Interpretation of x-ray rocking-curve broadening caused by lattice relaxation around metastable point defects

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The x-ray rocking-curve broadening accompanying the transfer to and from the metastable state of $EL2$ and DX centers in GaAs and $Al_xGa_{1-x}As$ has recently been observed experimentally [Leszczynski *et al.*, Semicond. Sci. Technol. 6, B66 (1991)]. This paper gives a more quantitative analysis of the experimental results. Computer simulations of rocking curves based on the dynamical theory of x-ray diffraction for various models of the real crystal structure made it possible to evaluate the conditions in which the lattice relaxation could be observed in experiment. The general conclusion is that in all the materials examined, the inhomogeneities played a decisive role. The possible range of the inhomogeneities and the strains around $EL2$ and DX centers is discussed in relation to their microscopic models.

I. INTRODUCTION

Recently a series of papers devoted to the x-ray-diffraction observation of lattice relaxation related to metastable point defects has been published. Three kinds of defects were examined: $EL2$ in semi-insulating (SI) GaAs,[1] $EL2$-like in low temperature (LT) grown GaAs,[2–4] and DX centers in $Al_xGa_{1-x}As$ doped with Te,[2,5] and with Si and Sn.[6,7] For low concentrations of defects (10^{16}–10^{18} cm^{-3} range) the transfer to and from metastable states was accompanied by a few arc sec change either of the peak half-width (SI GaAs and $Al_xGa_{1-x}As$:Te) or of the peak angular position ($Al_xGa_{1-x}As$:Si,Sn). For a high concentration (about 10^{20} cm^{-3}) of $EL2$-like defects, the transfer of these defects into a metastable state resulted in a dramatic broadening and peak shift into higher Bragg angles by tens of arc sec.

The microscopic models of both $EL2$ and DX defects predict a shift of defect atoms in the (111) direction.[8–13] In the case of $EL2$ it is a shift of the antisite arsenic atom ($EL2=As_{Ge}$ model[10,11]) or interstitial atom from second neighbor to a closer position ($EL2$ is the $As_{Ga}+X_i$ model, X_i an interstitial atom, presumably arsenic[12,13]). For DX centers it is a shift of a dopant atom (when the donor is from the IV group) or Ga/Al atom (when the donor is from the VI group).[8,9]

However, the significant difference between these two defects is that DX centers are supposed to transfer into metastable configurations after capturing two electrons[9] from the conduction band, whereas for $EL2$ defects the charge transfer is internal, without a pronounced change of the free-electron concentration. Therefore it is instructive to compare these two kinds of defects, as this can help in separating two factors influencing the lattice state: the lattice relaxation around the defects and the free charge concentration.

The aim of this paper is to give a more quantitative analysis of already published experimental results. In Sec. II simulations of the rocking curves for various models of crystal real structure will be presented. The simulations were based on the dynamical theory of x-ray diffraction for distorted crystals,[14–16] and also took its statistical approach.[17,18] The results give a basis for a discussion in Secs. III–V about possible explanations for the experimental results as well as possible strains caused by the point defects considered before and after transfer to the metastable states.

II. DIFFRACTION PEAK BROADENING

The peak broadening can be caused by (a) lattice spacing gradients, (b) destruction of wave coherence, (c) diffuse scattering, and (d) misorientation of lattice planes. The simulations of diffraction peaks were performed in order to obtain information about how these factors can influence the shape of diffraction peaks.

The calculations were done within the Takagi-Taupin approximation,[14,15] which can be solved analytically if a lamella model of a crystal is assumed.[16] Figure 1 shows a hypothetical crystal division into lamellas of thickness τ_0. Each lamella has a lattice constant

$$a_i = a + p\langle \Delta a \rangle , \tag{1}$$

where p is the probability function, for which

$$\langle p \rangle = 0 ,$$
$$\int |p(x)| dx = 1 .$$

The choice of p function turned out to be insignificant (only the orders of magnitude were of interest), but usually a Gaussian shape function was used.

