THEORETICAL DESCRIPTION OF THE INFLUENCE OF DISLOCATIONS ON THE LUMINESCENCE OF LIGHT-EMITTING DIODES

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THEORETICAL DESCRIPTION OF THE INFLUENCE OF DISLOCATIONS ON THE LUMINESCENCE OF LIGHT-EMITTING DIODES

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Résumé - Dans l'hypothèse qu'une dislocation isolée décorée par des impuretés peut être considérée comme une inhomogénéité macroscopique, on propose un modèle simple qui décrit l'influence de dislocations non corrélées sur la luminescence de diodes électroluminescentes. L'accord de ce modèle avec les données expérimentales est raisonnable.

Abstract - Under the assumption that a single dislocation decorated by impurities can be considered as a macroscopic inhomogeneity a simple model is proposed which describes the influence of uncorrelated dislocations on the luminescence of LEDs in reasonable agreement with experimental data.

1. - INTRODUCTION

Measurements of the luminescent efficiency of light-emitting diodes (LEDs) have yielded a strong dependence of the efficiency on the dislocation density (e.g. /1,2/). However, up to now the theoretical fundamentals are not yet sufficient to provide an unambiguous interpretation of such measurements.

A first promising model was proposed by Lax /3/. His model is based on following two main assumptions: (i) A single dislocation is considered as a macroscopic inhomogeneity of cylindrical shape with recombination only at the surface of the cylinder. (ii) The diode is considered as a semi-infinite semiconductor, i.e. bounded only by the p-n junction at which the injected minority carrier density is assumed to be constant. Lax described furthermore, the ratio of the total number of carriers with dislocations to that without dislocations by

$$\frac{N}{N_o} = 1 - \sigma_N \cdot \rho_d \cdot c, \qquad (1)$$

where σ_N represents a cross section for reduction of N, and ρ_d is the dislocation density. The quantity c was introduced more sophisticated to take into account the correlation of the dislocations.
c was assumed to be

$$c = \frac{N}{N_0} ,$$

which leads to

$$\frac{N}{N_0} = \left(1 + \sigma_N \cdot \rho_d \right)^{-1} . \tag{2}$$

However, equation (2) is not consistent with the assumption (i) of the model. Eq. (2) yields

$$\frac{N}{N_0} \longrightarrow 0 \qquad \text{as} \qquad \rho_d \longrightarrow \infty ,$$

but according to assumption (i) the ration $\frac{N}{N_0}$ has to vanish if

$$\rho_d \longrightarrow \rho_d^{max} = \frac{1}{A_d} , \tag{3}$$

where A_d is the area of the cross-section of the cylindrical dislocation region. Besides, in usual LEDs the distance between surface and p-n junction is about one diffusion length. Thus, it is doubtful whether the effect of the surface on the luminescence can be neglected as assumed by Lax (see above (ii)).
In addition to the model described above Lax considered a second model in which the volume of the cylindrical dislocation region provides "bulk" recombination at a higher rate than that of the surrounding medium. Unfortunately, Lax was mistaken in his treatment what can be immediately seen in his result which does not yield the solution without dislocations if the recombination inside the cylinder is equal to that outside the cylinder /3/.
Therefore, in this paper Lax's second model is treated once more, considering additionally, the influence of the surface of the sample. This model has already been used successfully for the interpretation of the EBIC (electron beam induced current) contrast /4-7/.

2. - GENERAL MOTIVATION FOR THE MODEL USED

The assumption of the model presented here, i.e. the dislocation is considered as a macroscopic inhomogeneity is the most essential one. This assumption means, that the mean free path length ℓ of the carriers has to be small compared with the radius r_d of the dislocation cylinder. For a single dislocation which is not decorated by impurities the main effect on the carriers is expected to be inside the dislocation core with a radial dimension of some 10 Å. Thus, considering a "pure" dislocation as a cylindrical region, where the recombination rate is different from that outside the cylinder, the assumption $r_d > 1$ is not satisfied (see Tab. 1). In this case the

material	$\bar{l}_e$ /µm/	$\bar{l}_h$ /µm/
GaAs	0.12	0.02
GaP	0.02	0.01

Table 1: Mean free path lengths of the minority carriers in GaAs and GaP at 300 K.

dislocation is described more appropriately as a scattering center (e.g. /8/).

