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MONTE CARLO SIMULATIONS OF SPATIAL CORRELATIONS OF CHARGED CENTERS IN δ-DOPED LAYERS*

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Results of Monte Carlo simulations of a 2D system of charged donors are presented. They enable to study the effects related to a spatial correlation of donor charges located on a random donor matrix. A qualitative difference between DX^+ and DX^- models is observed. In the first case, strong temperature dependence of the correlations and a "freezing-like" behaviour is found. The origin of the freezing is traced to the random distribution of donor sites by comparing the system with a liquid-like model where the charges may assume arbitrary positions within a plane. In the second case only nearest-neighbour correlations are observed. The simulations have direct application in analysis of the behaviour of the DX centers in the GaAs planarly doped with Si.

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1. Motivation

Physics of δ-doped structures attracts a considerable amount of attention [1–5]. In such structures dopant atoms are localized within a narrow slab of a host material. Electrons from the ionized dopant atoms are spatially confined by the electrostatic potential of the charged centers and form a two-dimensional (2D) electron layer. At present most of the theoretical models describing the energy structure of such a system [3–5] neglect the discrete nature of the donor charges which bind electrons, and assume, instead, a continuous 2D uniform charge density. This, in turn, causes a neglect of possible correlation effects between the charges located on donors. The correlations significantly affect the properties of the 2D electron layer and should be taken into account.

In this work, a behaviour of a two-dimensional system of charges interacting via a screened Coulomb interaction is analyzed. The charges are assumed to occupy a fraction of a number of fixed donor sites distributed randomly in a plane. Two

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physical situations are considered: a) the donors may be either positively charged (when ionized) or neutral (with an electron on the center); b) the donors are either positively or negatively charged (with two electrons localized on the center). This corresponds to two competing models of the deep donor (DX) center in GaAs: the DX^+ ($U > 0$) model and the DX^- ($U < 0$) model, with U denoting the on-center electron correlation energy [6].

2. Method of calculation

We performed Monte Carlo (MC) simulations for both DX^+ and DX^- models, for various values of the ratio N_+/N_D, where N_+ is the density of positive centers and N_D is the total density of dopant atoms. The simulations used standard MC techniques [7, 8]. Similar simulations have been previously performed in the case of 3D doped semiconductors [9–12]. In this study we put emphasis on the pair correlation functions and the density of states (DOS) of charged and neutral sites, which reflects the local fluctuations of the electrostatic potential. Other results are presented elsewhere [13]. The results are given for a sample with planar doping concentration $N_D = 1 \times 10^{13}$ cm^{-2} , which is typical of Si δ-doped layers in GaAs.

3. Results

In the DX^+ model, the general shape of the pair correlation functions $g_{++}(R)$ shows a depletion at small distances resulting from repulsion between the charges. Beyond this region, the correlation functions show strong dependence on the N_+/N_D ratio. For high N_+/N_D, $g_{++}(R)$, at all studied temperatures, only these short-range correlations are observed. The same situation exists for $N_+/N_D < 0.5$ at high temperatures. There, however, at low temperatures a longer range structure appears in $g_{++}(R)$. For decreasing temperature one can observe an increase in correlations, illustrated by, e.g., the amplitude of the first neighbour peak in $g_{++}(R)$. This increase stops below a certain threshold temperature, which increases with increasing N_+/N_D. The same behaviour may be observed in the density of states of the occupied centers, which describes the local fluctuations of the electrostatic potential. This density, roughly Gaussian in shape, at first narrows with decreasing temperature, but remains constant below the threshold.