Calculations were done so that dynamical diffraction theory equations were solved in a well-established manner,[16] starting with zero intensity deep in the substrate, then through subsequent lamellas [of lattice con-

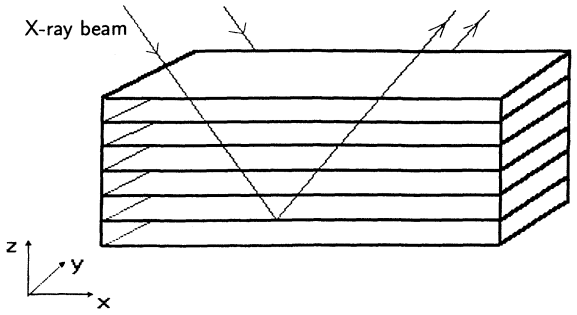

FIG. 1. Crystal division into lamellas in which the crystallographic parameters (see text) are constant.

stant as in Eq. (1)] until the surface was reached and the reflected intensity calculated. This corresponded to "adding waves." The procedure was repeated many times until no further change of the peak half-width was observed. This was "adding intensities."

The calculations were done for symmetrical (004) Cu $K\alpha 1$ and (008)Cu $K\beta$ reflections, taking into account the convolution with the first crystal of the monochromator in nondispersive double-crystal arrangements.

However, as the lateral coherence of the x-ray photon in the y direction is of the order 0.1 μm,[19] in that direction blocks of larger dimensions diffract independently, so the intensities, not waves, are added. In x-z directions the extinction length will govern the wave coherence. For the reflections considered [(004)Cu $K\alpha 1$ and (008)Cu $K\beta$], the extinction length is about 0.7 and 1.4 μm, respectively. Below these dimensions waves should be added [Eq. (1)], and above them intensities. It is important to note that the x-ray beam size in the experiment was about 0.5×0.5 mm^2.

A. Lattice spacing gradients

The results of numerical calculations for different lattice spacing gradients are illustrated in Fig. 2 and the first part of Table I. The curves in Fig. 2 correspond to the situation when the lamellas have the same average lattice constant and the same variation of it, but different thicknesses.

The values given in Table I are averaged over different spatial distributions (different p functions) of lattice constant gradients. Therefore these values shall be treated as the magnitude of broadening, which can vary for different setups of the lamellas, by not more than about 25%.

The values of peak broadening are given as a function of $\langle \Delta^2 a \rangle$, as there is a rough correspondence between this value and peak broadening and shift.

The following conclusions can be drawn.

(i) The broadening of the peak is significant when the grain size is higher than about 0.1 μm for (004) reflection, and 0.05 μm for (008) reflection.

(ii) Below a dimension of about 0.05 μm the internal strains practically influence only the peak height, and in the case of high Bragg angle reflection (008)Cu $K\beta$, there may also be a peak shift for rather large strains (as already reported[20]).

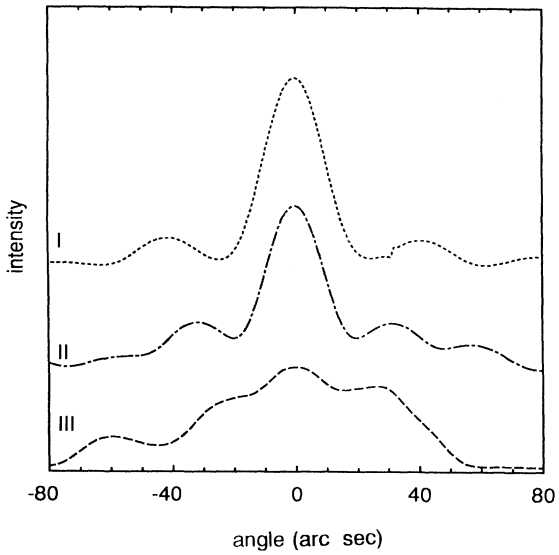

FIG. 2. Theoretical (004)Cu $K\alpha 1$ rocking curves from the GaAs crystal whose lattice parameter varies from 5.6530 to 5.6536 Å. These gradients appeared at the distances (I) 0.25, (II) 0.33, and (III) 0.50 μm. The Pendellosung fringes arise from a lamella model.

(iii) Above dimensions of about 1 μm (0.1 μm in the y direction), when intensities are added, the broadening of peaks can be easily derived from Bragg's law:

$$\Delta\omega(\text{arc sec}) = \Delta a\ (\text{Å})/0.000\,05 \quad \text{for (004)Cu } K\alpha 1 \text{ reflection}, \tag{2}$$

$$\Delta\omega(\text{arc sec}) = \Delta a\ (\text{Å})/0.000\,005 \quad \text{for (008)Cu } K\beta \text{ reflection}. \tag{3}$$

B. Destruction of wave coherence

Calculations were performed in the same manner as described above, but this time the perfect crystal lamellas were spaced with nondiffracting spacers (for example, dislocations) of average thickness $\langle t_s \rangle$, and a thickness variation of about 10%.

