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# A layer-by-layer study of CdTe(110) surface Debye temperature and thermal vibrations by low energy electron diffraction

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#### Abstract

The Debye temperature and the thermal vibrations of the first two surface layers of the CdTe(110) have been studied by low energy electron diffraction (LEED). The full dynamic LEED calculations were performed using the LEEDFIT code that allows one to carry out optimizations of the Debye temperature and vibrational amplitudes of each atom in each surface layer. © 1999 Elsevier Science B.V. All rights reserved.

*Keywords:* Cadmium telluride; Debye temperature; Low energy electron diffraction (LEED); Low index single crystal surfaces; Surface relaxation and reconstruction; Thermal vibrations

### 1. Introduction

It is well known nowadays that the diffracted intensities used in surface structural studies by low energy electron diffraction (LEED) depend on temperature, i.e. on the thermal vibrations of the atoms in the surface. In the kinematic approximation we can take this into account by introducing a Debye–Waller factor. Although this is a good approximation in X-ray diffraction, the dominance of the multiple scattering in LEED requires a more sophisticated approach. The standard procedure is to assume that the motions of the surface atoms are not correlated and that the atomic thermal vibrations are isotropic. These considerations lead us to use temperature-dependent phase shifts [1– 3]. This treatment of thermal vibrations usually

\* Corresponding author. Fax: +55-31-499-5600. *E-mail address:* edmar@fisica.ufmg.br (E.A. Soares) works well for the purpose of determining the structural parameters, but it is certainly one of the factors that limits the accuracy of the structural determination. The limitation to isotropic vibrations does not allow the determination of vibrational parameters via LEED with reliability comparable to the standard in X-ray or neutron diffraction. As the surface is for itself an anisotropic ambient we can expect that the extension of the multiple scattering theory to include anisotropic and anharmonic vibrations should lead to a better agreement between experimental and theoretical I(V) curves.

One of the attempts to take vibrational effects into account in a more realistic way in the structural determination by LEED was done by Löffler and coworkers [4,5]. In these studies, the tensor LEED formalism [6–9] was extended to handle thermal isotropic [4] and anisotropic [5] vibrations of surface atoms. This thermal tensor LEED

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method was applied to the adsorbate system  $Ni(100)c(4 \times 3)$ -K and allowed the authors to test the influence of atomic vibrations in a fast effective way. A quite different approach was proposed by Over and coworkers, namely the concept of split positions, in which the anisotropic probability distribution function is approximated by a small number of distinct sites [10,11]. This concept has the advantage of being able to treat correlated motions, as frequently observed in molecule vibrations, and can easily be inserted into standard LEED programs. This approach was applied to several representative adsorbate systems and improved considerably the agreement between experimental and theoretical I(V) curves. More recently Moritz and Landskron [12] have extended the multiple scattering theory of LEED in order to include anisotropic thermal vibrations. This method is based on the multipole expansion of the probability density function and leads to thermally averaged atomic scattering *t*-matrices with offdiagonal terms to be inserted in the current multiple scattering formalism. Although it was shown that these approaches work properly on adsorbate metal systems, only a very small number of semiconductor systems have been analysed. So, in this work we have applied the approach proposed by Moritz and Landskron [12] on the study of the surface Debye temperature and thermal vibrations of CdTe(110).

The properties of the (110) surfaces of zincblende semiconductors have been studied for more than two decades. However, this is still an active research field, mainly because of the scientific and technological importance of systems involving metal-semiconductor and semiconductor-semiconductor interfaces. Despite their importance, very little is known about the chemistry and physics of such systems and how the detailed knowledge of atomically clean surfaces of semiconductors can play an important role in the understanding of the interface formation and their unique properties.

