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Surface Science 487 (2001) 15–27

SURFACE SCIENCE

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The fast simulated annealing algorithm applied to the search problem in LEED

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Received 5 February 2001; accepted for publication 16 April 2001

Abstract

In this work we present new results obtained from the application of the fast simulated algorithm (FSA) to the surface structure determination of the Ag(1 1 0) and CdTe(1 1 0) systems. The influence of a control parameter, the "initial temperature", on the FSA search process was investigated. A scaling behaviour, that measures the efficiency of a search method as a function of the number of parameters to be varied, was obtained for the FSA algorithm, and indicated a favourable linear scaling (N^1). © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Low energy electron diffraction (LEED); Electron–solid diffraction; Surface structure, morphology, roughness, and topography

1. Introduction

The surface structure determination by low energy electron diffraction (LEED) is based on a comparison between experimental and theoretical intensity versus energy $I(V)$ curves of the diffracted beams. This comparison is performed with the utilization of a reliability factor (R-factor) that quantifies the experimental–theoretical agreement. The minimization of this R-factor allows the determination of the best structure among all proposed structural models. So, the surface determination by LEED consists on a search problem: to locate the global R-factor minimum in the explored volume of the parameters space.

An exhaustive exploration (trial and error) was first employed in the LEED search problem, where all feasible combinations of structural parameters are investigated on a grid that extends over a representative part of the parameters space. But the exhaustive search demands a lot of computational effort, which scales exponentially with the number of varied parameters, and belongs to the class of the NP-complete optimization problems [1].

More recently local directed search methods have been employed in surface structure

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PII: S0039-6028(01)01096-2

determination. These methods are based on descent methods, converting the N-dimensional search into a sequence of N one-dimensional searches [2]. The first gradient method with fully dynamical calculations was developed by Cowell and de Carvalho [3]. After that several descent methods have been employed by the Berkeley group (Tensor-LEED approach) [4] and by the Munich group (gradient expansion that goes beyond a simple descent method) [5,6]. Although the directed search methods present a more favourable scaling relation (approximately given by N^2), they have a serious limitation that consists on the inability to distinguish between local and global minima.

The problems associated with local search methods motivated the interest in the possibility of applying global search algorithms to the LEED structural determination of surfaces. An adequate search method for this purpose ought to be capable of identifying the global R-factor minimum among all the local minima and to present a reasonable scaling behaviour. Three recent works related to this subject have been published: Rous [7] has proposed the utilization of the simulated annealing algorithm. Döll and Van Hove [8] have suggested the use of the genetic algorithm, while Kottcke and Heinz [9] proposed a modified random sampling algorithm.

In a previous work [10] we have presented preliminary results obtained with the so-called fast simulated annealing (FSA) [11] global search method. These results indicated that the FSA method seems to be a good scheme to be applied to the surface structure determination by LEED. In order to continue our investigation on the convenience of using the FSA algorithm for LEED studies, in the present work we present more results obtained with the application of this algorithm to the surface structure determination of the Ag(1 1 0) and CdTe(1 1 0) systems using experimental data sets. The effects of the choice of the "initial temperature" on the FSA search process were also investigated. A scaling behaviour, necessary to evaluate the efficiency of the FSA method in comparison to other techniques, was also obtained using the CdTe(1 1 0) system in a theory–theory comparison.

2. The fast simulated annealing

The FSA [11,12] is, in fact, an improvement of the very well known simulated annealing algorithm that has been applied to solve different optimization problems in several branches of science [2,13–15]. This improvement can be achieved by using a Cauchy–Lorentz visiting distribution instead of a Gaussian or uniform distribution, as is commonly used for the choice of the random moves [2,12,16].

At the heart of the simulated annealing algorithm is the Metropolis criterion [16], which controls the acceptance probability of every step of the search process. Starting from an initial point A, a random step δX is chosen, leading to a new point B. The change of the cost function $\Delta C = C(B) - C(A)$ is then evaluated. If the cost function change is negative or zero ($\Delta C \leqslant 0$), the move will be accepted (a downhill move): if $\Delta C > 0$ the uphill move will be accepted with a probability given by the Boltzmann distribution $P(\Delta C) = e^{-\Delta C/T}$. This probability is controlled by the dimensionless parameter T (an artificial temperature), which is gradually decreased during the search. The simulated annealing algorithm is basically a search based on randomly chosen steps, accepted or rejected according to the Metropolis criterion, together with a gradual reduction of the "temperature" T.

In the case of the FSA the search distribution is semi-local, i.e., the random moves are frequently local, but occasionally long moves can be also considered. With this scheme the cooling cycle can be much faster when compared to the other implementations, making the search quite more efficient. In order to illustrate the visiting probability of the FSA and of the commonly employed implementations of the simulated annealing (Gaussian and uniform distributions), one can use an one-dimensional double-well cost function, as presented in Fig. 1. The Cauchy–Lorentz and the Gaussian distributions (which are "temperature" dependent) and the uniform distribution ("temperature" independent) are also plotted over the shallower minimum (Fig. 1 – point A), representing a "trapping" in the local minimum. We can see that while the "wing" of the Cauchy/Lorentzian