However, it was found that a single dislocation is only detectable by EBIC-measurements if it is decorated by impurities /9/. Such a decorated dislocation can be regarded more appropriately as a macroscopic inhomogeneity. Further, it appears to be reasonable to assume that only dislocations decorated by impurities as a result of various heat treatments occur in LED-materials, so that the macroscopic model presented here should be sufficiently justified.

3. - INJECTED CARRIER DENSITY IN PRESENCE OF A SINGLE DISLOCATION

Let us consider a semiconductor sample with a junction parallel to the surface in a distance d and with a single dislocation perpendicular to the surface (Fig. 1). Inside a cylindrical dislocation region of space Ω_d both the radiative (τ'_{rad}) and the

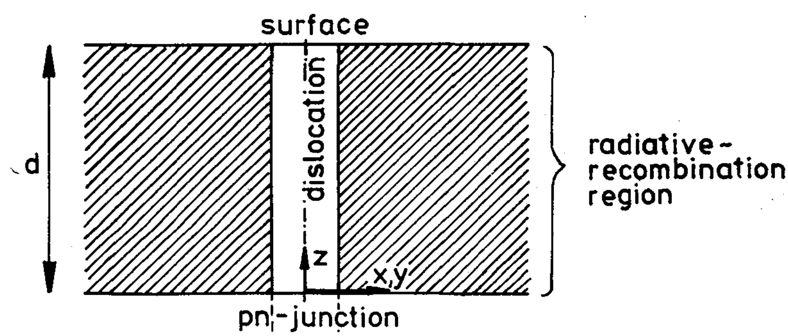

Fig. 1 - Schematic representation of the sample considered in the calculation of the luminescent efficiency

non-radiative lifetime (τ'_{nrad}) are assumed to be different from those (τ_{rad} , τ_{nrad}) outside the dislocation. At the junction the injected minority-carrier density $n(\underline{r})$ is assumed to be constant (cf. /3/). Then, for the bulk $n(\underline{r})$ obeys in steady state the following two differential equations

$$D\,\nabla^2 n(\underline{r}) = n(\underline{r}) \cdot \begin{cases} \frac{1}{\tau'} & \text{for } \underline{r} \text{ inside } \Omega_d \,, \\ \frac{1}{\tau} & \text{elsewhere} \,, \end{cases} \tag{4}$$

where

$$\frac{1}{\tau'} = \frac{1}{\tau'_{rad}} + \frac{1}{\tau'_{nrad}} \quad \text{and} \quad \frac{1}{\tau} = \frac{1}{\tau_{rad}} + \frac{1}{\tau_{nrad}} \,. \tag{5}$$

At the surface, z=d

$$-\frac{\partial n}{\partial z} = \frac{S}{L} \cdot n \,, \tag{6}$$

where $L=\sqrt{D\tau}$, and

$$S = \frac{v_s}{L/\tau} \tag{7}$$

is the surface recombination velocity v_s in units of the diffusion velocity.

At the junction, z=0

$$n = \bar{n} = \text{const.} \tag{8}$$

In the absence of the dislocation the solution of the problem is known /10/:

$$n_o(z,L) = \bar{n} \left(\frac{e^{-z/L} + \varepsilon_s \cdot e^{-(2d-z)/L}}{1 + \varepsilon_s \cdot e^{-2d/L}} \right) \tag{9}$$

with

$$\varepsilon_s = \frac{1-S}{1+S} \,.$$

Mathematically, the expression (9) is also a special solution of the general problem (eqs. (4-8)) obeying the boundary conditions and each of the two differential equations (4) separately, but it does not describe the additional radial dependence of the carrier density resulting from the coupling of the two differential equations.