The coherence of waves in the crystal is disturbed by the presence of these nondiffracting boundaries, if their thickness exceeds the dimension of a unit cell by about 0.5 Å for (004) reflection, or 0.2 Å for (008) reflection, and if the boundaries separate grains thinner than about 1 μm. If the boundaries grow thicker than the unit cell dimension by 2 [(004) reflection] or 0.5 Å [(008) reflection], coherence is lost completely and the peak width is equal [even higher for (008) reflection] to the one corresponding to the single-layer thickness between the boundaries.

Calculation results are visualized in Fig. 3, and the second part of Table I. These results indicate that for

point defect concentrations lower than about 10^{18} cm^{-3}, this mechanism of peak broadening is rather improbable (even if all defects are present in these boundaries).

C. Diffuse scattering

The third part of Table I shows the influence of diffuse scattering, when the lattice parameter is constant, and the crystal is characterized by only two statistical parameters:[17] the Debye-Waller factor E and correlation length τ_0.

As can be seen, diffuse scattering can significantly modify the peak shape (excluding the tails, which have not been examined in the experiments) if the correlation length is bigger than about 0.5 μm, and the static Debye-Waller factor is much less than unity (not the case for the

TABLE I. The peak shift $\Delta\omega$ and broadening at half maximum $\Delta\sigma$ as a function of lamella thickness (correlation length) τ_0, lattice constant variation Δa, and Debye-Waller factor E. It is assumed that the crystal consists of a number of such identical lamellas and has a thickness much larger than the extinction length. In the first column is given the average thickness $\langle t_s \rangle$ of nondiffracting spacers between lamellas of the same thickness as in the fourth column.

$\langle t_s \rangle$ (Å)	$\langle \Delta^2 a \rangle$ 10^{-8} Å^2	E	τ_0 (Å)	$\Delta\omega$ (sec) (004)	$\Delta\omega$ (sec) (008)	$\Delta\sigma$ (sec) (004)	$\Delta\sigma$ (sec) (008)	Remarks
0	0	1	any	0	0	0	0	Perfect crystal
0	2500	1	100	0	15	0	0	various gradients
0	5000	1	100	0	30	0	3	of lattice constant
0	10000	1	100	0	80	0	10	in direction perpendicular to
0	500	1	500	0	0	0	0	the surface
0	1000	1	500	0	5	0	2	
0	5000	1	500	0	30	0	10	
0	10	1	1000	0	0	0	10	
0	25	1	1000	0	0	2	100	
0	100	1	1000	0	0	20	220	
0	500	1	1000	0	0	40	400	
0	10	1	2000	0	0	2	80	
0	25	1	2000	0	0	10	230	
0	100	1	2000	0	0	25	300	
0	500	1	2000	0	0	50	500	
0	1	1	5000	0	0	0	1	
0	10	1	5000	0	0	10	180	
0	25	1	5000	0	0	20	320	
0	100	1	5000	0	0	45	400	
0	1	1	10000	0	0	3	10	
0	10	1	10000	0	0	10	220	
0	25	1	10000	0	0	22	400	
5.9	0	1	2500	0	0	1	200	different
6.2	0	1	2500	0	0	30	400	nondiffracting
7.5	0	1	2500	0	0	50	600	spacers
5.9	0	1	5000	0	0	1	200	
6.2	0	1	5000	0	0	20	150	
7.5	0	1	5000	0	0	30	50	
5.9	0	1	10000	0	0	1	150	
6.2	0	1	10000	0	0	6	50	
7.5	0	1	10000	0	0	10	10	
0	0	0.9	1000	0	0	0	0	influence of
0	0	0.9	5000	0	0	2	2	diffuse scattering
0	0	0.9	10000	0	0	5	10	
0	0	0.6	5000	0	0	4	7	
0	0	0.6	10000	0	0	12	22	