The first LEED study of the CdTe(110) surface was carried out by Duke et al. [13]. In their analysis, experimental data collected at 110 K were used and the calculations were carried out by using an approximate multiple scattering treatment, where the amplitudes scattered from the uppermost three atomic layers were evaluated exactly and a modified kinematical calculation was used for deeper layers. Also, they used an energy-dependent (Hara) exchange potential and considered the surface as a rigid lattice, i.e. no vibrational effects were investigated. The best model was obtained by refining the structural parameters so as to minimize the X-ray r-factor defined using the quadratic form [14] and was characterized by a bond-length-conserving rotation of  $\omega \approx 30.5^{\circ}$  and a contraction of  $0.05 \pm 0.05$  Å towards the substrate. In a more recently study, Cowell and de Carvalho [15,16] using the direct search method proposed by Hooke and Jeeves [17] adapted to the LEED problem, have investigated this surface. The experiment-theory comparison was done by the Pendry's r-factor  $(R_{\rm P})$  [18] and the CdTe crystal was cleaved in vacuum to produce the (110) surface. The structure corresponding to the minimum value of  $R_{\rm P}$  is characterized by a first-layer bond rotation of  $\omega \approx 30.5^{\circ}$ , a first-layer relaxation of 0.24 + 0.05 Å towards the bulk and a second layer rumple of 0.18 + 0.02 Å. The results are very similar to the one obtained by Duke et al. [13]. The effective Debye temperature of the CdTe(110) surface was also studied by LEED [19] using both X-ray (quadratic) r-factor  $(R_2)$  [14] and  $R_P$ . An rfactor behaviour similar to that reported for InSb(110) [20] was obtained and a value of 150 K was determined for the effective surface Debye temperature. The structural model obtained for this surface by LEED is also supported by recent studies using X-ray standing wave (XSW) measurements conjugated to first-principles total-energy calculations [21] and low energy positron diffraction (LEPD) (crystal cleaved in situ) [22].

Although the several results from different techniques agree with respect to the structural model of the (110) surface of CdTe, only a few attempts have been made in order to obtain information about the surface Debye temperature and thermal vibrations of this compound. In this paper, we firstly present a layer-by-layer study of the CdTe(110) surface Debye temperature by LEED. After that the thermal vibrations are explored in order to try to obtain some information about thermal vibrations of the surface atoms at room temperature.

## 2. Experimental details

The CdTe(110) experimental data set used was collected using an ultrahigh vacuum (UHV) chamber equipped with a range of facilities for sample preparation and surface characterization together with a computer-controlled LEED diffractometer at the Physics Department of UFMG, Brazil. The base pressure of the chamber was typically  $5 \times 10^{-10}$  Torr. The CdTe crystal was cleaved in air and the exposed (110) surface showed a planar and mirror finish. After insertion in vacuum, the sample was cleaned using 500 eV Ar<sup>+</sup> ions at grazing incidence for 10 min. Although the surface was not annealed after the sputtering cleaning process — that could have produced a surface with a high degree of structural disorder — the CdTe(110) surface exhibited a sharp  $(1 \times 1)$ pattern (with very low background) and no carbon, oxygen or sulphur were detectable using Auger electron spectroscopy. The LEED patterns for the CdTe(110) surface were then recorded from 20 eV up to 150 eV using an Omicron videoleed system in a scattering geometry near normal incidence. The sample was mounted on the manipulator in such a way that the parallel component of the incident wave vector laid on the surface mirror plane. With this setup, the symmetry between symmetric beams, (h, k) = (h, k), was preserved and the value of the angle  $\phi$  was constrained to either  $0^{\circ}$  or  $180^{\circ}$ . This setup was improved by comparing the symmetrically equivalent experimental beams using the  $R_{\rm P}$  factor. The I(V) curves for ten diffracted beams  $[(0, 1)=(0, \overline{1})-R_{\rm P}=$ 0.067,  $(\bar{1}, 1) = (\bar{1}, \bar{1}) - R_{\rm P} = 0.109, (2, 1) = (2, \bar{1}) - 0.067, (1, 1) = (2, \bar{1}) - 0.067, (1, 1) = (2, \bar{1}) - 0.067, (2, 1$  $R_{\rm p} = 0.130, (1, 1), (2, 0), (1, 0) \text{ and } (\overline{2}, 0)$  were then obtained from the digitized LEED patterns, normalized with respect to the incident beam current and smoothed using a five-point least-squares cubic polynomial algorithm.

