Loughborough University

FUNCTIONAL MATERIALS
(23MPC321)

Semester 2 2024 In-Person Exam paper

This examination is to take place in-person at a central University venue under exam conditions. The standard length of time for this paper is **2 hours**.

You will not be able to leave the exam hall for the first 30 or final 15 minutes of your exam. Your invigilator will collect your exam paper when you have finished.

Help during the exam

Invigilators are not able to answer queries about the content of your exam paper. Instead, please make a note of your query in your answer script to be considered during the marking process.

If you feel unwell, please raise your hand so that an invigilator can assist you.

You may use a calculator for this exam. It must comply with the University's Calculator Policy for In-Person exams, in particular that it must not be able to transmit or receive information (e.g. mobile devices and smart watches are not allowed).

Answer THREE questions.

A formulae sheet is included.

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1. (a) It is required to dope Si with B to create a material with a resistivity of $1\,\Omega\,\mathsf{cm}$, calculate the concentration of B required to achieve this, take the electron mobility to be $1350\,\mathsf{cm}^2/\mathsf{V}\,\mathrm{sec}$ and the hole mobility to be $450\,\mathsf{cm}^2/\mathsf{V}\,\mathrm{sec}$ and assume the resistivity is given by the majority carrier only. [6 marks]

   (b) The material is diffusion doped with a surface concentration $\phi_{\mathsf{surface}} = 1 \times 10^{18}\,\mathsf{cm}^{-3}$ at a temperature of $1200\,^{\circ}\mathsf{C}$. Calculate the time taken to diffuse enough dopant atoms into the material to achieve the required electron carrier concentration to a depth of $5\,\mu\mathsf{m}$, assume the final dopant concentration is uniform. Use the graph in figure 1 to determine the diffusion constant. [6 marks]

   (c) Calculate the depth at which the concentration would fall to 1% of the surface concentration given your solution to part (b), if you don't have a solution take a time of $30\,\mathrm{sec}$. [6 marks]

   (d) Discuss how you could process the material to increase the depth of penetration of the dopant into the semiconductor. [2 marks]

2. (a) At 300 K the lattice constants of silicon is 5.429 Å:

      (i) calculate the number of atoms per cubic centimetre and the density. Give your answers to three significant figures. [4 marks]

      (ii) if the silicon is doped with boron at a concentration of $1 \times 10^{16}\,\mathsf{cm}^{-3}$ what is the atomic percentage of boron in the material? [4 marks]

      The atomic weight of silicon is $28.0855\,\mathsf{g\,mol}^{-1}$.

   (b) Show that the density of states for a two-dimensional semiconductor has no dependence on the energy of the carriers. [12 marks]

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3. (a) Calculate the theoretical capacity of the following electrode materials:
   (i) LiC_6 [3 marks]
   (ii) $LiFePO_4$ [3 marks]
   (iii) $Li_{22}Si_5$ alloy [3 marks]

   (b) Consider a battery consisting of a LiC_6 electrode and a $LiFePO_4$ electrode calculate its capacity using the results from part (a), ignore the electrolyte and battery hardware. [4 marks]

   (c) Consider a battery consisting of a $Li_{22}Si_5$ alloy electrode and a $LiFePO_4$ electrode calculate its capacity using the results from part (a), ignore the electrolyte and battery hardware, compare to part (b). [4 marks]

   (d) Given the results of parts (b) and (c) explain the current choices of electrodes in commercial batteries. [3 marks]

   Useful data:
   The molar mass for the following elements in units of g/mol:
   C = 12.011
   O = 15.9994
   Fe = 55.847
   P = 30.97376
   Si = 28.0855

4. Calculate the polarisation per unit volume of $BaTiO_3$ by:

   (a) Calculating the polarisation per unit cell based on a distortion of the Ti^{4+} ion of 0.11Å. [4 marks]

   (b) Calculate volume of a unit cell, the density of $BaTiO_3$ is $6.02\,\mathrm{g\,cm^{-3}}$ and the mass of $BaTiO_3$ is $233.212\,\mathrm{g\,mol^{-1}}$. [4 marks]

   (c) Calculate the polarisation per cubic metre. [4 marks]

   (d) Given the density of $PbTiO_3$ is $7.52\,\mathrm{g\,cm^{-3}}$ and the mass of $PbTiO_3$ is $303.09\,\mathrm{g\,mol^{-1}}$ and a polarisation of $0.8\,\mathrm{C\,m^{-2}}$, calculate the distortion of the Ti^{4+} ion. [8 marks]