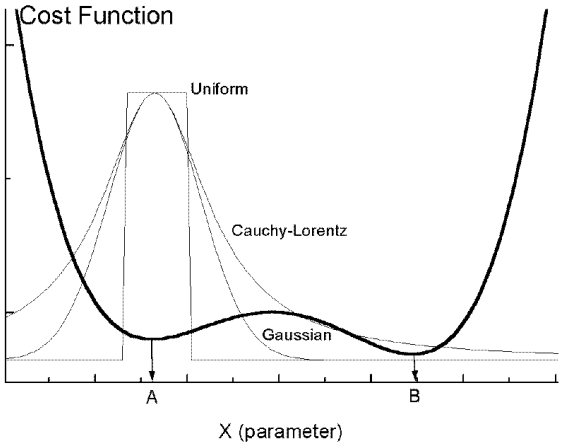

Fig. 1. Comparison between the Cauchy–Lorentz, Gaussian and uniform distribution sampling. The Cauchy–Lorentz and Gaussian distributions are plotted at the same "temperature".

distribution has reached the deeper minimum (Fig. 1 – point B), the normal (Gaussian) distribution has a negligible value at the deeper minimum and thus offers much less chance to escape from the initial local minimum. The uniform distribution will only be capable of escaping from the local minima after several favourable steps and, therefore, also presenting a lower probability. In the Cauchy–Lorentz scheme a higher "temperature" implies a faster sampling in a much more coarse grained fashion. As the "temperature" is gradually reduced the search becomes more refined in its sampling.

3. Experimental details

The Ag(1 1 0) data set was collected at the Department of Physics of UFMG, Brazil using an UHV chamber equipped with a range of facilities for sample preparation and surface characterization. This system was also provided with a TV camera system combined with a rear-view LEED optics and the base pressure of the chamber was typically 5×10^{-10} Torr. The Ag single crystal was supplied by Monocrystals Company (Richmond Heights, OH), with a nominal purity of 99.995% and previously oriented in the $\langle 1\,1\,0 \rangle$ direction ($\pm 1°$) and showing a mirrorlike (1 1 0) surface. After insertion in the vacuum chamber, the sample was cleaned using cycles of ion bombardment (Ar^- ions at 0.5 keV) and annealing (450°C for 20 min). The temperature was monitored using a chromel–alumel thermocouple in contact with the sample. The cleaning cycles were repeated until no carbon, oxygen or sulphur were detectable using Auger electron spectroscopy, while LEED indicated a sharp (1×1) pattern. The temperature of the Ag(1 1 0) sample was fixed at 27°C and the diffracted beam intensities of the LEED patterns from 40 to 350 eV were digitized using an Omicron LEEDStar video system at nominal normal incidence. The $I(V)$ curves of a total of 17 diffracted beams were obtained, normalized with respect to the incident beam current, and smoothed using a five-point least-square cubic polynomial algorithm. The symmetrically equivalent beams were averaged, leading to a total of seven independent data sets.

The experimental details for the CdTe(1 1 0) data set collection was described elsewhere [19]. Shortly, the $I(V)$ curves for 10 diffracted beams were obtained from the digitized LEED patterns, normalized with respect to the incident beam current and smoothed using a five-point least-squared cubic polynomial algorithm. No average of symmetrical beams was performed.

4. Theoretical details

The theoretical analysis was performed using the muffin-tin model for the potential of the Ag(1 1 0) and CdTe(1 1 0) systems. Muffin-tin radii of 1.45 Å for Ag atoms and 1.40 Å for Cd and Te atoms were assumed. Atomic wavefunctions were used to calculate the scattering potential, and a Slater parameter $\alpha = 2/3$ was assumed for the local exchange approximation. The phase shifts were evaluated by integration of the radial part of the Schrödinger equation in the muffin-tin spheres. The theoretical $I(V)$ curves were calculated using the Van Hove–Tong conventional LEED code [17] in the reverse forward scattering approximation. The calculations were performed on personal computers (AMD K6 II-500 MHz, AMD K6 II-300 MHz, Pentium II-500 MHz and

Pentium II-700 MHz) running the Linux operating system, on an Alpha-Dec workstation, and on an IBM RS-6000 SP machine (CENAPAD MG/CO – Brazil). Eight phase shifts were employed in the calculations and inner potentials of $Vo = (-10 + 5i)$ eV for Ag and $Vo = (-1 + 5i)$ for the CdTe were assumed, with their real parts being optimized during each structural analysis. Debye temperatures of 225, 140 and 140 K were assumed for the Ag, Cd and Te atoms, respectively, and these values were not optimized.

The simulated annealing algorithm was implemented using a modified Van Hove–Tong conventional LEED code according to the scheme proposed by Rous [7] (Fig. 2), with the necessary changes in the program being part of this work. The necessary modifications for the FSA variation were based on the original scheme proposed by Szu and Hartley [11], that will be discussed in Section 5.1, and on a recent study by Tsallis and Stariolo [12].

5. Results and discussion

As our main goal in this work was a more detailed investigation of the usefulness of the FSA to the LEED problem, the FSA algorithm was applied to the LEED data sets collected for the Ag(1 1 0) and CdTe(1 1 0) surfaces. Basically two aspects have been explored: the "temperature" parameter and the scaling with respect to the