### 3. Theoretical details

The theoretical analysis was performed assuming the muffin-tin model for CdTe crystal. Muffintin radii of 1.40 Å were assumed for both atoms. The atomic wavefunction [23] for each atom was used on the scattering potential calculation and a Slater parameter  $\alpha = 2/3$  was assumed in the local exchange approximation. As the I(V) curve calculation depends on the phase shifts, these were evaluated by numerical integration of the radial part of the Schrödinger equation in the muffintin spheres.

The full dynamic LEED calculations were performed on an AlphaDec Station, and the LEEDFIT code [10,12,24-26] was used to evaluate the I(V) curves. Besides the automatic optimization of the structural parameters, this code allows the optimization of non-structural parameters such as Debye temperature and atomic vibrations for each atom in each layer. In order to do that, the multiple scattering theory of LEED was extended to include anisotropic vibrations. The method is based on the multipole expansion of the probability density function. This treatment of anisotropic vibrations leads to thermally averaged atomic scattering *t*-matrices with off-diagonal terms to be inserted in the current multiple scattering formalism. The Marquardt procedure [27], which combines the steepest descent and expansion methods, was used on the r-factor minimizations. A set of ten phase shifts and a sample temperature of 293 K were assumed for the crystal. The surface was considered as being formed by three layers. Two different *r*-factors were used in this work, the  $R_{\rm P}$  factor proposed by Pendry [17] and the  $R_{\rm DE}$ factor proposed by Kleinle and coworkers [24,25]. A bulk Debye temperature of 140 K was assumed for the CdTe. Initially, the inner potential was assumed to be equal to  $V_0 = (-1+4i) \text{ eV}$ , but the real part of this potential was optimized during the analysis. All beams were treated independently and no average was carried out.

### 4. Results and discussions

As we have used a new LEED data set collected at off-normal incidence, we started our CdTe(110) analysis by determining the value of the angle of incidence. As described in the Section 2, the sample was mounted on the manipulator in such a way that the component of the incident wave vector parallel to the surface laid on the surface mirror plane. Therefore, the value of the azimuthal angle  $\phi$  was constrained to 0° or 180°. Then, using the structure obtained by Cowell and de Carvalho [16], we calculated the I(V) curves for several values of the incidence angle  $\theta$  (in steps of 1° in the range 0 to  $15^{\circ}$ ) for the two possible values of  $\phi$ . During this step no structural or non-structural parameter optimizations were performed. A welldefined minimum for both r-factors ( $R_{\rm P} = 0.50$  and  $R_{\rm DE} = 0.54$ ) was found for  $\theta = 4^{\circ}$  and  $\phi = 180^{\circ}$ . As the r-factor reported by Cowell and de Carvalho [16] ( $R_{\rm P} = 0.54$ ) was obtained by a different LEED program and a different experimental data set was used, it is difficult to compare their absolute values. This difficulty arises from the fact that some programs carry out a smoothing of the experimental data before the comparison with theoretical data or use different integration subroutines in order to evaluate the r-factors. Therefore, from now on, any changes in the *r*-factors will be measured with respect to those values obtained by LEEDFIT and presented in the second column of Table 1 and labelled 'earlier LEED'.

As the thermal vibration optimization provided by the LEEDFIT code is a very fine refinement we cannot start an optimization procedure at a point very far from the minimum. So, we have decided to use the following strategy in order to be able to obtain some information on how the atoms are moving due to thermal effects. First, we carried out optimizations of the structural parameters and the Debye temperatures of each atom in the first two surface layers where no anisotropic or anharmonic effects were taken into account. Once the values for the Debye temperature were obtained, they were used to calculate the isotropic vibrational amplitudes of the two first-layer atoms. These amplitudes were used as an input to anisotropic thermal vibrations optimizations.