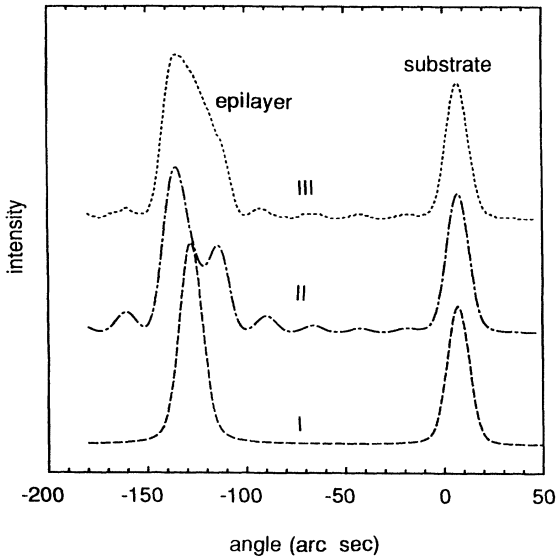

FIG. 3. Theoretical (004)Cu $K\alpha 1$ rocking curves of GaAs epilayers of perpendicular lattice constant 5.6590 Å (peaks on the left) on GaAs substrate ($a=5.6533$ Å). The epilayer contained nondiffracting spacers at 1-μm distance and average thickness (I) 5.9, (II) 6.2, and (III) 7.5 Å.

high-quality semiconductors which were used in the experiments).

Examples of the influence of diffuse scattering on the peak shape can be seen in Fig. 4 and the third part of Table I. More information about the influence of diffuse scattering on the peak shape can be found in Refs. 18 and 21.

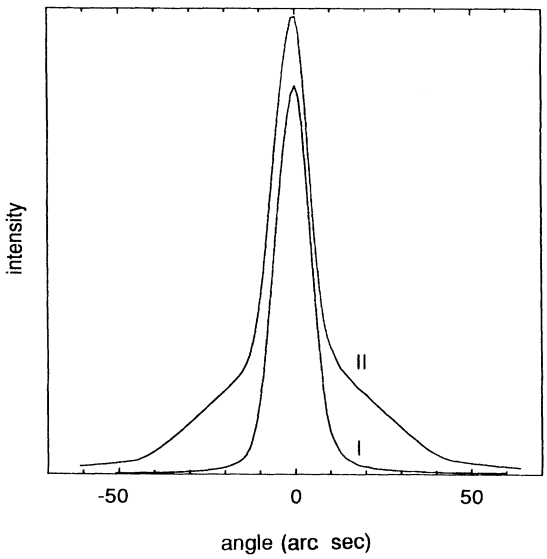

FIG. 4. Theoretical (004)Cu $K\alpha 1$ double crystal rocking curves: (I) perfect GaAs crystal; (II) GaAs crystal with the correlation length $\tau_0=0.6$ μm and static Debye-Waller factor $E=0.9$. Peak I was shifted by 2 arc sec to visualize the difference in halfwidth of the peaks.

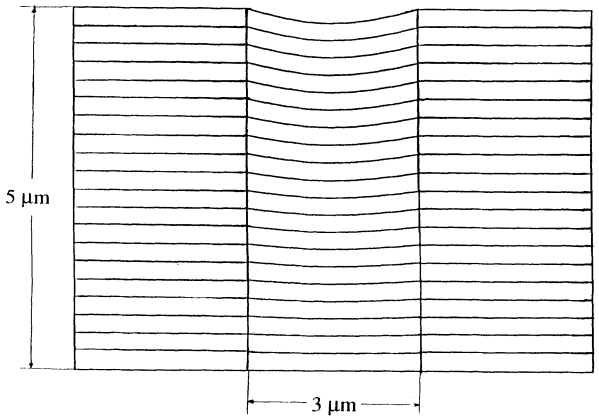

FIG. 5. Illustration of lattice plane bending when two blocks have a slightly larger lattice constant than the block in the middle.

D. Misorientation of lattice planes

The real crystal consists of grains which can be disoriented in space. This can be considered a factor similar to the lattice constant change [Eqs. (2) and (3)].

If the misorientations (in the angular seconds range) are within grains smaller than about 0.05 μm, there will be no broadening of the peak. For dimensions larger than about 0.5 μm the broadening will be approximately equal to the grain misorientation.