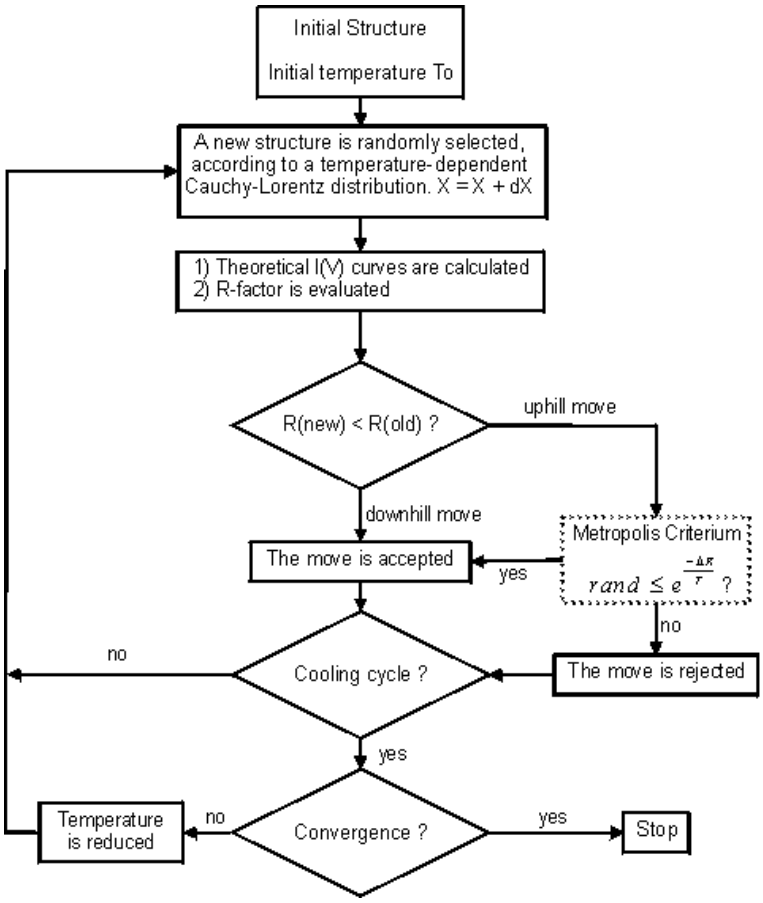

Fig. 2. Flowchart of the FSA algorithm implementation for the LEED structure search [7,11]. In the FSA cooling scheme, at every new structure (rejected or not by the Metropolis criterion) the "temperature" is reduced.

number of surface structural parameters to be investigated.

5.1. The initial "temperature"

The FSA algorithm used is that defined by the search scheme proposed by Szu and Hartley [11]:

- Random steps: chosen according to a Cauchy–Lorentz distribution $G(\delta X) \approx T_n/(T_n^2 + \delta X^2)$, allowing occasional long steps, where $T(n)$ corresponds to the "temperature" in the nth cooling cycle.
- Cooling scheme: a fast cooling scheme was adopted so that at every new structure (rejected or not) the "temperature" was decreased according to $T_n = T_0/n$.

The initial structure is arbitrarily chosen within the parameters space explored.

One important search control parameter is the initial "temperature", T_0. In order to investigate the influence of this parameter in the FSA search process we have carried out several structural searches using a theory–theory comparison, for the minimization of the Pendry R-factor [18], where two structural parameters of the CdTe(1 1 0) system were varied. The repeated structural searches were performed with initial "temperatures" equal to 1, 5, 10, 50 and 90, and some typical results ($T_0 = 1$, 10 and 50) are presented in Fig. 3. As can be seen in this figure for $T_0 = 1$ the FSA method was able to quickly locate the global minimum, but long range random steps (that would permit the search to escape from local minima, performing uphill moves) were not observed. When an initial "temperature" equal to 10 was adopted the search method could not reach the global minimum as quickly as before, but the occurrence of long random steps was observed (Fig. 3 – point A for example). Higher initial "temperatures", as $T_0 = 50$ for example, have increased the number of long steps without allowing the search to reach the global minimum. The same behaviour was observed for structural searches associated with the optimization of a larger number of parameters. As the effectiveness of the FSA method depends not only on a fast convergence, but also on its ability to escape from local minima, an optimum value for the initial "temperature" is about 5 or 10. Based on this investigation, an initial "temperature" of 10 was used in all structural investigations performed in this work.

5.2. Scaling behaviour

The most important feature of any search algorithm applied to the LEED search problem is how it scales with the total number of parameters N that are sought, i.e, its efficiency as a function of the number of parameters varied, the so-called scaling behaviour. As previously pointed out, the exhaustive search method (trial and error) scales exponentially with N [1], while the directed-search (descent) methods present a quadratic scaling (N^2) [4]. But, as mentioned before, the most important problem presented by all descent methods is the inability to distinguish between local and global minima. This problem motivates the application of global search methods to the LEED search problem. In a recent work Rous [7] has applied the simulated annealing algorithm to the LEED search problem, and the scaling behaviour of this method was obtained (N^6). More recently two other works related to global search methods have been published. Döll and Van Hove [8] have proposed the application of the genetic algorithm, which simulates the natural evolution of living organisms to the LEED structural search problem. Although the results obtained with the optimization of three structural parameters indicated that the genetic algorithm is able to find the final structure 10 times faster than an exhaustive grid search, a scaling behaviour was not obtained. Another approach to the global optimization problem was proposed by Kottcke and Heinz [9]. A modified random sampling algorithm which only allows downhill steps (in contrast to the simulated annealing) was suggested, and the results obtained indicate a scaling relation given by $N^{2.5}$. In our previous work [10] we have implemented the simulated annealing algorithm as well as the FSA variation and applied both to the structural searches for the Ag(1 1 1) and CdTe(1 1 0). Several tests have been performed, and the preliminary results indicated that the FSA

