air.

3. Results and discussion

The outer fibre glide strain rate in bending was of the order of 10^{-5} sec^{-1}, and specimens were tested at temperatures, T, in the range between 31° C and 92° C (approximately $0.35T_m^0$, where T_m^0 is the absolute melting point of $Cd_{0.2}Hg_{0.8}Te$). Adjacent slices from an ingot contained sections of the same grains, so that test-pieces could be cut from them having the same orientations of the vectors **a** and **b** (Fig. 1). Pairs of such samples were bent in opposite senses, and deformed to similar glide strain overall. After bending, specimen dimensions were measured, away from the deformed region, with a micrometer. The outer fibre glide stress–glide strain curves were derived using elastic bending theory, the results being corrected for the elasticity of the jig itself. Typical plots for two pairs of oppositely-bent samples are shown in Fig. 4. They display a yield drop and an easy glide region, and resemble the curves found for Group IV [11, 12] and III–V [12, 13] semiconductors. The ratio of upper yield stress to lower yield stress is consistently about 3:2. Table I summarizes the results.

The strain rate varied between tests, as a result of differences in sample thickness. In order to correct for this, the values of τ_{ly} have been normalized to a strain rate of 5×10^{-5} sec^{-1} using the relation [14, 15],

$$\tau_{ly} = C\left(\dot{\epsilon} \exp \frac{E}{kT}\right)^{1/(m+2)}, \qquad (1)$$

where $\dot{\epsilon}$ is the glide strain rate, C is a constant and E is the activation energy for dislocation motion. The quantity m usually lies between 1 and 2, and is taken as 1.0 here since values for diamond structure materials are commonly close to 1 [15]. The normalized values of lower yield stress (see Table II) are used in Fig. 5, which shows ln τ_{ly} plotted

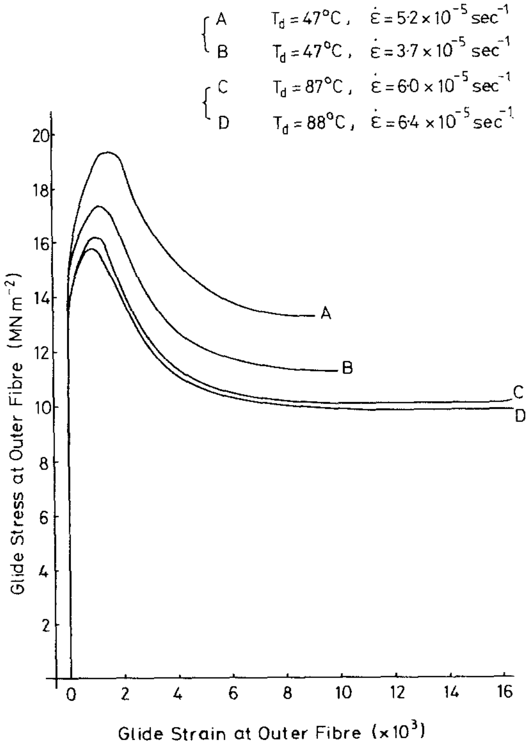

Figure 4 Experimental stress–strain curves, calculated assuming single slip on the primary system.

TABLE I Glide strain and glide stress data for samples of $Cd_{0.2}Hg_{0.8}Te$, typically of dimensions 3 mm × 0.3 mm × 10 mm, deformed at varying temperatures between 304 K (31° C) and 365 K (92° C).

Testing temperature, T (° C)	Orientation code (see Fig. 2)	Glide strain rate, $\dot{\epsilon}$ ($\times 10^5$ sec^{-1})	Overall* glide strain (%)	Outer fibre glide stress	
				Upper yield stress (MN m^{-2})	Lower yield stress (MN m^{-2})
{91†	1	6.5	1.9	15.7	9.9
92		6.7	2.0	14.8	9.9
{88	2	6.4	1.7	15.7	9.8
87		6.0	1.7	16.1	10.1
{57	3	5.0	0.9	15.5	10.5
58		5.8	1.0	16.0	10.8
{47	3	5.2	0.9	19.3	13.3
47		3.7	1.0	17.4	11.2
{31	4	3.8	1.1	23.4	17.0
33		3.8	3.1	24.6	14.0

*All tests stopped prior to fracture.

†Brackets indicate pairs of samples, deformed to the same extent, in opposite crystallographic senses.

against T^{-1} (K). Although there is considerable scatter in the data, the closest straight line fit to this plot yields a value of E, calculated using Equation 1, of about 0.3 eV. This is rather lower than the value of 0.45 eV found by Kurilo *et al.* [5] for $Cd_{0.15}Hg_{0.85}Te$ using microhardness measurements, and significantly smaller than the corresponding activation energies for other compound semiconductors of around 1 eV (e.g. InSb [13, 15, 16], InAs [17], GaSb [12, 17].

It is not felt that great significance can be attached to the apparent deviations of the present results from Equation 1; that is, deviations from linearity in Fig. 5. The possible variations in initial dislocation density, the known variations in orientation of the bend axes, and random inhomogeneities in the test-pieces (to which the three-point bend-test is especially sensitive) may all contribute to fluctuations in the yield stress.

