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Atomistic Analysis of the Vacancy Diffusion Mechanism

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There is still a large amount of disagreement concerning the basic diffusion mechanisms in silicon. Especially, there has been a long standing controversy about the macroscopic diffusion equations in case of the vacancy mechanism. If both dopant and vacancy gradients act as driving forces, the dopant flux J_d can be written in the general form

$$-\underline{J}_d = D_d \nabla C_d + T_d \nabla C_v = D_d^0 \frac{C_v}{C_{Si}} \nabla C_d + T_d^0 \frac{C_d}{C_{Si}} \nabla C_v \qquad (1)$$

where C_d, C_v, and C_{Si} denote the concentrations of dopants, vacancies, and lattice sites. D_d and T_d are the diffusion coefficient and the transport coefficient of the dopants, the superscript '0' indicates divison by the site fraction of vacancies or dopants, respectively. As long as particle concentrations are low D_d^0 and T_d^0 are constants whereas D_d and T_d depend linearly on C_v and C_d, respectively. Pair diffusion models [1] predict that the relation $\alpha=T_d^0/D_d^0$ must be +1 whereas other authors [2] claim that α= -1 and hence state that the pair diffusion models that are frequently used in process simulation are inconsistent with the vacancy mechanism. To clarify this discrepancy, we have performed calculations of D_d^0 and T_d^0 that account for the actual crystal structure of silicon. The results depend on the modification of the vacancy potential energy in the vicinity of the dopant atom. Since no accurate data for this interaction is available, we performed calculations with a number of model interaction potentials with different depth, range and shape to outline the possible range of the factor α. For the sake of simplicity, we started with a simple rectangular shape which allows for an easy parameterization according to depth and range, and already provides most of the important results. For comparison, also other potential shapes were considered. Some of the basic principles of the calculation are described in [3]. However, large improvements of the numerical and theoretical methods have been achieved since then that made it possible to examine a variety of interactions in a reasonable time and to obtain quantitative values that do not suffer from the very limited accuracy of the preliminary results of [3]. The errors of the simulation results shown here were below 1% for a given potential and therefore error bars were omitted in the graphs.

An interesting first result of the investigation was that a reduction of the actication energy of dopant diffusivity with respect to self-diffusivity (which is experimentally found to be 1 to 2 eV for the usual dopants) does not require a real binding of the vacancy to the dopant. An interaction that only reduces the height of the potential barriers in the neighborhood of the dopant was found to give similar results and therefore this kind of interaction was also included in the analysis. A schematic drawing of the two types of interaction is shown in Fig.1 for a simple rectangular (box-shaped) potential. They are of course only two extreme cases of the general situation. The simulation results for the reduction of the activation energy of D_d compared to D_{self} are shown in Fig.2 for different rectangular interaction potentials and one potential that depends linearly on the distance to the dopant atom. It can be seen that for a given potential depth this reduction is only comparable to the depth if the potential extends to at least the 3rd coordination number. This is in agreement with earlier results from the literature [4]. The calculated values for the relation $\alpha=T_d^0/D_d^0$ from the different model potentials are shown in Fig.3 as a function of potential range and in Fig.4 as a function of the potential depth for a range to the 3rd coordination number. The comparison of the results for the box-shaped and the linear potentials shows that the shape does not affect very much the qualitative behavior. However, since the results show the largest sensitivity on the potential in the vicinity of the 3rd nearest neighbor site (as can be seen from the results of the rectangular potentials), the total depth of the linear potential (measured at zero distance) must be larger to give similar quantitative values. Also other potentials (including coulomb potentials) have been investigated and confirmed these findings. As the figures show, the obtained results for α range from -2 (for tracer diffusion) to values very close to 1 if both the potential depth as well as its range lie above a certain value.

From the results shown in Fig.3 and Fig.4, the following conclusions can be drawn: The prediction α=-1 [2] may be fullfilled for very special interaction potentials but obviously this model has no general validy. On the

other hand, the prediction α=+1 from pair diffusion [1] can be considered as the limit to which the value of α converges for any potential shape if both the depth and the range of the interaction is increased. Moreover, the simulation results shown above demonstrate that for all the potential types considered here the value of α lies very close to +1 if the reduction of the activation energy of D_d with respect to the activation energy of tracer diffusion is larger than about 0.5eV. Since this reduction is experimentally found to be in the range 1 to 2 eV for the commonly used dopants, it may be concluded even without the knowledge of the real interaction potential that the pair diffusion model is very likely to be a valid description of diffusion via the vacancy mechanism.