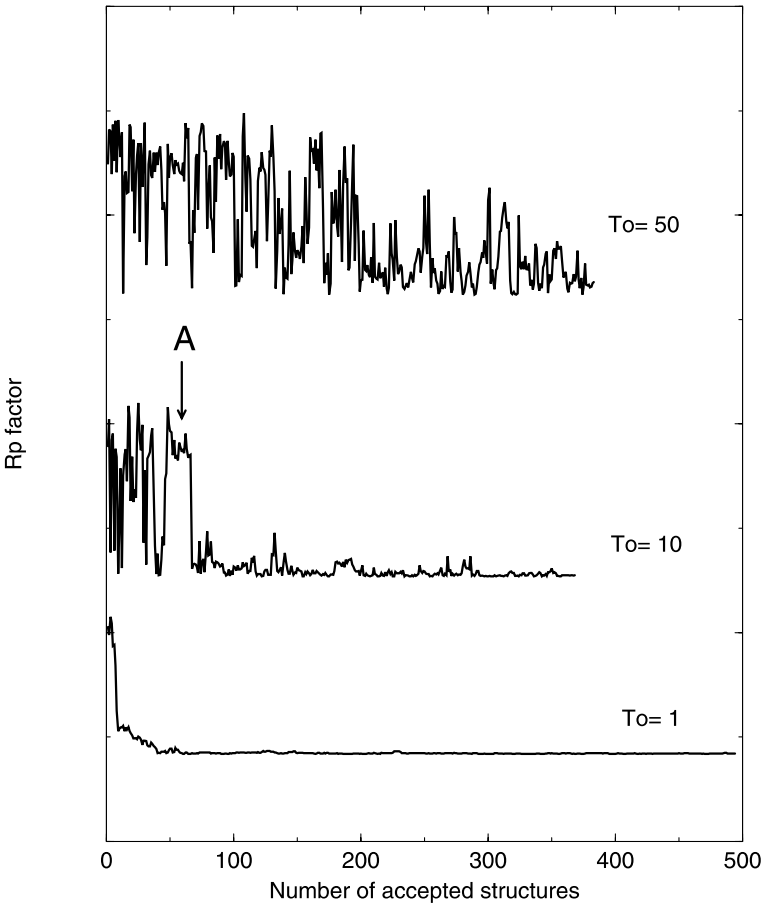

Fig. 3. Typical FSA structural search results for initial "temperatures" T_0 of 1, 10 and 50. The point A is an example of a long-range step, related to an uphill move.

algorithm presents a faster convergence to the global minimum than the original simulated annealing scheme. The FSA algorithm have also demonstrated an impressive ability to escape from local *R*-factor minima. However, a scaling behaviour, that could measure the efficiency of the FSA search method as a function of the number of varied parameters could not be presented at that time.

So, in order to investigate the scaling behaviour for the FSA algorithm we have applied the algorithm to the structural search for the CdTe(1 1 0). This choice comes from the fact that this surface exhibits a complex surface relaxation involving several parameters (Fig. 7) and also that it has been the subject of a recent structural investigation carried out in our laboratory [19]. So, it is a good reference system. Repeated FSA searches were performed allowing the optimization of 2, 4, 6 and 8 parameters associated to the first and second layers of Cd and Te atoms, in a theory–theory comparison (Pendry *R*-factor minimization). An initial "temperature" of 10, as previously discussed in Section 5.1, was adopted for all the searches, which have started from many different initial positions. The first four structural parameters (associated to the first layer) were varied in a range of 1.0 Å around their 'bulk terminated' values, while for the other four parameters (second layer) a range of 0.5 Å was adopted. Typical results of