Now, introducing cylinder coordinates (ρ , z) and using for the special solution (9) the integral representation /11/

$$n_o(z,L) = \frac{2\bar{n}}{\pi}\int_0^\infty \frac{\sin(\lambda z/L)}{1+\lambda^2}\left[\lambda + 2\,q(L)\cdot\sin(\lambda d/L)\right]d\lambda \tag{10}$$

with

$$q(L) = \frac{\varepsilon_s\cdot e^{-d/L}}{1+\varepsilon_s\cdot e^{-2d/L}}\ , \tag{11}$$

then for the internal solution ($\underline{r}$ inside the cylinder) one finds

$$\begin{aligned} n_i(\rho,z) = \int_0^\infty \sin(\lambda z/L)\cdot\Big\{ & I_o\left(\sqrt{\lambda^2+\tau/\tau'}\,\rho/L\right)\cdot h(\lambda) \ + \\ & + \frac{2\bar{n}/\pi}{\lambda^2+\tau/\tau'}\left[\lambda + 2\left(\frac{L}{L'}\right)\cdot q(L')\cdot\sin(\lambda d/L)\right]\Big\}\,d\lambda \end{aligned} \tag{12}$$

($L'=\sqrt{D\tau'}$) and for the external solution ($\underline{r}$ outside the cylinder)

$$\begin{aligned} n_a(\rho,z) = \int_0^\infty \sin(\lambda z/L)\cdot\Big\{ & K_o\left(\sqrt{\lambda^2+1}\,\rho/L\right)\cdot g(\lambda) \ + \\ & + \frac{2\bar{n}/\pi}{\lambda^2+1}\left[\lambda + 2\,q(L)\cdot\sin(\lambda d/L)\right]\Big\}\,d\lambda\ . \end{aligned} \tag{13}$$

Here, I_o and K_o are the modified Bessel functions of the order zero of first and second kind, respectively, and ρ denotes the radial distance from the dislocation line. The unknown coefficients **h** and **g** are obtained by the matching conditions at the surface of the cylinder. Let r_d be the radius of the cylinder it must hold

$$\begin{aligned} n_i\big|_{\rho=r_d} &= n_a\big|_{\rho=r_d}\ , \\ \frac{\partial n_i}{\partial\rho}\Big|_{\rho=r_d} &= \frac{\partial n_a}{\partial\rho}\Big|_{\rho=r_d}\ . \end{aligned} \tag{14}$$

Inserting (12) and (13) into (14) one obtains finally for the injected minority-carrier density:

$$n(\rho\le r_d,z) = n_i(\rho,z) = n_o(z,L') + \bar{n}\int_0^\infty \sin(\lambda z/L)\ \frac{I_o(\alpha_1\rho/L)}{I_1(\alpha_1 r_d/L)}\cdot\phi(\lambda)\,d\lambda\ , \tag{15a}$$

$$n(\rho>r_d,z)=n_a(\rho,z)=n_o(z,L)-\bar{n}\int_0^{\infty}\sin(\lambda\tfrac{z}{L})\left(\frac{\alpha_1}{\alpha_2}\right)\frac{K_o(\alpha_2\rho/L)}{K_1(\alpha_2 r_d/L)}\cdot\phi(\lambda)\,d\lambda, \tag{15b}$$

where

$$\phi(\lambda)=\frac{(2/\pi)\left\{(\frac{\tau}{\tau'}-1)\lambda+2\cdot\sin(\lambda d/L)\left[\alpha_1^2\cdot q(L)-\frac{L}{L'}\cdot\alpha_2^2\cdot q(L')\right]\right\}}{\alpha_1^2\cdot\alpha_2^2\left[\frac{\alpha_1\cdot K_o(\alpha_2 r_d/L)}{\alpha_2\cdot K_1(\alpha_2 r_d/L)}+\frac{I_o(\alpha_1 r_d/L)}{I_1(\alpha_1 r_d/L)}\right]} \tag{16}$$

with

$$\alpha_1=\sqrt{\lambda^2+\tau/\tau'}\qquad \text{and}\qquad \alpha_2=\sqrt{\lambda^2+1}\ .$$