In Fig. 5 we show an example of how the dilation of one grain can cause lattice plane bending in adjacent grains. Such a dilation (or contraction) can be caused by an inhomogeneous change of lattice spacings in the crystal. It is of importance to note that even very small (but inhomogeneous) changes of the lattice constant can produce a significant misorientation of lattice planes. In the example shown in Fig. 5 the change of lattice constant by 2×10^{-6} Å [not observed for the (004) reflection] makes a 0.1-Å change of 5-μm size of two blocks with respect to the one in the middle. This causes a plane misorientation of 2–4 arc sec within a distance 0.1–1 μm, which results in observable peak broadening.

This estimation was obtained by applying a formula for bending of a plane, which is fixed at the ends and subjected to a constant, perpendicular force:[22]

$$\Delta z = A(L^3-2Lx^2+x^3)\ ,$$

where A is the coefficient dependent on the force, and L is the block length. Coefficient A was obtained by assuming that the lattice constant in the middle block is unaffected in its position by the presence of two neighboring blocks of different lattice constant. This assumption is justified, as the length of 3 μm is much larger than the deformation.

III. SMALL BROADENING OF PEAKS FOR SI GaAs AND $Al_xGa_{1-x}As$:Te

In these samples the experimental results were as follows:[1,5]

(i) Cooling the samples in the dark down to 77 K resulted in 3–5 arc sec broadening of (004)Cu $K\alpha 1$ peaks. It was understood for $Al_xGa_{1-x}As$:Te to be caused by the transfer of *DX* centers into a metastable configuration (two electrons were captured and a Ga/Al atom shifted from substitutional to interstitial position). It was not understood for SI GaAs.

(ii) Illumination with white light caused the peak to recover (narrowing to the room-temperature shape). For *DX* centers this situation meant two electrons were released and returned to the stable configuration (the Ga/Al atom moved back to its substitutional position). For SI GaAs it corresponded to the transfer of *EL*2 into a metastable configuration (a shift of the As_{Ga} atom into interstitial position, or of the X_i atom into first-neighbor position).

The concentration of defects was about 2×10^{16} cm^{-3} for SI GaAs, and 2×10^{17} cm^{-3} for $Al_xGa_{1-x}As$:Te, which corresponds to an average distance between them of 400–200 Å. In Sec. II it was shown that for such distances internal deformations (until the distance between lattice planes does not change more than about 0.5 Å) should not cause any (004) peak broadening. Therefore experimental results can be understood only if a large spatial nonuniformity of the samples is assumed (as it was suggested in Ref. 7).

In SI GaAs the natural grains are those of cellular structure. As indicated in, e.g., Ref. 23, the differences in *EL*2 concentration at places separated by distances of some microns can range from 0.5 to 2×10^{16} cm^{-3}. In that case we would expect that transfer into the metastable state would result in a slightly different lattice constant and possibly different orientation of the grains.

The samples of $Al_xGa_{1-x}As$:Te were grown by the LPE (liquid-phase epitaxy) method, which is quite likely to produce large inhomogeneities of the dopant concentration. However, this is difficult to measure, as a resolution of better than 1 μm would be necessary.

The broadening and narrowing of (004) reflection peaks by 3–5 arc sec means an apparent difference in the lattice constant $\Delta a/a=2\times10^{-5}$ and/or the grain misorientation by 3–5 arc sec.

For a considered defect concentration, if we assume that the transfer of a single defect to the metastable state produces a volume change $\Delta V/V$, the change of lattice constant would be about:

$$\Delta a/a=(\tfrac{1}{3})\times\Delta V/V\times10^{-6} \text{ for SI GaAs}, \quad (4)$$

$$\Delta a/a=(\tfrac{1}{3})\times\Delta V/V\times10^{-5} \text{ for } Al_xGa_{1-x}As\text{:Te}, \quad (5)$$

if the strain around the defect decreases as $1/r^2$ and Vegard's law is obeyed. Such an estimation would lead to improbably high values of $\Delta V/V$.

Therefore, only the effect of grain misorientation can be helpful in understanding the experimental results. As was shown in Fig. 5, the broadening of the peak by 3–5 arc sec can be caused by a lattice constant change of about 2×10^{-6} Å in a grain of a few μm size. This would mean that a coefficient $\Delta V/V$ can be of order 0.1 for $Al_xGa_{1-x}As$:Te and 1.0 for SI GaAs, which can be compared with 0.2–0.4 for $Al_xGa_{1-x}As$:Si,Sn as was proposed in the work of Cargill *et al.*[7]

The similar change of the peak half-width for (004) and (008) reflections is additional important evidence that these are the misorientations of grains (caused by small lattice constant gradients) such as were seen in x-ray-diffraction measurements.