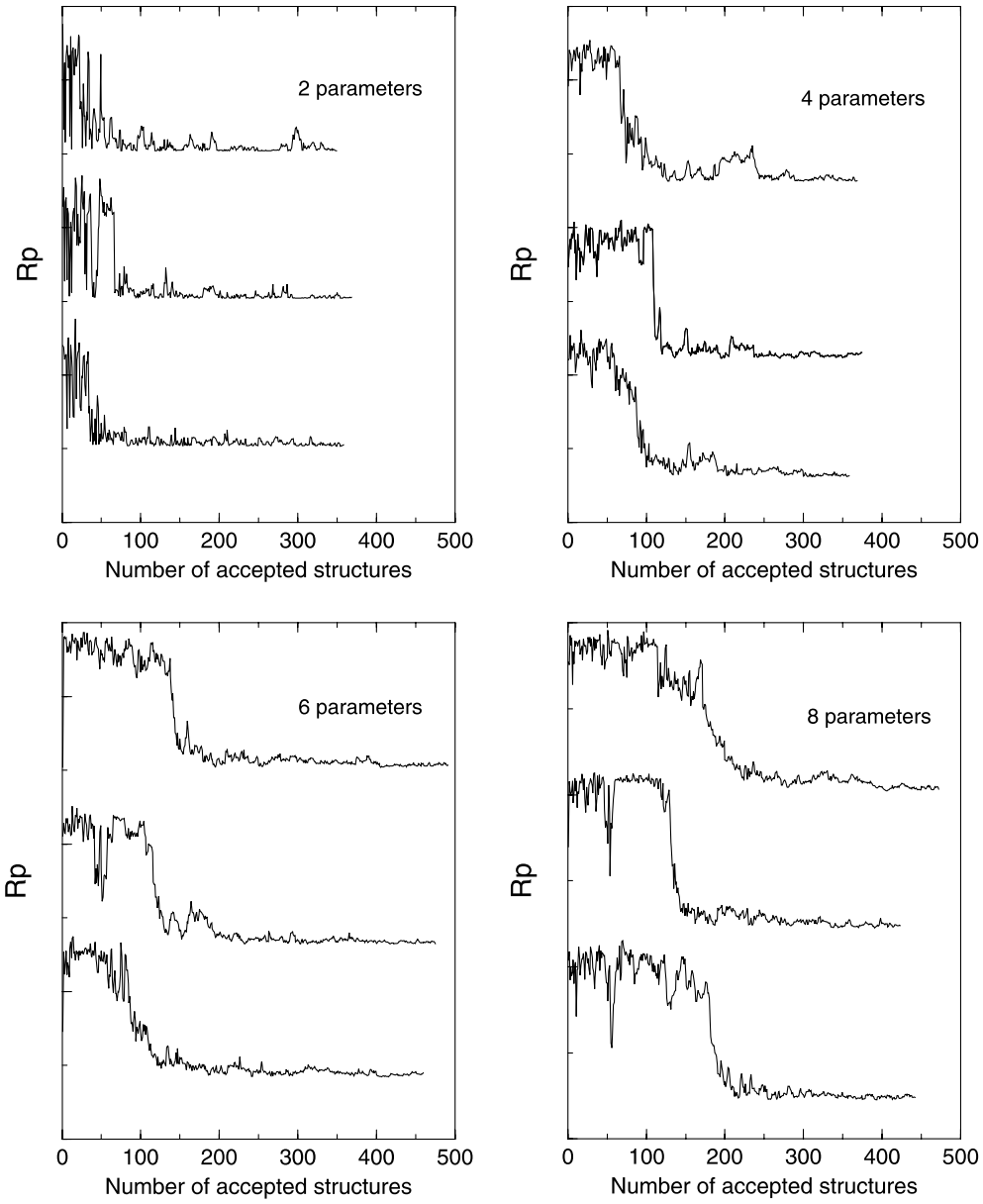

Fig. 4. Typical FSA structural searches performed for the optimization of 2, 4, 6 and 8 parameters for the CdTe(1 1 0) system in a theory–theory comparison, obtained from three different starting points.

these structural searches can be seen in Fig. 4. Each panel on this figure presents plots of the R_P as a function of the number of accepted structures for three different structural searches, that have started from distinct points, arbitrarily chosen within the explored region of the parameter space. The results obtained from the repeated FSA searches have indicated probabilities of locating the global R_P minimum equal to 99%, 90%, 80% and 75% for 2, 4, 6 and 8 parameters, respectively. The probabilities for 6 and 8 parameters searches could not be improved by adjusting the search

parameters (as initial "temperature" and parameters space volume) and we believe that these lower probabilities can be explained by the intrinsic property of the FSA algorithm to perform long steps even at low "temperatures" and to the lower sensitivity of the $I(V)$ theoretical curves to the structural parameters associated with the second layer.

The mean number of accepted structures examined before convergence to the global minima for 2, 4, 6 and 8 parameters were determined, and are shown in a linear plot in the Fig. 5a. As can be seen the good fit to a straight line (with a correlation equal to 0.995) indicates that the scaling relation is given by a first order polynomial in the range of parameters investigated and is given by: $N_{\mathrm{Accepted}} = (17 \pm 1)n_{\mathrm{P}} + (20 \pm 7)$, where N_{Accepted} and n_{P} corresponds to the number of accepted structures and number of parameters, respectively.

However, in the simulated annealing algorithm several structures are rejected by the Metropolis criterion during the structural search, and do not appear as part of the accepted structures. But, in fact theoretical $I(V)$ curves are also calculated for these structures requiring some computational effort. So, we believe that a more realistic scaling behaviour can be obtained if we use the total number of trial structures examined before convergence – that includes the accepted structures (accepted by the Metropolis criterion) as well as the rejected ones – and not only the number of accepted structures. We have obtained the mean number of trial structures as a function of the number of structural parameters varied. The results are presented in Fig. 5b. Here again a good fit to a straight line is observed (correlation equal to 0.993) indicating a scaling relation given by: $N_{\mathrm{Trial}} = (88 \pm 7)n_{\mathrm{P}} + (68 \pm 40)$, where N_{Trial} and n_{P}

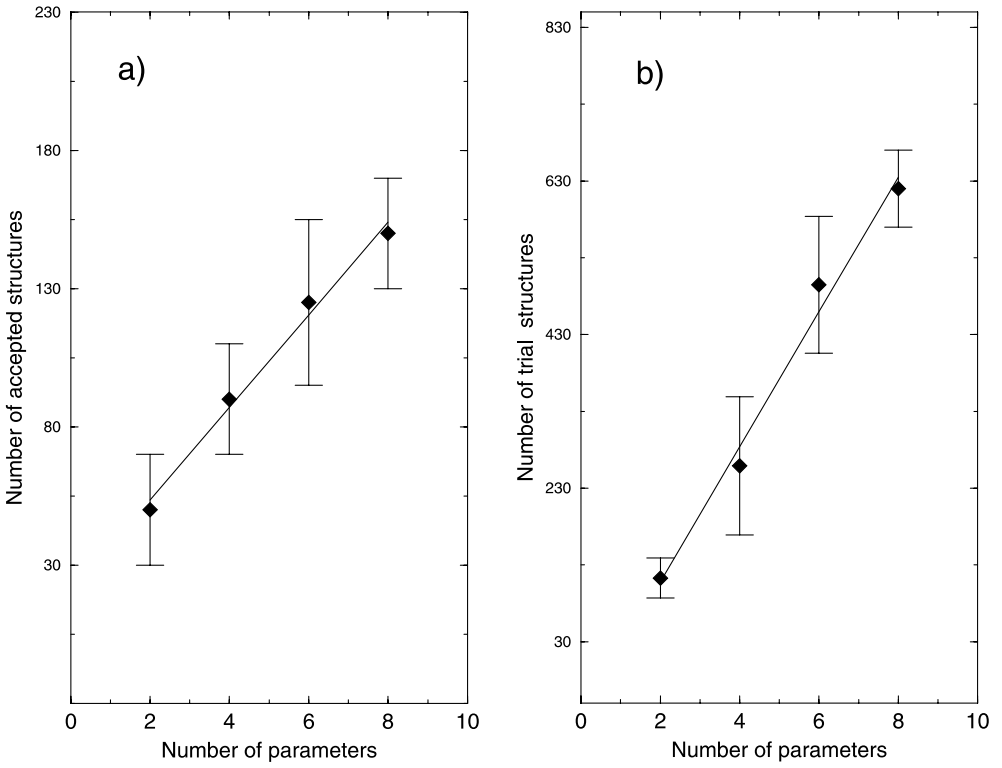

Fig. 5. Mean number of accepted (a) and trial structures (b) as a function of the number of varied structural parameters. The straight lines in both graphs correspond to the results obtained with least-squares fittings. The errors were obtained from a standard mean deviation from the mean values.