4. - INFLUENCE OF UNCORRELATED DISLOCATIONS ON THE LUMINESCENCE

According to Lax /3/ the luminescent efficiency can be expressed by

$$\eta=\eta_o\frac{J}{J_o}\,\frac{I_o}{I} \tag{17}$$

where η_o is the efficiency without dislocations, J/J_o is the ratio of the current of photons with dislocations to that without dislocations, and I_o/I is the ratio of the diffusion current across the p-n junction surface without dislocations to that with dislocations. Using (15) and considering only the layer between surface and junction as radiative recombination region (Fig. 1) in presence of a single dislocation one obtains for the integrated quantities:

$$\frac{J}{J_o}=1-\sigma_N\cdot\rho_d^{(1)} \tag{18}$$

and

$$\frac{I_o}{I}=\left[1+\sigma_I\cdot\rho_d^{(1)}\right]^{-1}\quad, \tag{19}$$

where

$$\sigma_N = L^2\left\{\left[1-\beta\,\frac{L'}{L}\,\frac{(1-e^{-d/L'})(1+\varepsilon_s\cdot e^{-d/L'})\,(1+\varepsilon_s\cdot e^{-2d/L})}{(1-e^{-d/L})(1+\varepsilon_s\cdot e^{-d/L})\,(1+\varepsilon_s\, e^{-2d/L'})}\right]\times\right. \tag{20}$$

$$\times\pi\left(\frac{r_d}{L}\right)^2 + 2\pi\,\frac{r_d}{L}\,\frac{(1+\varepsilon_s\cdot e^{-2d/L})}{(1-e^{-d/L})(1+\varepsilon_s\cdot e^{-d/L})}\int_0^\infty \frac{(1-\cos(\lambda d/L))}{\lambda}\left(\frac{\alpha_1}{\alpha_2^2}-\frac{\beta}{\alpha_1}\right)\times$$

$$\left.\times\phi(\lambda)\,d\lambda\right\}$$

$$\sigma_I = L^2\left\{\left[\frac{L}{L'}\;\frac{(1-\varepsilon_s\cdot e^{-2d/L'})(1+\varepsilon_s\, e^{-2d/L})}{(1+\varepsilon_s\cdot e^{-2d/L'})(1-\varepsilon_s\, e^{-2d/L})} - 1\right]\times\pi\left(\frac{r_d}{L}\right)^2 + \right.$$

$$\left. + 2\pi\,\frac{r_d}{L}\left(\frac{\tau}{\tau'}-1\right)\left(\frac{1+\varepsilon_s\cdot e^{-2d/L}}{1-\varepsilon_s\cdot e^{-2d/L}}\right)\int_0^\infty \frac{\lambda}{\alpha_1\cdot\alpha_2^2}\,\phi(\lambda)\,d\lambda\right\} \tag{21}$$

with $\beta = \tau_{rad}/\tau'_{rad}$,

and

$$\rho_d^{(1)} = \frac{1\ \text{dislocation}}{\text{p-n junction area}} \tag{22}$$

From this it follows for the efficiency:

$$\eta = \eta_0\,\frac{1-\sigma_N\cdot\rho_d^{(1)}}{1+\sigma_I\cdot\rho_d^{(1)}}\ . \tag{23}$$

The quantity σ_N can be regarded as a cross section which describes the variation of J in presence of one dislocation, and analogously, σ_I is a cross section for the variation of the junction current in presence of one dislocation.
Now, an arbitrary number of dislocations is considered, where the distance between two neighbour dislocations should be sufficiently large, so that no correlation exists between them. In this case the efficiency can be written as

$$\eta = \eta_0\,\frac{1-\sigma_N\cdot\rho_d}{1+\sigma_I\cdot\rho_d}\ , \tag{24}$$

where

$$\rho_d = \frac{\text{no. of dislocations}}{\text{p-n junction area}} \tag{25}$$

Exactly, ρ_d describes the average dislocation density of the sample.