The structural parameters and the Debye temperatures were optimized using the scattering geometry defined by  $\theta = 4^{\circ}$  and  $\phi = 180^{\circ}$ . Several optimizations were carried out using different starting points, including the structure proposed by Cowell and de Carvalho [16]. Both  $R_{\rm P}$  and  $R_{\rm DE}$ factors were used as the r-factor to be minimized. The structural parameters optimized were: atomic displacements perpendicular to the surface  $(\Delta_{z_1}^{\rm Te}, \Delta_{z_1}^{\rm Te})$ 

 $\Delta_{z_1}^{Cd}$ ,  $\Delta_{z_2}^{Te}$  and  $\Delta_{z_2}^{Cd}$ ) and atomic displacements parallel to the x direction  $(\Delta_{x_1}^{\text{Te}}, \Delta_{x_1}^{\text{Cd}}, \Delta_{x_2}^{\text{Te}}, \Delta_{x_2}^{\text{Cd}})$ . The displacements of the atoms are defined with respect to the bulk positions as shown in Fig. 1. The nonstructural parameters optimized in this step were the Debye temperature of each atom of the first two layers  $(\Theta_{D_1}^{Te}, \Theta_{D_1}^{Cd}, \Theta_{D_2}^{Te}$  and  $\Theta_{D_2}^{Cd})$  and the real part of the optical potential. Displacements in the y direction are forbidden by the symmetry of the (110) surface. Therefore, a total of 13 parameters were simultaneously optimized. In these optimizations only isotropic vibrations were taken into account to calculate the Debye temperature. The best models corresponding to each of the two rfactors minimized are presented in Table 1 as Model 1 and Model 2. From Table 1 we can clearly see that both r-factor minimizations have found nearly the same structure. This was expected as different r-factors should find the same structural parameters. Although the  $R_{\rm P}$  factor obtained in both minimizations remained nearly constant (changed from 0.50 to 0.48 only), the  $R_{\rm DE}$  resultant from the optimization based on the  $R_{\rm DE}$  minimization showed a significant improvement (from 0.54 to 0.37). The main difference between the two best structural models found is the first-layer rumple and consequently the first layer bond rotation  $\omega_1$ . The rumple found by the  $R_{\rm DE}$  minimization is about 12% higher than that obtained by the  $R_{\rm P}$ minimization. The structural parameters are in qualitative agreement with previously reported results including LEED studies using UHV-cleaved surfaces [15,16], LEPD [22] and XSW - firstprinciples total-energy calculation [21] analysis as can be seen from Table 2. From Table 2 we can see that our results obtained using a sputtered sample are very close to that obtained using samples cleaved in situ. In Fig. 2a we show, for illustration, the variation of both r-factors as a function of the vertical displacement of the firstlayer Te atoms  $(\Delta_{z_1}^{Te})$  for Model 2 in Table 1. All the other structural parameters were kept fixed at their optimum values. As we can see, both rfactors have the same behaviour and the deepest minima are at the same optimum value. Similar curves to the one presented in Fig. 2a provided the basis for estimating the precision of our strucTable 1

The best models obtained by minimization of the  $R_P$  (Model 1) and  $R_{DE}$  (Model 2) factors using the structure proposed by Cowell and de Carvalho [16] (earlier LEED) as one of the starting points. The atomic displacements are defined from the bulk positions and are shown in Fig. 1

	Earlier LEED [16]	Model 1	Model 2
First layer			
$\Delta z_1^{\text{Te}}$ (Å)	10.17	$(0.15 \pm 0.05)$	$\uparrow (0.21 \pm 0.05)$
$\Delta z_1^{\rm Cd}$ (Å)	0.65	$\downarrow (0.65 \pm 0.05)$	$\downarrow (0.71 \pm 0.04)$
$\Delta x_1^{\text{Te}}$ (Å)	-0.17	$-0.13 \pm 0.06$	$-0.11 \pm 0.06$
$\Delta x_1^{\rm Cd}$ (Å)	-0.39	$-0.38 \pm 0.06$	$-0.42 \pm 0.06$
$\omega_1$ (deg)	30.3	30.3	35.0
Rumple (Å)	0.82	0.80	0.92
Relaxation (Å)	-0.24	-0.25	-0.25
$\Theta_{D_1}^{Te}(K)$	140	$141 \pm 200$	$122 \pm 80$
$\Theta_{D_1}^{Cd}(K)$	140	$144 \pm 200$	$126 \pm 100$
Second layer			
$\Delta z_2^{\text{Te}}$ (Å)	↓0.03	$\downarrow$ (0.03 ± 0.06)	$\downarrow$ (0.02 $\pm$ 0.05)
$\Delta z_2^{\rm Cd}$ (Å)	10.06	$\uparrow(0.04\pm0.05)$	$\uparrow (0.04 \pm 0.05)$
$\Delta x_2^{\text{Te}}$ (Å)	0.00	$0.06 \pm 0.07$	$0.05 \pm 0.07$
$\Delta x_2^{\rm Cd}$ (Å)	0.00	$0.02 \pm 0.07$	$0.02 \pm 0.07$
$\omega_2$ (deg)	3.2	2.4	2.0
Rumple (Å)	0.09	0.07	0.06
Relaxation (Å)	0.02	0.01	0.01
$\Theta_{D_2}^{Te}(K)$	140	$144 \pm 250$	$142 \pm 120$
$\Theta_{\mathrm{D}_{2}}^{\mathrm{Cd}}(\mathrm{K})$	140	$142 \pm 250$	$115 \pm 150$
r-factors			
R <sub>P</sub>	0.50	$0.48 \pm 0.06$	$0.48 \pm 0.05$
R <sub>DE</sub>	0.54	$0.55 \pm 0.05$	$0.37 \pm 0.05$