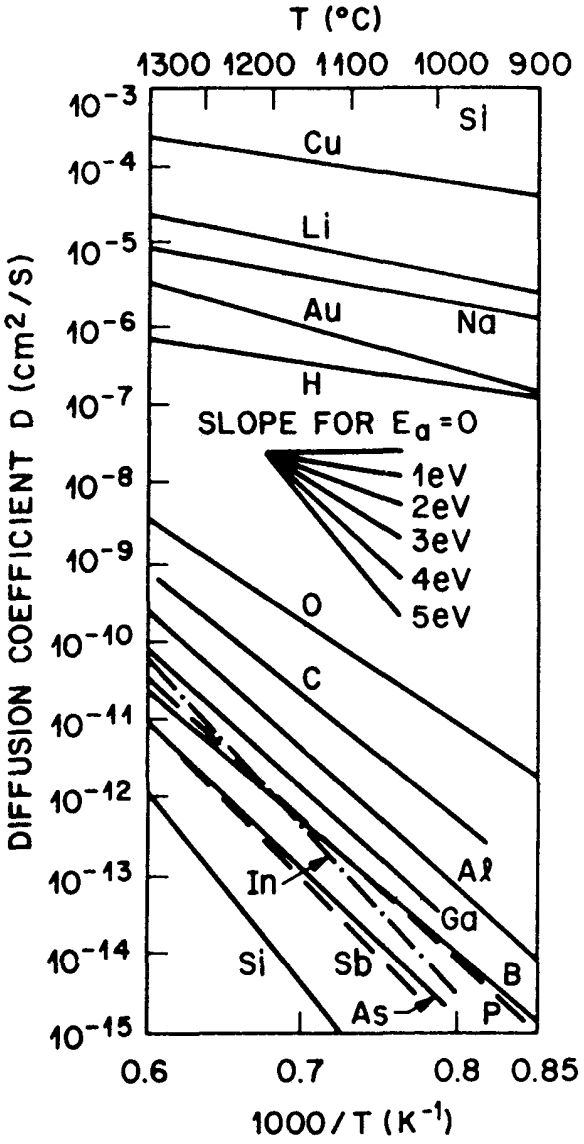

Figure 1: Diffusion constants for various dopants in Si.

continued. . .