The spatial nonuniformity means that there must be parts of a crystal at least 0.5–1 μm in size, with a much lower defect concentration and grains containing most of the defects. The size of the latter cannot be deduced from the experiment—if we have smaller size, the concentration of defects in the grains is higher (the lattice constant change is larger), and a similar change of the diffraction peak half-width would be obtained.

The nonuniformity of samples does not have to mean only result in the inhomogeneous distribution of defects. It can also be the cause of inhomogeneous elastic properties in crystals (e.g., in the vicinity of dislocations or other defects).

IV. LARGE BROADENING OF PEAKS FOR LT GaAs

The examinations of 190–220 °C MBE (molecular-beam epitaxy) grown GaAs on semi-insulating GaAs substrates performed at room temperature (x-ray-diffraction plus step etching) revealed a small gradient of lattice constant,[24] with the biggest mismatch at the interface. This can be seen as a tail at the left side of the peak (008)Cu $K\beta$ [curve *I* in Fig. 6 (b)]. Curves *II* and *III* of that figure show the (004)Cu $K\alpha 1$ and (008)Cu $K\beta$ peak shapes change after cooling in the dark down to 77 K, and illumination with 950-nm infrared light. The peak shift and dramatic broadening can be seen. The broadening and curve shape were slightly different for the various samples and spots examined, but on average the peak broadening was 30 arc sec for (004) reflection, and 300 arc sec for (008) reflection. The positions of the center of the broad peaks were shifted to higher angles, which can mean an average lattice constant diminution by about 0.001 Å.

The concentration of *EL*2-like defects in this material is about 10^{20} cm^{-3}, which means an average distance between defects of about 20 Å and gives

$$\Delta a/a=(\tfrac{1}{3})\times(\Delta V/V)\times5\times10^{-3}. \quad (6)$$

Also in this case, the broadening of the peaks can be attributed only to the nonuniformity of the layers.

However, this large peak broadening can be explained by a large variety of different microscopic models. The simplest are based on gradients of the lattice constants, which would be about $\Delta a=0.002$ Å at distances of 0.1–1 μm. This and the average lattice constant change would mean that value $\Delta V/V$ is about 0.2.

The gradients can be caused by a nonuniform distribution of defects (a highly probable situation) or different elastic properties. However, for that defect concentration we can also expect that inhomogeneous distribution of defects can produce deformations so large that they could destroy the wave coherence (as the distance between lattice planes can be changed more than 0.2 Å).

This, as well as possible misorientations of grains, shows the complexity of the problem of interpretation of the broad rocking curves for such a high defect concentration (with the presence of other defects).

One should also keep in mind that the small distance between defects and eight possible (111) directions can result in a smaller lattice deformation, as might be expected. Such a lattice behavior was observed[25] in $Pb_xGe_{1-x}Te$ crystals where phase transition into the rhombohedral phase [a shift of atoms in the (111) direction] was obstructed by internal strains.

V. DISCUSSION

The basic question that should first be discussed is whether the relaxation around point defects really was observed with x-ray diffraction—the method that "sees" an average lattice state.

For variously doped $Al_xGa_{1-x}As$ it seems to be well proven that it was *DX* centers which produced the lattice relaxation. No such effects were observed in samples in which the *DX* level was unoccupied, and full correspondence could be found between x-ray and electrical measurements. For these defects it was also possible (by electrical measurements) to exclude the possibility of significant influence of the x-ray beam on the state of *DX* centers during the experiment (x-ray-induced emission of electrons from *DX* centers).