corresponds to the number of trial structures and number of parameters, respectively.

The results obtained for the CdTe(1 1 0) system in the range of the number of structural parameters investigated indicate that the FSA algorithm scales as N^1. This scaling behaviour is very favourable, especially when compared with the other global search techniques previously discussed. So, the FSA presents not only an impressive ability to escape from local minima and locate the global minimum but also a very satisfactory scaling behaviour. These two important features indicate that the FSA method is an adequate method to be applied to the search problem in the crystallography of surfaces by LEED.

In the next section we will present the results obtained with the application of the FSA algorithm to actual structure determinations of the Ag(1 1 0) and CdTe(1 1 0) systems, i.e. in a theory–experiment comparison.

5.3. Application of the FSA: Ag(1 1 0) and CdTe(1 1 0) systems

5.3.1. Ag(1 1 0)

The existence of an "oscillatory" relaxation of the topmost three interlayer spacings of Ag(1 1 0) (with a contraction, an expansion and a contraction in the first, second and third interlayer spacings, respectively), is well stabilised by LEED [20,21] and Rutherford backscattering spectroscopy (RBS) studies [22,23]. As the FSA algorithm has been applied only to the Ag(1 1 1) system [10] it was important to verify if reasonable results could be obtained with another system, such as Ag(1 1 0) ("oscillatory relaxation"), in order to gain confidence in the method.

So, an Ag(1 1 0) LEED experimental data set was used in order to test the performance of the FSA algorithm, when the first three interlayer spacings were allowed to vary in a parameter space volume of $1.0 \times 1.0 \times 1.0$ Å^3 using the bulk-terminated surface structure as a reference. The FSA algorithm was then run to search for the R_P (Pendry R-factor) global minimum, launched from many different starting structures.

A large number of structural searches was then performed, starting from many different initial structures, with an initial "temperature" equal to 10 and all of them have led to the same final structure. The results of the structural analysis are presented in Table 1 and, as can be seen, are in good agreement with a previous published work [20], and with an structural determination performed using the SATLEED code [24] for the same experimental data set, when a directed search method (Powell directed search) was employed. A comparison between experimental and theoretical $I(V)$ curves (obtained with SATLEED and FSA codes) is presented in Fig. 6, for some typical beams.

Table 1
Percent variation of vertical spacings for the best R_P structural model for the Ag(1 1 0) system, where d_{12}, d_{23} and d_{34} correspond to the distances between the first and second, the second and third and the third and fourth layers, respectively. The structural results obtained with the FSA algorithm are compared with a structural search performed for the same experimental data set, using a directed search method (Powell directed search) and with a previous work performed by Lindroos et al. [20]. The + and − signs corresponds to an increase and a decrease in the vertical spacings (relative to bulk values), respectively

Vertical spacing	This work (FSA)	This work (SATLEED)	Lindroos et al. [20]
Δd_{12}	$(-7 \pm 2)\%$	$(-6 \pm 2)\%$	$(-7 \pm 2)\%$
Δd_{23}	$(+1 \pm 2)\%$	$(+0.7 \pm 2)\%$	$(+1 \pm 2)\%$
Δd_{34}	$(-1 \pm 3)\%$	$(-1 \pm 2)\%$	$(-2 \pm 2)\%$
Δd_{45}			$(0 \pm 2)\%$
Final R_P	0.23	0.22	0.18[a]

[a] Different Debye temperatures were adopted for surface and bulk layer atoms.

So the FSA algorithm was able to quickly locate the global R-factor minimum, after a typical number of 80 accepted structures, exploring the parameters space volume investigated in a more detailed way if compared with local search methods commonly employed.

5.3.2. CdTe(1 1 0)

In order to test the performance of the FSA when a greater number of structural parameters ought to be optimized, we have applied the algorithm to the CdTe(1 1 0) structural determination. This surface, as indicated by previous works [3,19], presents a complex reconstruction (Fig. 7). The top layer is characterized by a

