Bridging accuracy and simplicity: ML-based models for carrier mobility estimation in silicon

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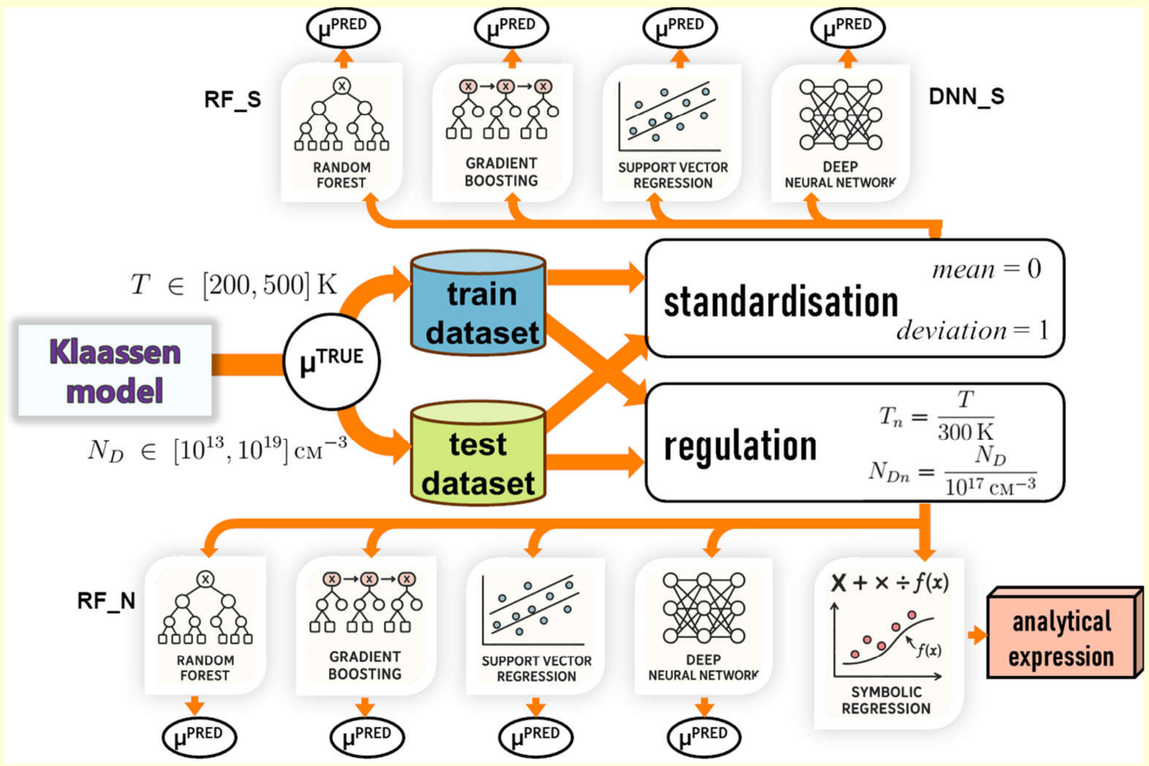
Introduction. Carrier mobility is a fundamental parameter in semiconductor physics because it determines conductivity, operating speed, and energy efficiency while reflecting microscopic scattering effects on charge transport. Its description relies on both fundamental approaches, including the Boltzmann transport equation, and empirical models such as the Caughey–Thomas, Masetti, Arora, and Klaassen formulations. Although the last model provides high accuracy, its practical use is limited by its mathematical complexity and large number of fitting parameters. To address this issue, this work proposes machine-learning regression models for predicting carrier mobility in monocrystalline silicon as a function of temperature and doping concentration. The developed approach combines the simplicity of Arora-type models with the predictive accuracy of the Klaassen formulation. In addition, symbolic regression was used to derive compact analytical expressions suitable for TCAD simulations and semiconductor device optimization.