As a measure for the nearest distance between two uncorrelated dislocations the radial distribution

$$Q(\rho) = \int_0^d n_d(\rho, z)\, dz = Q_o - L\bar{n} \int_0^\infty \frac{[1-\cos(\lambda d/L)]}{\lambda} \frac{\alpha_1 K_o(\alpha_2 \frac{\rho}{L})}{\alpha_2 K_1(\alpha_2 r_d/L)} \times \phi(\lambda)\, d\lambda \tag{26}$$

of the injected minority carriers around a single dislocation can be analysed, where

$$Q_o = \int_0^d n_o(z, L)\, dz = L\bar{n}\, \frac{(1-e^{-d/L})(1+\varepsilon_s \cdot e^{-d/L})}{1+\varepsilon_s \cdot e^{-2d/L}} \tag{27}$$

is the constant radial distribution of the carriers in a sample without dislocations. Two dislocations are regarded to have no influence upon another if

$$\frac{Q_o - Q}{Q_o} \leqslant 0.01. \tag{28}$$

Now, the theoretical results may be applied to interpret experimental data. Roedel et al. /1/ have published a plot of electroluminescent efficiency versus dislocation density for 45 individual GaAs-LEDs (Fig. 2). In order to get a reasonable agreement of the calculated $\eta - \rho_d$-behaviour with the experimental one the both unknown quantities (r_d/L) and (τ/τ'), which characterize a single dislocation within the model, were varied within the interval $0.02 \leqslant r_d/L \leqslant 1$ and within $2 \leqslant \tau/\tau' \leqslant 10^3$, respectively. As fixed input parameters $L=L_e=10\ \mu m$, $d=10\ \mu m$ and $S = \infty$ were used, and additionally,

$$\frac{\tau_{rad}}{\tau'_{rad}} = 0,$$

i.e. the radiative recombination rate inside the dislocation region was assumed to be zero what appears to be reasonable in GaAs-material.

Only one pair of values which is consistent with the assumptions of the model was obtained, namely

$$(r_d/L) = 0.55 \text{ and } (\tau/\tau') = 100$$

to fit the experimental plot (see Fig. 2). For the cross sections the values

$$\sigma_N = 2.13\ L^2 = 213\ \mu m^2$$

and

$$\sigma_I = 8.97\ L^2 = 897\ \mu m^2$$

were calculated.

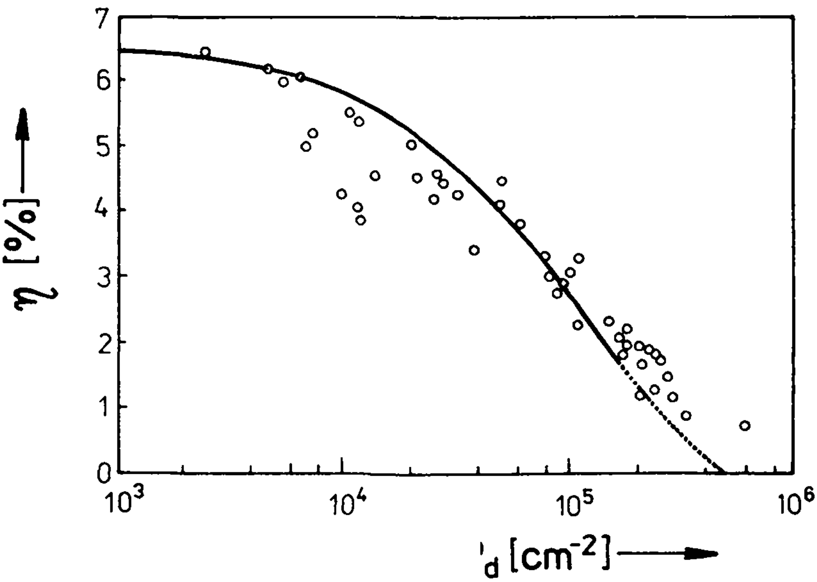

Fig. 2 - Experimental plot of the luminescent efficiency (from Roedel et al. /1/) versus dislocation density for 45 GaAs-LEDs (the circles) and theoretical values (solid line) obtained using $L = 10\ \mu m$, $d = 10\ \mu m$, $S = \infty$, $r_d/L = 0.55$, $\tau/\tau' = 100$, $(\tau_{rad}/\tau'_{rad}) = 0$. The dotted line describes the theoretical behaviour beyond the maximum density of uncorrelated dislocations ($\rho_{d,uc}^{max} = 1.6 \cdot 10^5 cm^{-2}$).