References

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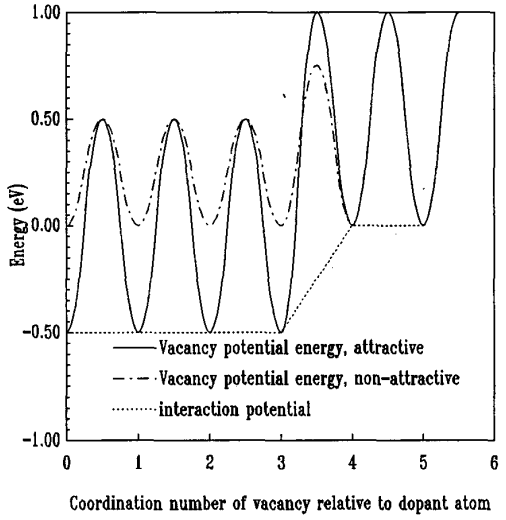

Fig.1 : Schematic drawing of the vacancy potential as function of the distance to the impurity. The dotted line shows the interaction potential with the impurity at coordination number 0.

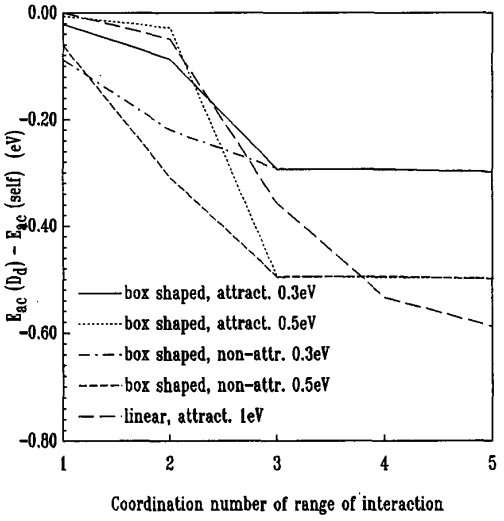

Fig.2: Reduction of activation energy of dopant diffusivity with respect to self-diffusion for different model interaction potentials.

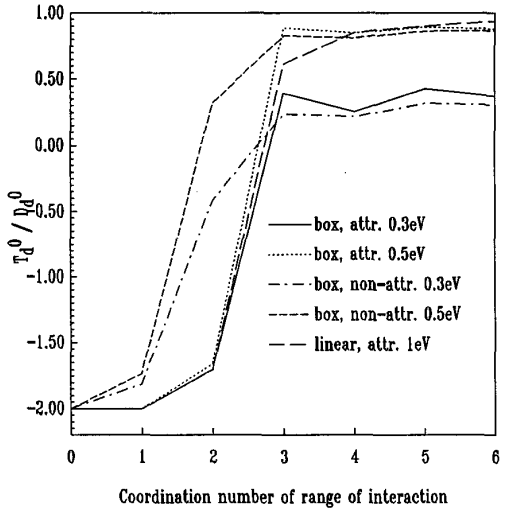

Fig.3: Relation $\alpha = T_d^0/D_d^0$ as function of range of the model interaction potentials.

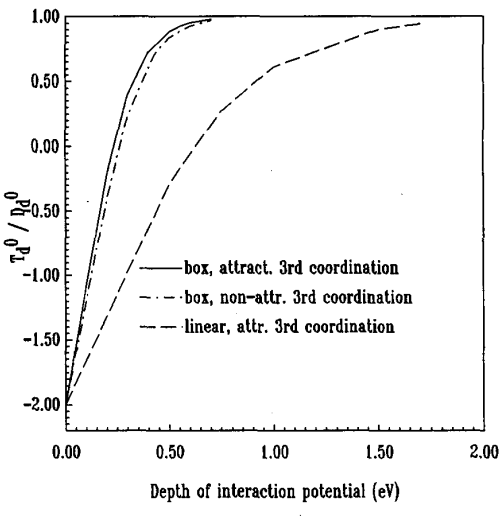

Fig.4: Relation $\alpha = T_d^0/D_d^0$ as function of the depth of the model interaction potentials.