tural parameter determination. Positive displacements are inward to the crystal.

With respect to the Debye temperatures, the values obtained by the  $R_{\rm P}$  minimization are nearly the bulk values, i.e.  $\Theta_{D_1}^{Te} = 141 \text{ K}$ ,  $\Theta_{D_1}^{Cd} = 144 \text{ K}$ ,  $\Theta_{D_2}^{Te} = 144 \text{ K}$  and  $\Theta_{D_2}^{Cd} = 142 \text{ K}$ . On the other hand, the  $R_{\rm DE}$  minimization seems to be able to distinguish the Debye temperature of each atom in each layer. As the Debye temperature enters into the LEED intensity calculations through the Debye-Waller factor, it appears by multiplying the atomic amplitudes when one takes into account the lattice vibrations. In this way, this parameter has a great influence on the diffracted beam intensities, but has little influence on the peak positions that are present in the I(V) curves. Since the peak positions do not change very much when the surface Debye temperature  $\Theta_{D_s}$  is varied, this nearly constant  $R_P$ behaviour may be expected. As the  $R_{\text{DE}}$  is more sensitive to peak intensities, this factor should be able to detect changes that appear on the intensities

when  $\Theta_{D_e}$  is varied. These *r*-factor behaviours are in agreement with the results reported in Refs. [19,20]. We can also note that the optimization of the Debye temperature did not spoil a previous optimization of the structural parameters using the  $R_{\rm P}$  factor. That was expected since it is known that structural parameters and the Debye temperature are largely decoupled, so that a structure refinement can be performed in two independent steps: first the structural parameters are optimized and then the Debye temperature [11]. The variation of the  $R_{\rm DE}$  factor as a function of the Debye temperatures of the first-layer atoms ( $\Theta_{D_1}^{Te}, \Theta_{D_1}^{Cd}$ ) is shown in Fig. 2b. The Debye temperatures of the second layer atoms  $(\Theta_{D_2}^{Te}, \Theta_{D_2}^{Cd})$  were kept fixed at the optimum values found by the  $R_{\rm DE}$  minimization (Model 2 in Table 1). From Fig. 2b we are able to see that there is only one well-defined minimum corresponding to the optimum values found by the  $R_{\rm DE}$  factor. Orthogonal projections passing through the minimum of Fig. 2b were used to



Fig. 1. Side view of the CdTe(110) surface showing a model for top- and second-layer reconstruction. Open circles: bulk atom sites. Black circles: Te atoms. Grey circles: Cd atoms. The *y*-axis points into the paper.

estimate the uncertainties in the Debye temperatures,  $\Delta \Theta_{D_1}^{Te} = 80 \text{ K}$  and  $\Delta \Theta_{D_1}^{Cd} = 100 \text{ K}$ . In Fig. 3 we show the theoretical I(V) curves