Flowchart of calculations



Klaassen model

$$\mu^{\mathrm{K}} = \frac{\mu_L\,\mu_{DA}}{\mu_L + \mu_{DA}} \qquad \mu_L = \mu_{\max}\left(\frac{300}{T}\right)^{2,25}$$

$$\mu_{DA} = \frac{\mu_{\max}^2}{\mu_{\max} - \mu_{\min}} \cdot \frac{N_{sc}}{N_{\mathrm{eff}}} \cdot \left(\frac{N_{ref}}{N_{sc}}\right)^{\alpha} \cdot \left(\frac{T}{300}\right)^{3\alpha-1,5} + \frac{\mu_{\max}\,\mu_{\min}}{\mu_{\max} - \mu_{\min}} \cdot \frac{n+p}{N_{\mathrm{eff}}} \cdot \left(\frac{300}{T}\right)^{0,5}$$

electrons:

$$N_{\mathrm{sc}} = N_d^+ + N_a^- + p\,,$$

$$N_{\mathrm{eff}} = N_d^+ + N_a^- \cdot G_n(P_n, T) + \frac{p}{F_n(P_n, T)}$$

holes:

$$N_{\mathrm{sc}} = N_a^- + N_d^+ + n\,,$$

$$N_{\mathrm{eff}} = N_a^- + N_d^+ \cdot G_p(P_p, T) + \frac{n}{F_p(P_p, T)}$$

$$G_n = 1 - S_1 \cdot \left[S_2 + \left(\frac{m_0}{m_e}\frac{T}{300}\right)^{S_4} P_n\right]^{-S_3} + S_5 \cdot \left[\left(\frac{m_e}{m_0}\frac{300}{T}\right)^{S_7} P_n\right]^{-S_6},$$

$$G_p = 1 - S_1 \cdot \left[S_2 + \left(\frac{m_0}{m_h}\frac{T}{300}\right)^{S_4} P_p\right]^{-S_3} + S_5 \cdot \left[\left(\frac{m_h}{m_0}\frac{300}{T}\right)^{S_7} P_p\right]^{-S_6},$$

$$F_n = \frac{r_1 P_n^{r_6} + r_2 + r_3 \frac{m_e}{m_h}}{P_n^{r_6} + r_4 + r_5 \frac{m_e}{m_h}};\quad F_p = \frac{r_1 P_p^{r_6} + r_2 + r_3 \frac{m_h}{m_e}}{P_n^{r_6} + r_4 + r_5 \frac{m_h}{m_e}},$$

$$P_n = (P_{bn} + P_{cn})^{-1};\quad P_p = (P_{bp} + P_{cp})^{-1},$$

$$P_{bn} = \frac{3.83\left(\frac{m_0}{m_e}\right)}{\frac{1,36\cdot 10^{26}}{N_d^+ + p}\left(\frac{T}{300}\right)^2};\quad P_{bp} = \frac{3.83\left(\frac{m_0}{m_h}\right)}{\frac{1,36\cdot 10^{26}}{N_a^- + n}\left(\frac{T}{300}\right)^2},$$

S_1	S_2	S_3	S_4	S_5	S_6	S_7
0,89233	0,41372	0,19778	0,28227	0,005978	1,80618	0,72169
r_1	r_2	r_3	r_4	r_5	r_6	
0,7643	2,2999	6,5502	2,3670	-0,01552	0,6478	