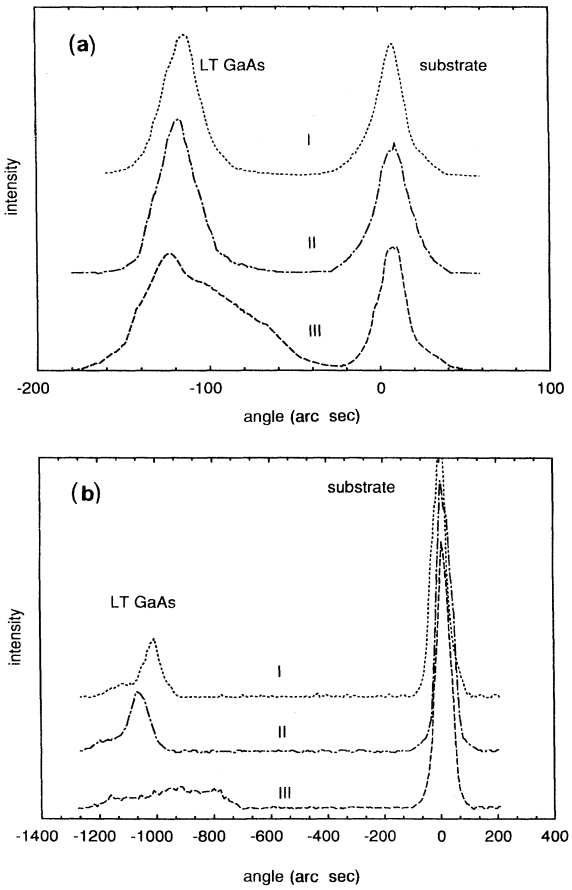

FIG. 6. The experimental rocking curves from LT GaAs. (a) (004)Cu $K\alpha 1$ reflection. (b) (008)Cu $K\beta$ reflection. (I) 295 K. (II) 77 K in dark. (III) 77 K after 950-nm illumination.

For LT GaAs the transfer into the metastable state, as observed with x-ray diffraction and with infrared light absorption,[26] occurred at almost identical conditions of temperature and illumination. The quickest transfer into the metastable state occurred for 950-nm illumination. The recovery occurred at 130–140 K or 1350-nm illumination. These results indicate strongly that this was an *EL*2-like defect transfer to the metastable configuration which was observed in the x-ray experiment.

However, for SI GaAs it is not clear what caused peak broadening when samples were cooled in the dark. The authors failed to find a better explanation (than *EL*2 metastability) for the peak narrowing after illumination at low temperature, and peak recovery after increase of the temperature to 110–120 K (characteristic for *EL*2 in SI GaAs). Also, an improbably high value for $\Delta V/V$ (at least 1) indicates that understanding of experimental data is far from satisfactory.

In the paper by Cargill *et al.*[7] the authors explain the observed lattice constant decrease in $Al_xGa_{1-x}As$:Si,Sn by the decrease of the free-electron concentration via the deformation potential,[27] and by dopant atom shift into interstitial position. As it is not possible to separate these two effects, it is interesting to compare it with the *EL*2-like case of LT GaAs, where there is no significant change in the free-electron concentration. For that defect the As atom shift from substitutional to interstitial positions results in a decrease of the lattice constant. This means that the creation of a vacancy causes more significant distortion than is caused by an interstitial dopant atom [there is empty space in the (111) direction in diamond lattice]. The quantitative analysis of experimental data leading to the verification of the deformation potential is not yet possible.

This paper has not discussed the validity of the *EL*2 and *DX* center models. But it should be noted that these models still have not been adequately verified experimentally.[28,29] Also, it is not clear if *EL*2 in SI GaAs and *EL*2-like defects in LT GaAs are the same defects, as some properties are identical, and some different.[30] However, the latter also can be caused by strains or different electrical properties.

X-ray diffraction examination of metastable defects is in its initial stage. It seems that more advanced studies are necessary. For example, it would be desirable to study the changes of peak tails, not only their position and half-width. Also, reciprocal-lattice mapping, which is possible in triple-axis diffractometry, will permit the separation of diffuse scattering, bending of crystallographic planes, and lattice spacing gradients. Such experiments are planned, but they will be extremely time consuming.

VI. CONCLUSIONS

Computer simulations of rocking curves for various microscopic models made it possible to conclude that the

broadening of peaks accompanying the transfer of point defects (of concentrations lower than 10^{18} cm^{-3}) into their metastable states can only be attributed to the spatial nonuniformity of samples.

Analysis of peak shifts and broadening for variously doped $Al_xGa_{1-x}As$ and LT GaAs samples showed that the transfer of *DX* centers into their ground state, and *EL*2 defects into their metastable state, results in a volume decrease of order $\Delta V/V=0.2$.

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