To clarify the origin of the above "freezing" effects we performed Monte Carlo studies for a system with the same density of charges and interactions, but allowing the charges to assume arbitrary positions. In this liquid-like system the structures in the pair correlation function continued to increase without any threshold temperature, whereas the width of the energy distribution decreased. The comparison of the second moment of the energy distribution, σ^2, vs. temperature for various values of N_+/N_D in the random impurity model and the corresponding "liquid" counterparts is shown in Fig. 1. The differences between the temperature behaviour of the random impurity and liquid-like models clearly point out that the "freezing" originates in the *random* distribution of donors at fixed positions, which we will call "positional disorder". A simple empirical formula has been fitted to the $\sigma^2(T)$ for the random impurity model (see Fig. 1, solid

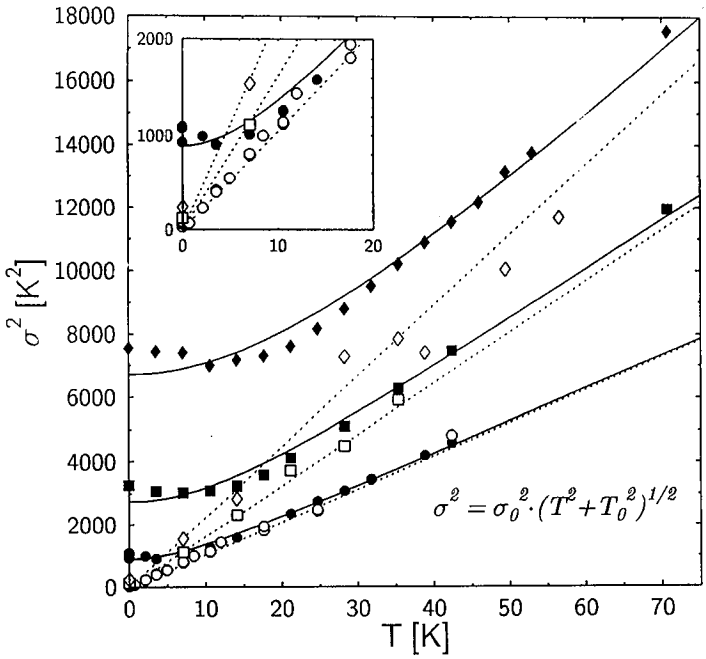

Fig. 1. Second moment of the energy distribution of the charged sites σ^2 for the DX^+ model as a function of temperature. Full symbols: impurity model, open symbols: liquid-like equivalent systems. Diamonds: $N_+/N_D = 0.4$, squares: $N_+/N_D = 0.3$, circles: $N_+/N_D = 0.2$. For decreasing temperature σ^2 for the liquid-like model tends to zero, whereas for the model with random distribution of impurities saturates at values depending on N_+/N_D. Solid lines are best fits of an empirical formula $\sigma^2 = \sigma_0^2\sqrt{T^2 + T_0^2}$ for each value of N_+/N_D. Dotted lines are calculated with the same σ_0 but with T_0 set to zero.

lines). The dotted lines are calculated by simply putting $T_0 = 0$, without changing the σ_0 value, and reproduce the results for the liquid model fairly well. The symmetric form of the empirical formula reflects the interplay between thermal and positional disorder and allows to treat T_0 as a thermal measure of the positional disorder.

We turn now to the DX^- model. There is much weaker temperature dependence of pair correlation functions and lack of any significant long-range correlations for all values of the N_+/N_D ratio. This is due to the nature of the correlations in the DX^- model: the most important effect is grouping of + and − charges in closest pairs of sites. Such process then significantly lowers the electrostatic energy of the system. Moreover, such +− pairs act as electric dipoles, interacting only weakly with other charges, which diminishes the importance of long-range correlations. At the same time large values of electrostatic energies within the pairs reduce the importance of the temperature [13].

4. Conclusions

The results of Monte Carlo simulations of spatial correlation of charges on donors in δ-doped layers presented in this work yield useful physical characteristics of the system: pair correlation functions, DOS etc. We show here that the effects of correlations can be quite substantial. A qualitative difference between the DX^+ and DX^- models is found. In the first case, for low values of the N_+/N_D ratio, correlations at low temperatures extend beyond the nearest neighbours, whereas in the latter case in all cases only the nearest neighbour correlations are observed. The DX^- model shows little or no temperature dependence, while in the DX^+ model an "freezing" behaviour is found: The long-range correlations increase with decreasing temperature. However, below a certain threshold temperature, the correlations become practically temperature independent, which reflects the inability of the system to develop true long-range order.

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