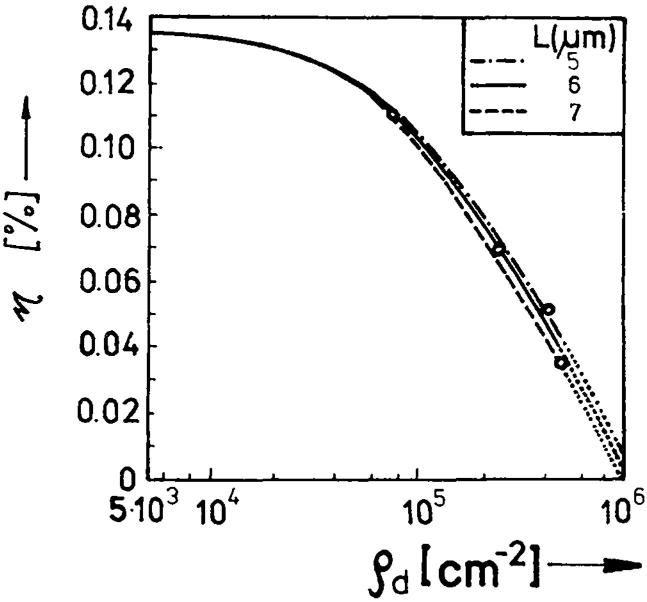

Fig. 3 - Experimental data (from Brantley et al. /2/; the circles) and theoretical values obtained using d = 6 μm, $S = \infty$, $(\tau_{rad}/\tau'_{rad}) = 0$, and $\frac{r_d}{L} = 0.7$, $\frac{\tau}{\tau'} = 35$ for L = 6 μm, $\frac{r_d}{L} = \frac{6}{5} \cdot 0.7$, $\frac{\tau}{\tau'} = \frac{25}{36} \cdot 35$ for L = 5 μm, $\frac{r_d}{L} = \frac{6}{7} \cdot 0.7$, $\frac{\tau}{\tau'} = \frac{49}{36} \cdot 35$ for L = 7 μm. The dotted lines point out the range beyond the maximum density of uncorrelated dislocations ($\rho_{d,uc}^{max} = 4.5 \cdot 10^5 cm^{-2}$). η_o was found to be 0.138%.

For GaP-LEDs

$$(r_d/L) = 0.7 \text{ and } (\tau/\tau') = 35$$

were found in the same manner as described for GaAs in order to fit the experimental data measured by Brantley et al. /2/ (the circles and the solid line in Fig. 3). Here, the following input parameters were used: L = 6 μm, d = 6 μm, $S = \infty$, $(\tau_{rad}/\tau'_{rad}) = 0$.
In /2/ the diffusion lengths are given for the 4 specimens considered in Fig. 3: L = 5 ... 6 μm for the electrons in the p-type layer. To examine the dependence of the η-ρ_d -behaviour on the diffusion length $\eta(\rho_d)$ was calculated for L = 5 μm (dot-dash line in Fig. 3) as well as for L = 7 μm (dashed line in Fig. 3) in addition to the case of L = 6 μm. One sees a relatively weak dependence of the $\eta(\rho_d)$ -behaviour on the diffusion length. For the cross sections σ_N and σ_I the calculated values are given in Tab. 2.

