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ANALYSIS OF SHAPES OF RHEED INTENSITY OSCILLATIONS OBSERVED FOR GROWING FILMS *

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A new method of analysing shapes of RHEED intensity oscillations observed during epitaxial growth of ultrathin films is presented. The intensity of the specular electron beam is computed by solving the one-dimensional Schrödinger equation. The method can be used for interpreting data collected at very low glancing angle ($< 1°$) of the incident electron beam. In the paper we show numerically determined shapes of the intensity oscillations for different cases of settling of atoms at surfaces of growing films.

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The phenomenon of RHEED oscillations was first observed in the early eighties [1]. Since that time RHEED has been established as a very helpful technique for preparing ultrathin films and investigating their structural arrangements. Some authors proposed qualitative explanations of the origin of the RHEED intensity oscillations [2–5]. However, so far, only one quantitative approach was introduced. This approach proposed by Cohen and coworkers [6] is based on the kinematical theory of diffraction and is expected to work properly when so-called off-Bragg condition is fulfilled by the value of the glancing angle of incident electron beam. In this paper we propose another quantitative approach. We suggest to solve the one-dimensional Schrödinger equation to describe the changes of the intensity of the specular electron beam. Appriopriately adopted numerical methods of three-dimensional RHEED dynamical theories [7–13] can be applied to solve the above-mentioned equation. The idea of the use the one-dimensional wave equation for the RHEED case is well-known in literature [5, 14–15]. However, this concept leads to a conclusion that the specular beam intensity does not depend on the

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azimuth of the incident beam direction. Many experimental results do not confirm this conclusion (for example [16]). Because of these facts pointing out conditions determining when the proposed description of diffraction processes can be applied should be considered as the significant part of the proposed approach. Below we present such conditions.

(1) In few cases experimental results weakly depend on the azimuth of the incident beam direction [17]. Using the one-dimensional equation may be suggested for such cases.

(2) When the "random" azimuth of the incident beam direction is chosen then in some cases cancellations of diffraction effects connected with lateral distributions of atoms may occur as it has been shown by A. Ichimiya [15].

(3) It was find by us [18] that for low glancing angles of the primary electron beam ($< 0.5^{\circ}$ for electrons of the energy of 20 keV) results of three-dimensional dynamical theory calculations can be well approximated by results obtained on the basis of one-dimensional dynamical theory calculations.

The last condition we consider the most important and theoretically satisfactory one. However, we foresee that in practical applications of the approach some combination of all conditions might turn out to be neccesary.

Below we demonstrate the use of our approach for simulations of the shapes of RHEED oscillations. It should be stressed that we show preliminary results of our research.

The description of settling of atoms at growing film surfaces was obtained by solving [19] the set of non-linear differential equations developed for the distributed model of growth [20]:

$$\frac{d\Theta_n}{dt} = \frac{1}{\tau}(\Theta_{n-1} - \Theta_n) + \frac{\alpha_n}{\tau}(\Theta_n - \Theta_{n+1}) - \frac{\alpha_{n-1}}{\tau}(\Theta_{n-1} - \Theta_n),$$

$$\alpha_n = A\frac{d_n(\Theta_n)}{d_n(\Theta_n) + d_{n+1}(\Theta_{n+1})}, \qquad d_n(\Theta_n) = \Theta_n(1 - \Theta_n)^{1/2}. \tag{1}$$

In these equations Θ_n is the coverage of the n-th surface monolayer, τ is the time of deposition one monolayer and A is the parameter that determines the coverage profile of the growing film surface. Figure 1 shows our results of calculations assuming the growth of ZnSe films.

The shapes of the oscillations obtained by us are noticeably different than those [20] obtained on the basis of the approach of Cohen and coworkers [6]. However, fulfilling different conditions on the value of the glancing angle of the primary electron beam is required for two considered approaches (for example: the kinematical approach is expected to be successful for the angle values greater than 2° [6], on the other hand we applied the one-dimensional dynamical approach for the value of 0.25°). This means that our results cannot be treated as opposite ones to the results of Cohen et al. [20].