Machine learning

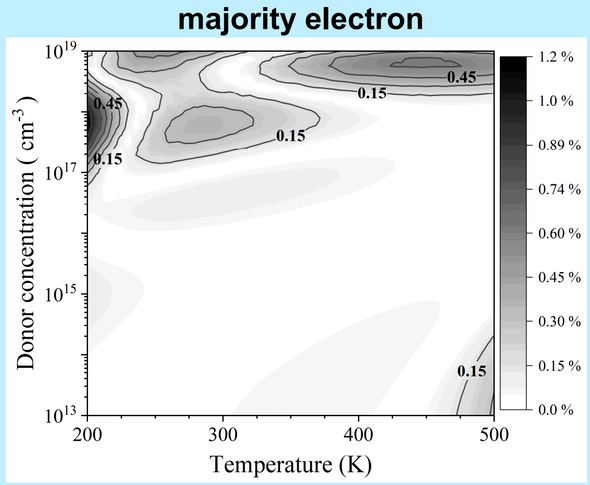
symbolic regression

$$\mu = \mu_0 + \frac{\mu_1}{T_n^{2,25} + a \cdot b / (a+b)}$$

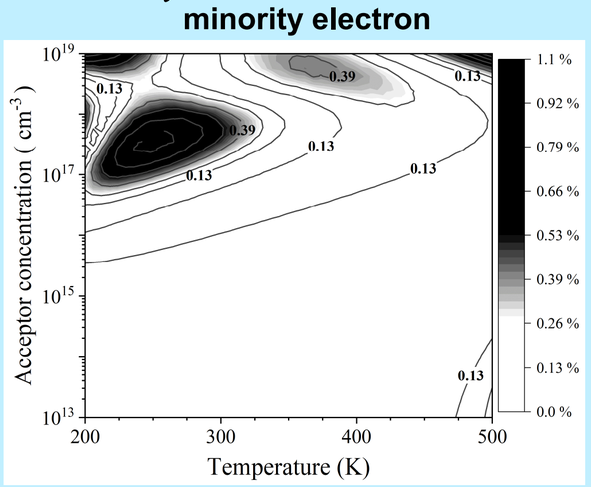
	majority electron	minority electron
μ_0	0	$26.3\left(\frac{N_{Dn}}{N_{Dn}+192}\right)^{0.62}$
μ_1	$N_{Dn}+1413.2$	1412.3
a	$\left(\frac{N_{Dn}}{0.873T_n+0.0727}\right)^{0.7212}$	$1.92\left(\frac{N_{Dn}}{T_n+0,071}\right)^{0.717}$
b	$0.215N_{Dn}^{0.58}+10.5T_n-1.342$	$5.7\cdot N_{Dn}^{0.103}\cdot T_n$