In Fig. 3 we show the theoretical I(V) curves for four different values of the Debye temperature of the first-layer atoms. The Debye temperatures of the Cd and Te atoms on the first layer were assumed to be equal just for simplicity. From Fig. 3 we can clearly see how changes in the Debye temperature affect the theoretical I(V) curves. As we increase the Debye temperature of the surface,

Table 2

The best fit models obtained for the CdTe(110) surface by different techniques. The first row corresponds to the results from an earlier LEED [16]. The second and third rows report results from XSW and first-principles calculations (FPS) [21]. The fourth row contains the results from a very recent LEPD study [22]. The last two rows show the results obtained in this work.  $\Delta_1$  and  $\Delta_2$  are the rumple in the first and second layer respectively. Rel<sub>1</sub> and Rel<sub>2</sub> are the first- and second-layer relaxations and are defined by Rel<sub>i</sub> =  $\frac{1}{2} (|\Delta_{z_i}^{Te}| - |\Delta_{z_i}^{Sb}|)$ 

	$\Delta_1$ (Å)	$\omega_1$ (deg)	$\Delta_2$ (Å)	$\omega_2$ (deg)	$\operatorname{Rel}_1(\operatorname{\AA})$	Rel <sub>2</sub> (Å)
Earlier LEED [16]	0.82	30.5	-0.09	-3.2	-0.24	0.02
XSW [21]	0.78	28.7	_	_	_	_
FPC [21]	0.73	29.5	-0.13	-4.5	_	_
LEPD[22]	0.75	30.5	-0.19	-6.7	_	_
Model 1	0.80	30.3	-0.07	-2.4	-0.25	0.01
Model 2	0.92	35.0	-0.06	-2.0	-0.25	0.01



Fig. 2. (a) Variation of  $R_{\rm P}$  and  $R_{\rm DE}$  factors as a function of the vertical displacement of the first-layer Te atoms for Model 2 of Table 1. (b) The variation of the  $R_{\rm DE}$  factor as a function of the Debye temperature of the first-layer atoms ( $\Theta_{\rm De}^{\rm Te}$ ,  $\Theta_{\rm De}^{\rm Cd}$ ).

the intensities of the peaks at higher energies also increase. This is already known and can be explained as follows: we can look at the Debye temperature as a measure of how much the surface atoms are displaced from their equilibrium positions due to thermal effects — the higher the  $\Theta_{\rm D}$ the less the atoms vibrate. In this way, the number of electrons inelastically scattered due to thermal vibrations decreases for high values of the surface Debye temperature and an increase in the number of electrons elastically scattered is observed. So, the LEED I(V) curves are really sensitive to changes in  $\Theta_{\rm D}$ .

In order to take into account anisotropy of the surface atom vibrations, the LEEDFIT code was allowed to optimize the atomic vibrational amplitudes of the first two layer atoms. The vibrational amplitudes corresponding to the Debye temperatures shown in Table 1 were used as starting points and the structural parameters were kept constant to their respective values. Optimizations based on minimizations of  $R_{\rm DE}$  and  $R_{\rm P}$  factors were performed. Results from the optimizations starting from the thermal vibrations corresponding to the Debye temperatures of Model 1 of Table 1 did not show any improvement in the r-factor values (both  $R_{\rm P}$  and  $R_{\rm DE}$ ) and, sometimes, the vibrations found were not physically acceptable. On the other hand, the atomic vibrational amplitudes obtained using as a starting point the Debye temperatures of Model 2, under minimization of  $R_{\rm P}$ , are more reasonable, as can be seen in Table 3. From Table 3 we can firstly note that the thermal vibrations found suggest that, at room temperature, there is no anisotropic behaviour parallel to the surface since  $\langle u_x \rangle \approx \langle u_y \rangle$  for the first two layer atoms. The perpendicular vibrations were found to be larger than the parallel vibrations as expected. The  $R_{\rm P}$  factor decreased from 0.48 to 0.43, whereas the  $R_{\rm DE}$  factor remained nearly constant. Considering the bulk Debye temperature as being equal to 140 K, the bulk harmonic isotropic vibrational amplitudes are about 0.14 Å for the Cd atom and 0.13 Å for the Te atom. The results obtained through the  $R_{\rm P}$  minimization show that the atoms in the first layer, at room temperature, undergo thermal vibrations, perpendicular to the surface  $\langle u_z \rangle$ , higher than those expected for bulk. Also, the second-layer atoms have vibrational amplitudes that are lower than the first-layer atoms and higher than those of the bulk. However, the vibrations parallel to the surface present a puzzling behaviour. Although they are nearly isotropic, the



Fig. 3. I(V) curves for four different values of first-layer Debye temperature. The dashed lines are the experimental curves.

