Influence of illumination spectrum on dissociation kinetic of iron-boron pairs in silicon

Oleg Olikh, Oleksandr Datsenko, Serhiy Kondratenko

*Taras Shevchenko National University of Kyiv, 64/13, Volodymyrska Street, 01601, Kyiv, Ukraine*

olegolikh@knu.ua

The iron-boron pair is one of the most extensively examined defects in silicon. The complex’s levels, carrier capture cross-sections, kinetic models, dissociation techniques, and even ultrasound influence on pairing have been established [1-3]. However, the exact mechanism underlying the second decay phase — iron ion recharge or a recombination-enhanced defect reaction — remains debatable. We believe that investigation of the illumination spectrum impact on light-induced dissociation may reveal which proposed model is correct.

To demonstrate our methodology, we focused on identifying iron-related defect concentrations in silicon SC. Fig. 1(a) presents the workflow. Using SCAPS-1D software, the performance of back surface field SCs under both standard AM1.5 and monochromatic (940 nm) illumination were modeled. Simulated IV curves captured the behaviour of iron-acceptor pairs and scenarios with only interstitial iron. Then the relative changes in short-circuit current ε*Isc*, open-circuit voltage ε*Voc*, efficiency εη, and fill factor ε*FF* were extracted. ML techniques – deep neural networks (DNN), random forest (RF), and gradient boosting (GB) – were employed to estimate iron concentrations. The accuracy of predictions from various models was compared using data obtained under different lighting conditions and with varying numbers (ranging from 4 to 7) of descriptors. In the simplest case, the descriptors included the SC's base depth and doping level, temperature, and ε*Isc*. For cases involving 5, 6, and 7 descriptors, the εη, ε*Voc*, and εFF, were added respectively. The results are shown in Tables 1 and 2 and Fig. 1(b).

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[3] C. Sun *et al.*, *Phys. Status Solidi RRL* **2021**, *15*, 2000520.

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**Fig. 1.** (a) Workflow. (b) Fraction of samples for which the error does not exceed the threshold versus the threshold value for neural networks and random forest models. Top and down panels correspond to standard and monochromatic illumination, respectively.

**Table 1.** Results of 5-fold cross-validation for train dataset

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Model | Illumination | Mean squared error (10-3) | | | |
| Number of descriptors | | | |
| 4 | 5 | 6 | 7 |
| DNN | AM1.5 | 42±5 | 9±3 | 4±2 | 2±1 |
| 940 nm | 10±5 | 6.1±0.4 | 6±2 | 1.5±0.7 |
| RF | AM1.5 | 33±2 | 11±3 | 5±2 | 4±1 |
| 940 nm | 6±1 | 4.6±0.2 | 3.0±0.5 | 3.0±0.8 |
| GB | AM1.5 | 34±2 | 9±2 | 5±2 | 4±1 |
| 940 nm | 4.2±0.6 | 3.5±0.2 | 2.3±0.6 | 2.1±0.5 |

**Table 2.** Prediction accuracy for test dataset

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Model | Number of descriptors | Mean squared error (10-3) | | Mean relative error (%) | | R2 | |
| Illumination | | | | | |
| AM1.5 | 940 nm | AM1.5 | 940 nm | AM1.5 | 940 nm |
| DNN | 4 | 58 | 6 | 53 | 10 | 0.905 | 0.977 |
| 5 | 4 | 33 | 7 | 36 | 0.988 | 0.881 |
| 6 | 0.9 | 0.6 | 5 | 5 | 0.992 | 0.993 |
| 7 | 5 | 0.8 | 11 | 5 | 0.990 | 0.988 |
| RF | 4 | 41 | 3 | 142 | 11 | 0.930 | 0.968 |
| 5 | 10 | 3 | 15 | 10 | 0.959 | 0.967 |
| 6 | 4 | 3 | 10 | 9 | 0.972 | 0.956 |
| 7 | 5 | 3 | 11 | 10 | 0.958 | 0.963 |
| GB | 4 | 33 | 3 | 43 | 8 | 0.947 | 0.965 |
| 5 | 9 | 2 | 13 | 8 | 0.955 | 0.980 |
| 6 | 5 | 2 | 10 | 7 | 0.969 | 0.967 |
| 7 | 5 | 2 | 10 | 8 | 0.960 | 0.961 |