percentage error in assessing mobility compared with Klaassen's theory

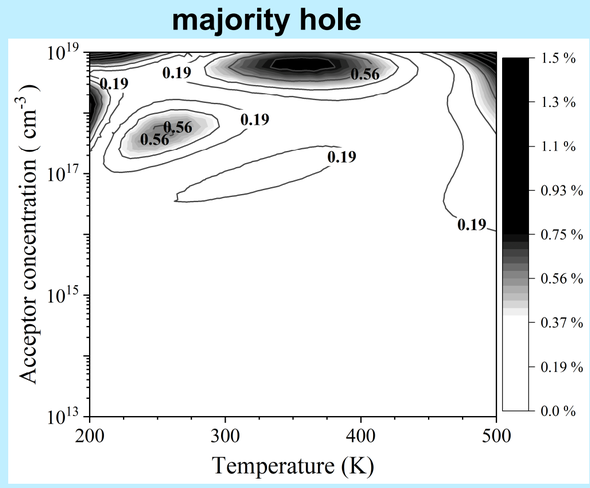
majority electron



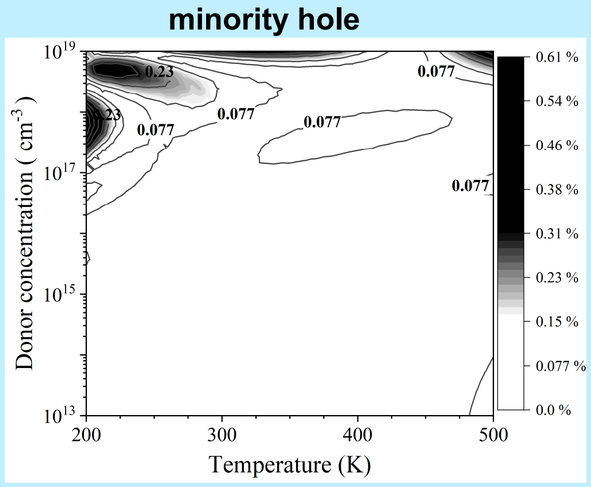
minority electron



majority hole



minority hole



Model	MAPE, %				APE_{MAX}, %				APE_{MED}, %				MAE, см^2/(В · с)			
	μ_{nn}	μ_{np}	μ_{pp}	μ_{pn}	μ_{nn}	μ_{np}	μ_{pp}	μ_{pn}	μ_{nn}	μ_{np}	μ_{pp}	μ_{pn}	μ_{nn}	μ_{np}	μ_{pp}	μ_{pn}
RF_N	1,29	1,69	1,52	1,47	9,33	14,5	4,60	10,9	0,805	0,994	0,264	0,913	11,0	13,5	4,50	4,76
RF_S	1,42	1,77	1,46	1,41	12,3	14,4	14,5	12,6	0,852	1,04	0,744	0,872	11,6	14,1	4,40	4,76
SVR_N	46,5	51,5	32,6	33,4	1630	1750	2070	1510	14,9	17,4	13,1	12,9	220	244	68,8	73,6
SVR_S	0,108	**0,087**	**0,098**	0,082	1,71	2,16	2,26	3,56	0,088	**0,064**	**0,069**	0,050	1,20	1,03	0,394	0,410
GB_N	2,20	1,46	1,60	1,55	58,2	10,8	17,3	11,0	1,46	0,939	0,905	1,15	15,43	10,85	4,75	5,24
GB_S	1,32	1,60	1,82	1,23	1,42	11,7	15,0	8,48	0,841	1,104	1,19	0,874	11,3	13,4	5,92	4,19
DNN_N	0,925	0,942	2,01	0,529	9,39	20,0	8,07	6,02	0,621	0,702	1,893	0,383	5,23	5,37	4,22	1,39
DNN_S	0,374	0,623	0,655	0,671	2,23	3,75	5,96	2,97	0,323	0,392	0,556	0,631	3,58	3,49	2,88	1,97
SR	**0,094**	0,137	0,140	**0,050**	**1,19**	**0,992**	**1,48**	**0,596**	**0,044**	0,077	0,079	**0,026**	**0,475**	**0,708**	**0,314**	**0,115**
Arora [11]	5,35	20,3	5,62	37,8	38,2	70,7	17,6	111	3,67	16,3	5,01	32,6	45,7	103	16,0	82,6

$$MAPE = \frac{1}{N}\sum_{i=1}^{N}\frac{|\hat{y}_i - y_i|}{y_i}\times 100\% \qquad MAE = \frac{1}{N}\sum_{i=1}^{N}|\hat{y}_i - y_i|$$

Conclusion. Using a symbolic regression algorithm, analytical expressions were derived to describe electron and hole mobilities in monocrystalline silicon over the temperature range of 200–500 K and the doping concentration range of 10^{13}–10^{19} cm^{-3} .Compared with the Klaassen model, the proposed expressions contain fewer than half as many parameters, eliminate the need for prior determination of the dopant ionization degree, and exhibit a simpler functional form. Importantly, the reduction in accuracy is minimal: for approximately 50% of all temperature and doping concentration combinations, the relative error does not exceed 0.044%, 0.077%, 0.079%, and 0.026% for $\mu_{n,n}$, $\mu_{n,p}$, $\mu_{p,p}$, and $\mu_{p,n}$, respectively. Furthermore, despite having a complexity comparable to that of the Arora model, the derived expressions provide substantially higher accuracy. These advantages demonstrate the strong potential of the proposed approach for practical applications.