Table 2: Cross sections in GaP

L /µm/	σ_N/L^2	σ_I/L^2
5	3.34	8.18
6	2.40	6.49
7	1.80	5.22

To be able to give the range of validity for the calculated $\eta(\rho_d)$-curves shown in Figs. 2,3 the maximum density of uncorrelated dislocations must be determined. For this reason the normalized radial distribution (Q/Q_0) of the injected minority carriers around a single dislocation was calculated both for GaAs and GaP (Fig. 4). As input parameters the values given above were used. Using the criterion (28) for the nearest distance a_d between two uncorrelated dislocations the values

$$a_d = \begin{cases} 27\ \mu m & \text{for GaAs,} \\ 16\ \mu m & \text{for GaP} \end{cases} \qquad (29)$$

were obtained. Now, the dislocations are

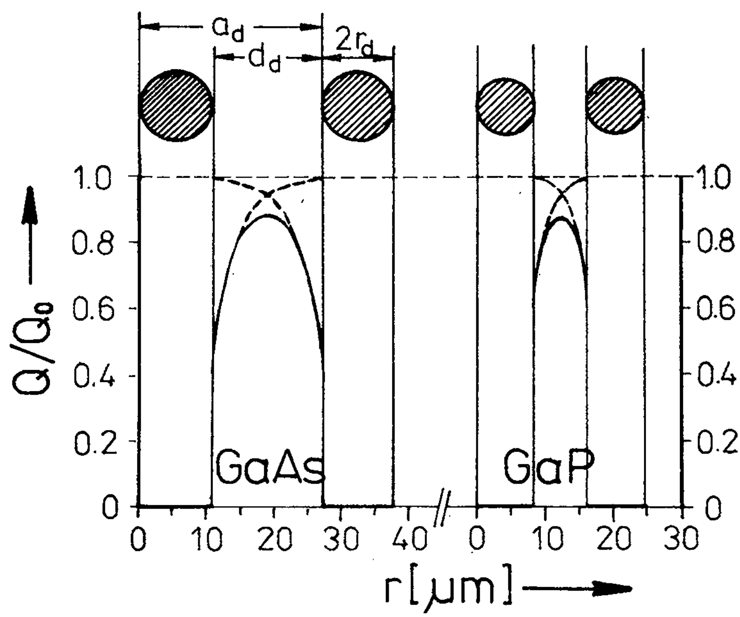

Fig. 4 - Determination of the nearest distance of two uncorrelated dislocations with the help of criterion (28) for GaAs and GaP. The dashed lines show the Q/Q_0 -behaviour arising from a single dislocation, the solid line represents the superposition of the contributions from two neighbour dislocations.

equidistantly distributed in the sample. In this way one gets a hexagonal lattice (Fig. 5) and, consequently,

$$\rho_{d,uc}^{max} = (2/\sqrt{3})\, a_d^{-2}$$

for the maximum density of uncorrelated dislocations. This gives

$$\rho_{d,uc}^{max} = \begin{cases} 1.6\times 10^5 \text{ cm}^{-2} \text{ for GaAs,} \\ 4.5\times 10^5 \text{ cm}^{-2} \text{ for GaP} \end{cases}$$

(cf. Figs. 2 and 3).

With the help of the model presented here the absolutely maximum dislocation density for which the luminescence should entirely extinguish can be given too (see eq. (3)):

$$\rho_{d,max} = \frac{1}{\pi r_d^2} = \begin{cases} 1.1\times 10^6 \text{ cm}^{-2} \text{ for GaAs,} \\ 1.8\times 10^6 \text{ cm}^{-2} \text{ for GaP.} \end{cases}$$

In comparison with the experimental plots shown in Figs. 2 and 3 these $\rho_{d,max}$ -values appear to be reasonable.

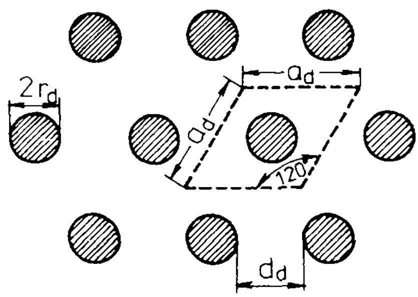

Fig. 5 - Arrangement of uncorrelated dislocations at maximum density, where a_d denotes the nearest neighbour distance. For GaP and GaAs the a_d-values are given by (29).

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