It is interesting to compare the present results on $Cd_{0.2}Hg_{0.8}Te$ with the parent binary compounds CdTe and HgTe. CdTe has been shown [18, 19] to yield in compression, at 298 K (25° C) and strain rates of 10^{-4} sec^{-1}, at stresses less than 10 MN m^{-2}. The present results indicate that $Cd_{0.2}Hg_{0.8}Te$ has a lower yield stress of about 1.7 MN m^{-2} at 30° C and a strain rate of 10^{-5} sec^{-1}, which again appears to be consistent with the work of Kurilo *et al.* [5], and that of Koman and Pashovskii [4], who found that the ternary, as

TABLE II Values of lower yield stress, τ_{ly}, for samples of $Cd_{0.2}Hg_{0.8}Te$, deformed at varying temperatures between 304 K (31° C) and 365 K (92° C), normalized for a constant glide strain rate, $\dot{\epsilon}$, of 5×10^{-5} sec^{-1}.

Testing temperature, T (° C)	Corrected lower yield stress, τ_{ly} (MN m^{-2})
91	9.1
92	9.0
88	9.0
87	9.5
57	10.5
58	10.3
47	13.1
47	12.4
31	18.6
33	15.3

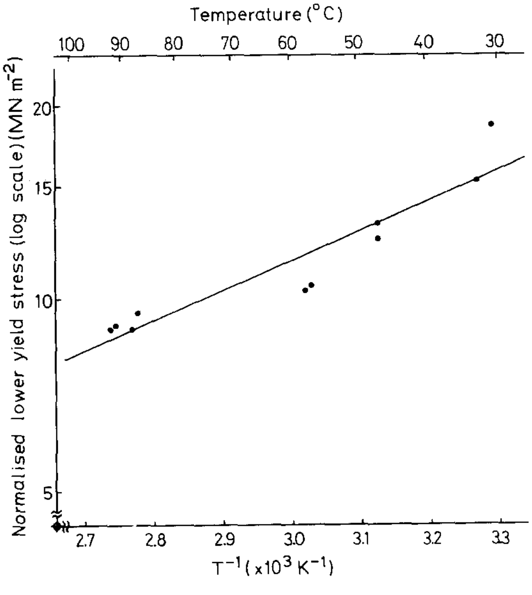

Figure 5 Plot of ln τ_{ly} against T^{-1} (K).

grown by the Bridgman method, is harder than CdTe, at about 298 K (25° C). However, it should be noted that the yield stress measured in compression is generally lower, for a given material, than that measured in bending under the same conditions of temperature and strain rate [15]. There appears to be no information available on the macroscopic plastic properties of HgTe; however, microhardness results [5] indicate that it is appreciably softer than CdTe and $Cd_{0.15}Hg_{0.85}Te$.

The present investigation provides insufficient data to facilitate determination of the origin of the yield relaxation, however, it may be significant that it occurs in the presence of 10^6-10^7 dislocations cm^{-2}. Further work is proposed which will investigate the yield and flow mechanisms of compounds in the CdTe–HgTe quasi-binary section.

The yield stress appears to differ for similarly-oriented samples, bent in opposite senses at the same temperature, but insufficient samples were tested to establish whether the observed variation is significant with respect to the random fluctuations in measurement. Several authors (for example [13, 20]) have observed an anisotropy of yield stress in bend tests on sphalerite-structure compounds, interpreting their results in terms of the model suggested by Haasen [1] that bending in opposite polar directions produces excesses of positive and negative edge dislocations, which have different mobilities. However, this concept applies unequivocally only when the test-piece is orientated for single slip (long axis $[\bar{1}\,2\,3]$, bend axis $[1\,2\,\bar{1}]$). The situation is very much more complex for other orientations [13]. A further problem in making a definitive study of such effects in $Cd_xHg_{1-x}Te$ is the lack of a calibration of the absolute polarity in the material.

4. Conclusions

New data on the mechanical properties of $Cd_xHg_{1-x}Te$ are reported.

(a) Plastic bending tests of single crystal samples of $Cd_xHg_{1-x}Te$, with a value of x about 0.2, conducted in air at strain rates of the order of $10^{-5}\,sec^{-1}$, show stress–strain curves with a pronounced yield drop similar to those found for Group IV and Group III–V semiconductors.

(b) Upper yield stresses from about 15 to $24\,MN\,m^{-2}$ and lower yield stresses from about 10 to $15\,MN\,m^{-2}$ for temperatures from about 363 K (90° C) to 303 K (30° C) were found.

(c) An approximate estimate of the activation energy, E, in the relation

$$\tau_{ly} = C\left(\dot{e}\exp\frac{E}{kT}\right)^{1/(m+2)}$$

gives a value of about $E = 0.3\,eV$.

(d) $Cd_{0.2}Hg_{0.8}Te$ appears to have a higher yield stress than CdTe under similar conditions of temperature and strain rate.

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