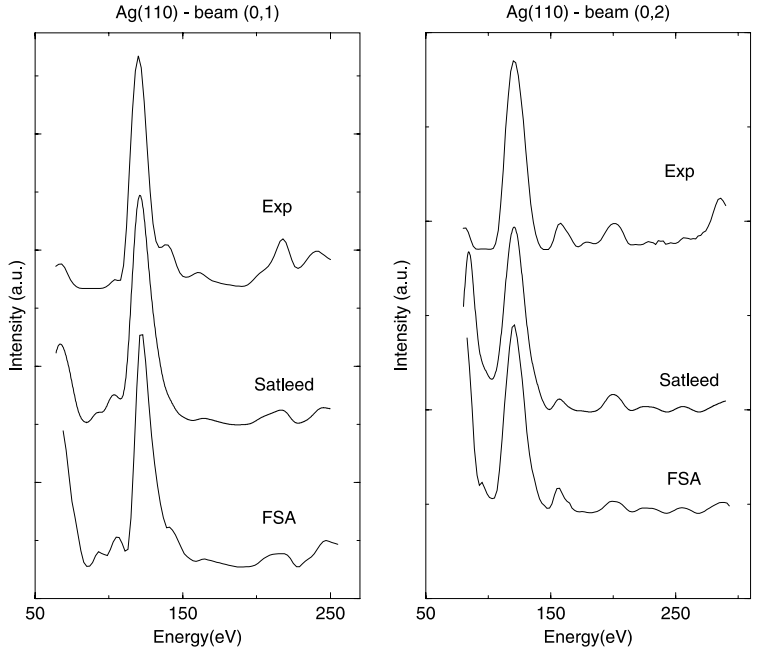

Fig. 6. Comparison between typical experimental and theoretical $I(V)$ curves obtained with the SATLEED and FSA codes for the Ag(1 1 0) system.

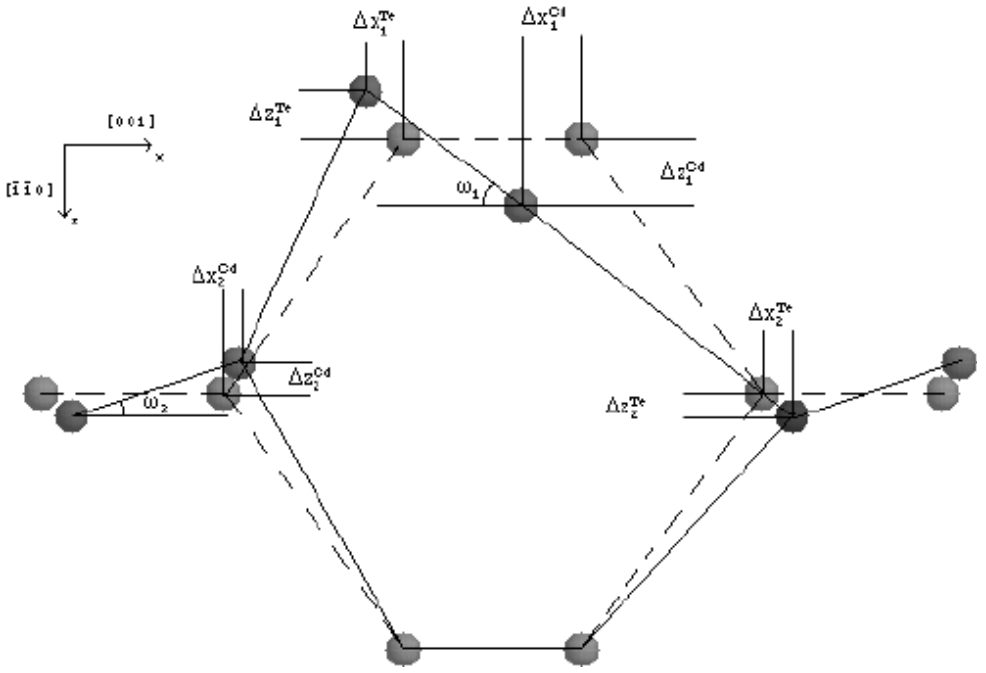

Fig. 7. Diagram showing the complex reconstruction presented by the CdTe(1 1 0) surface. The displacements of the Cd and Te atoms of the first two layers are shown, and their optimum values are presented in Table 2 [19].

bond-length-conserving rotation and a contraction towards the substrate. Because of the complexity of this reconstruction, the structure determination is quite complicated, with a large number of structural parameters to be optimized: eight parameters if the first two layers were allowed to vary.

For the CdTe(1 1 0) structural search the eight parameters associated to the first and second layer atoms were allowed to vary in a parameters space hypervolume of $(2.0 \times 2.0 \times 2.0 \times 2.0 \times 0.5 \times 0.5 \times 0.5 \times 0.5)$ Å^8, for the minimization of the Pendry R-factor. Several structural searches were then performed, following the scheme discussed in the previous section and starting from many different initial points. All searches have indicated the same final structure. But, because the number of structural parameters investigated was relatively large, and also of the fact that the theoretical $I(V)$ curves present a lower sensitivity to the structural parameters associated with the second layer, we have decided to refine the final structure obtained, performing a fast grid search. Each of the eight structural parameters were varied in a small range (0.1 Å, with constant steps of 0.01 Å, and 0.001 Å near the lowest R_P value) around their optimal values (obtained in the FSA searches). However, the final structure obtained with this refinement was basically the same one previously indicated by the FSA method.

The final results obtained (Table 2) are in good agreement with results obtained with a previous structural study, performed by our group [19] and using the LEEDFIT code [25–27] for the same experimental data set. Typical theoretical and experimental $I(V)$ curves are shown in Fig. 8.

As in the other system studied, the FSA algorithm was able to quickly locate the global R-factor minimum (after a typical number of 400 accepted structures), performing a more detailed exploration of the parameters space volume investigated if compared with local search methods.