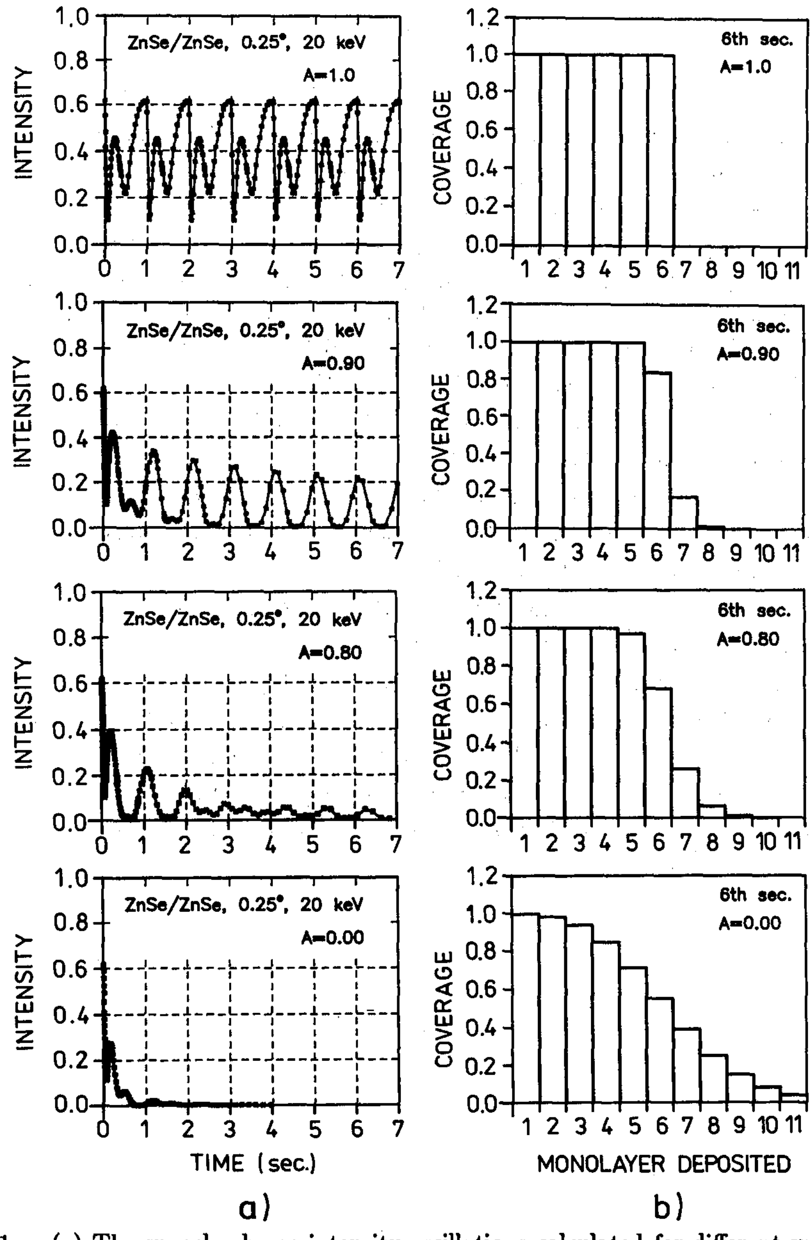

Fig. 1. (a) The specular beam intensity oscillations calculated for different values of the parameter A of the distributed growth model. (b) The coverage profiles for the surfaces at the chosen moment of time for the cases of growth shown in part (a). The following experimental situation was assumed for carrying out calculations: ZnSe(001) films deposited on Znse(001) substrates with the rate of one monolayer per one second, the electron energy equal to 20 keV and the glancing angle of the primary electron beam equal to 0.25°. It was assumed that one monolayer of ZnSe(001) consisted of one atomic Zn sublayer and one atomic Se sublayer.

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