Table 3 The mean vibrational amplitudes for the best  $R_{\text{DE}}$  model presented in Table 1.  $\Theta_{D_1}^{\text{Sb}} = 122 \text{ K}$ ,  $\Theta_{D_1}^{\text{In}} = 126 \text{ K}$ ,  $\Theta_{D_2}^{\text{Sb}} = 142 \text{ K}$ , and  $\Theta_{D_2}^{\text{In}} = 115 \text{ K}$ 

	Starting point	Final values
$\overline{\langle u_x \rangle_1^{\text{Te}}}$ (Å)	0.150	0.120
$\langle u_{v} \rangle_{1}^{\text{Te}}$ (Å)	0.150	0.115
$\langle u_z \rangle_1^{\text{Te}}$ (Å)	0.150	0.168
$\langle u_x \rangle_1^{\rm Cd}$ (Å)	0.155	0.118
$\langle u_v \rangle_1^{\rm Cd} ({\rm \AA})$	0.155	0.126
$\langle u_z \rangle_1^{\rm Cd}$ (Å)	0.155	0.172
$\langle u_x \rangle_2^{\text{Te}}$ (Å)	0.129	0.096
$\langle u_v \rangle_2^{\text{Te}}$ (Å)	0.129	0.095
$\langle u_z \rangle_2^{\mathrm{Te}}$ (Å)	0.129	0.117
$\langle u_x \rangle_2^{\text{Cd}} (\text{\AA})$	0.163	0.140
$\langle u_{\rm u} \rangle_2^{\rm Cd} (\rm \AA)$	0.163	0.137
$\langle u_z \rangle_2^{\rm Cd}$ (Å)	0.163	0.151
R <sub>P</sub>	0.48	$0.43 \pm 0.04$
R <sub>DE</sub>	0.37	$0.36 \pm 0.03$

Te atoms in the second layer present an unexpected low value for the parallel vibrations. This may be explained by taking into account the changes in the chemical bonds associated with Te atoms of the second layer, resulting from the significant distortion undergone by the atoms of the first layer. The final value obtained for the real part of the optical potential was -2.8 eV. Fig. 4. shows a comparison of four of the experimental I(V) curves used in this work with the theoretical curves obtained from the LEEDFIT code for the best structural model (Model 2) and thermal vibrations presented in Table 3. Clearly, there is a good agreement between the experimental and theoretical data.

### 5. Conclusion

In summary, we have successfully used the LEEDFIT code in order to study the thermal



Fig. 4. Representative CdTe(110) experimental (dashed lines) and theoretical I(V) curves for the best structural model.

vibrations of the CdTe(110) surface. It was observed that, at least for our data set, the  $R_{DE}$ factor seems to be more sensitive to the Debye temperature. It was also found that using the thermal vibrations corresponding to the Debye temperatures obtained by the  $R_{DE}$  factor as starting point, the  $R_P$  factor was able to find good values for the vibrational amplitudes of the first two layer atoms. The best structural model is characterized by structural parameters of Model 2 presented in Table 1. With respect to the thermal vibrations, no anisotropy was observed parallel to the surface at room temperature. Also, vibrations perpendicular to the surface were found to be greater than the parallel vibrations.

Despite the thermal vibrations optimizations, the *r*-factors are at relatively high values  $(R_{\rm P}=0.43 \text{ and } R_{\rm DE}=0.36)$ . So we can conclude that the remaining misfit between theory and experiment is not due to thermal vibrations. As CdTe is a covalent compound, which means that the electrons forming the bond tend to be partly localized in the region between the two atoms joined by the bond, the use of non-spherical potentials could produce a better theory–experiment agreement.

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