Table 2
Structural results obtained for the CdTe(1 1 0) system. The optimum structural values obtained with the FSA method are compared with results obtained in a previous work [19] using the LEEDIT code for the same experimental set. The up and down arrows corresponds to outward and inward atomic displacements (with respect to the bulk terminated values) perpendicular to the (1 1 0) surface. A definition of the atomic displacements is presented in Fig. 7

	Previous work (LEEDFIT code) [19]	This work
First layer		
Δz_1^{Te}(Å)	$\uparrow (0.15 \pm 0.05)$	$\uparrow (0.17 \pm 0.05)$
Δz_1^{Cd}(Å)	$\downarrow (0.65 \pm 0.05)$	$\downarrow (0.62 \pm 0.05)$
Δx_1^{Te}(Å)	(-0.13 ± 0.06)	(-0.11 ± 0.06)
Δx_1^{Cd}(Å)	(-0.38 ± 0.06)	(-0.39 ± 0.06)
$\omega_1(^\circ)$	30.3	30.9
Rumple (Å)	0.80	0.79
$\Theta_{D_1}^{Te}$ (K)	(141 ± 200)	(140)
$\Theta_{D_1}^{Cd}$ (K)	(144 ± 200)	(140)
Second layer		
Δz_2^{Te}(Å)	$\downarrow (0.03 \pm 0.06)$	$\downarrow (0.02 \pm 0.06)$
Δz_2^{Cd}(Å)	$\uparrow (0.04 \pm 0.05)$	$\uparrow (0.05 \pm 0.06)$
Δx_2^{Te}(Å)	(0.06 ± 0.07)	(0.05 ± 0.07)
Δx_2^{Cd}(Å)	(0.02 ± 0.07)	(0.02 ± 0.07)
$\omega_2(^\circ)$	2.4	2.5
Rumple (Å)	0.07	0.07
$\Theta_{D_2}^{Te}$ (K)	(144 ± 250)	(140)
$\Theta_{D_2}^{Cd}$ (K)	(142 ± 250)	(140)
R_P	(0.48 ± 0.06)[a]	(0.44 ± 0.08)

[a] The Debye temperatures of the first two layers atoms were optimized.

6. Conclusions

In this work we have presented some new results obtained from the application of the FSA algorithm to the search problem in the crystallography of surfaces by LEED.

Structural determinations were performed for the Ag(1 1 0) and CdTe(1 1 0) systems employing the FSA algorithm implemented with a modified Van Hove–Tong conventional LEED code. The final structures obtained were in good agreement with previous structural studies performed for these systems. In all cases the FSA algorithm was able to quickly locate the global minimum, although exploring the parameters space volume in a more detailed way when compared with local search methods.

An investigation of the initial "temperature" influence on the FSA search process was carried

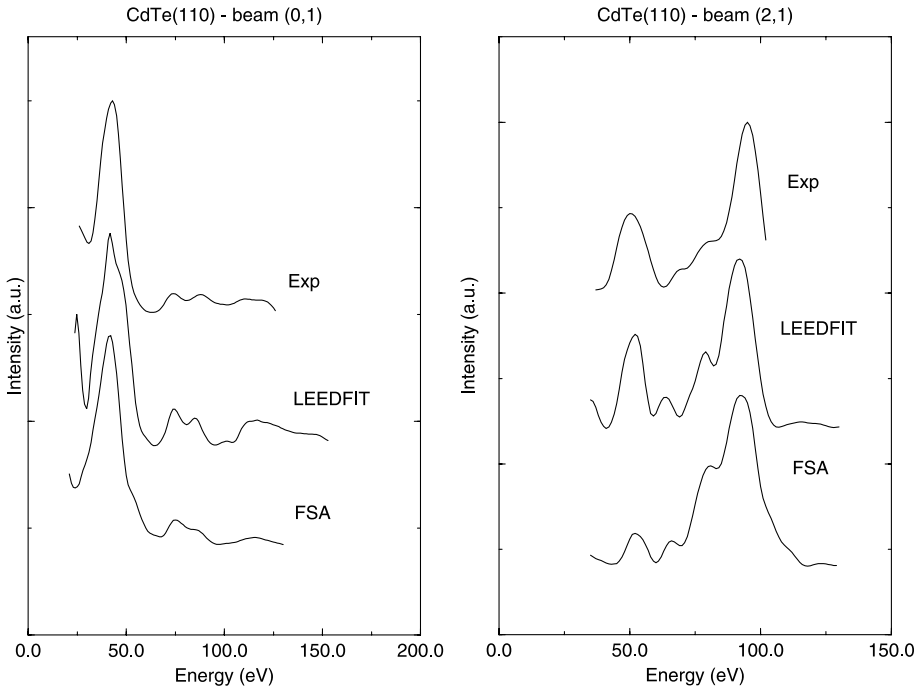

Fig. 8. Comparison between typical experimental and theoretical $I(V)$ curves obtained with the LEEDFIT and FSA codes for the CdTe(1 1 0) system.

out using data obtained from the optimization of two structural parameters of the CdTe(1 1 0) in a theory–theory comparison. The results obtained have indicated an optimum value of 10 for the initial "temperature".

The scaling behaviour presented by the FSA method was investigated, by performing structural searches for the optimization of 2, 4, 6 and 8 parameters in a theory–theory comparison for the CdTe(1 1 0) system. For the determination of the scaling relation we have used the mean number of accepted structures and the mean number of trial structures, and both results indicated an scaling with N in the range of structural parameters investigated. This result indicate a very favourable scaling behaviour (N^1), especially when compared with other local and global search methods. The FSA method is able to quickly locate the global R-factor minimum and can be easily associated with a local search method (to be applied in the final refinement of the structural parameters). Such an implementation suggests the FSA as an effective search method to be applied to the crystallography of surfaces by LEED.

Acknowledgements

The authors would like to thank FAPEMIG, CADCT and CNPq (Brazilian research agencies) for financial support. Special thanks to Prof. M.A. Van Hove for providing the Van Hove-Tong conventional and the SATLEED codes. We would like to thank A.B. Lima and F.J. Resende (UFMG) for many helpful discussions. One of us (E.A.S.) would like to thank FAPESP.

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