Complementary Error Function Table													
x	erfc(x)	x	erfc(x)	x	erfc(x)	x	erfc(x)	x	erfc(x)	x	erfc(x)	x	erfc(x)
0	1.000000	0.5	0.479500	1	0.157299	1.5	0.033895	2	0.004678	2.5	0.000407	3	0.00002209
0.01	0.988717	0.51	0.470756	1.01	0.153190	1.51	0.032723	2.01	0.004475	2.51	0.000386	3.01	0.00002074
0.02	0.977435	0.52	0.462101	1.02	0.149162	1.52	0.031587	2.02	0.004281	2.52	0.000365	3.02	0.00001947
0.03	0.966159	0.53	0.453536	1.03	0.145216	1.53	0.030484	2.03	0.004094	2.53	0.000346	3.03	0.00001827
0.04	0.954889	0.54	0.445061	1.04	0.141350	1.54	0.029414	2.04	0.003914	2.54	0.000328	3.04	0.00001714
0.05	0.943628	0.55	0.436677	1.05	0.137564	1.55	0.028377	2.05	0.003742	2.55	0.000311	3.05	0.00001608
0.06	0.932378	0.56	0.428384	1.06	0.133856	1.56	0.027372	2.06	0.003577	2.56	0.000294	3.06	0.00001508
0.07	0.921142	0.57	0.420184	1.07	0.130227	1.57	0.026397	2.07	0.003418	2.57	0.000278	3.07	0.00001414
0.08	0.909922	0.58	0.412077	1.08	0.126674	1.58	0.025453	2.08	0.003266	2.58	0.000264	3.08	0.00001326
0.09	0.898719	0.59	0.404064	1.09	0.123197	1.59	0.024538	2.09	0.003120	2.59	0.000249	3.09	0.00001243
0.1	0.887537	0.6	0.396144	1.1	0.119795	1.6	0.023652	2.1	0.002979	2.6	0.000236	3.1	0.00001165
0.11	0.876377	0.61	0.388319	1.11	0.116467	1.61	0.022793	2.11	0.002845	2.61	0.000223	3.11	0.00001092
0.12	0.865242	0.62	0.380589	1.12	0.113212	1.62	0.021962	2.12	0.002716	2.62	0.000211	3.12	0.00001023
0.13	0.854133	0.63	0.372954	1.13	0.110029	1.63	0.021157	2.13	0.002593	2.63	0.000200	3.13	0.00000958
0.14	0.843053	0.64	0.365414	1.14	0.106918	1.64	0.020378	2.14	0.002475	2.64	0.000189	3.14	0.00000897
0.15	0.832004	0.65	0.357971	1.15	0.103876	1.65	0.019624	2.15	0.002361	2.65	0.000178	3.15	0.00000840
0.16	0.820988	0.66	0.350623	1.16	0.100904	1.66	0.018895	2.16	0.002253	2.66	0.000169	3.16	0.00000786
0.17	0.810008	0.67	0.343372	1.17	0.098000	1.67	0.018190	2.17	0.002149	2.67	0.000159	3.17	0.00000736
0.18	0.799064	0.68	0.336218	1.18	0.095163	1.68	0.017507	2.18	0.002049	2.68	0.000151	3.18	0.00000689
0.19	0.788160	0.69	0.329160	1.19	0.092392	1.69	0.016847	2.19	0.001954	2.69	0.000142	3.19	0.00000644
0.2	0.777297	0.7	0.322199	1.2	0.089686	1.7	0.016210	2.2	0.001863	2.7	0.000134	3.2	0.00000603
0.21	0.766478	0.71	0.315335	1.21	0.087045	1.71	0.015593	2.21	0.001776	2.71	0.000127	3.21	0.00000564
0.22	0.755704	0.72	0.308567	1.22	0.084466	1.72	0.014997	2.22	0.001692	2.72	0.000120	3.22	0.00000527
0.23	0.744977	0.73	0.301896	1.23	0.081950	1.73	0.014422	2.23	0.001612	2.73	0.000113	3.23	0.00000493
0.24	0.734300	0.74	0.295322	1.24	0.079495	1.74	0.013865	2.24	0.001536	2.74	0.000107	3.24	0.00000460
0.25	0.723674	0.75	0.288845	1.25	0.077100	1.75	0.013328	2.25	0.001463	2.75	0.000101	3.25	0.00000430
0.26	0.713100	0.76	0.282463	1.26	0.074764	1.76	0.012810	2.26	0.001393	2.76	0.000095	3.26	0.00000402
0.27	0.702582	0.77	0.276179	1.27	0.072486	1.77	0.012309	2.27	0.001326	2.77	0.000090	3.27	0.00000376
0.28	0.692120	0.78	0.269990	1.28	0.070266	1.78	0.011826	2.28	0.001262	2.78	0.000084	3.28	0.00000351
0.29	0.681717	0.79	0.263897	1.29	0.068101	1.79	0.011359	2.29	0.001201	2.79	0.000080	3.29	0.00000328
0.3	0.671373	0.8	0.257899	1.3	0.065992	1.8	0.010909	2.3	0.001143	2.8	0.000075	3.3	0.00000306
0.31	0.661092	0.81	0.251997	1.31	0.063937	1.81	0.010475	2.31	0.001088	2.81	0.000071	3.31	0.00000285
0.32	0.650874	0.82	0.246189	1.32	0.061935	1.82	0.010057	2.32	0.001034	2.82	0.000067	3.32	0.00000266
0.33	0.640721	0.83	0.240476	1.33	0.059985	1.83	0.009653	2.33	0.000984	2.83	0.000063	3.33	0.00000249
0.34	0.630635	0.84	0.234857	1.34	0.058086	1.84	0.009264	2.34	0.000935	2.84	0.000059	3.34	0.00000232
0.35	0.620618	0.85	0.229332	1.35	0.056238	1.85	0.008889	2.35	0.000889	2.85	0.000056	3.35	0.00000216
0.36	0.610670	0.86	0.223900	1.36	0.054439	1.86	0.008528	2.36	0.000845	2.86	0.000052	3.36	0.00000202
0.37	0.600794	0.87	0.218560	1.37	0.052688	1.87	0.008179	2.37	0.000803	2.87	0.000049	3.37	0.00000188
0.38	0.590991	0.88	0.213313	1.38	0.050984	1.88	0.007844	2.38	0.000763	2.88	0.000046	3.38	0.00000175
0.39	0.581261	0.89	0.208157	1.39	0.049327	1.89	0.007521	2.39	0.000725	2.89	0.000044	3.39	0.00000163
0.4	0.571608	0.9	0.203092	1.4	0.047715	1.9	0.007210	2.4	0.000689	2.9	0.000041	3.4	0.00000152
0.41	0.562031	0.91	0.198117	1.41	0.046148	1.91	0.006910	2.41	0.000654	2.91	0.000039	3.41	0.00000142
0.42	0.552532	0.92	0.193232	1.42	0.044624	1.92	0.006622	2.42	0.000621	2.92	0.000036	3.42	0.00000132
0.43	0.543113	0.93	0.188437	1.43	0.043143	1.93	0.006344	2.43	0.000589	2.93	0.000034	3.43	0.00000123
0.44	0.533775	0.94	0.183729	1.44	0.041703	1.94	0.006077	2.44	0.000559	2.94	0.000032	3.44	0.00000115
0.45	0.524518	0.95	0.179109	1.45	0.040305	1.95	0.005821	2.45	0.000531	2.95	0.000030	3.45	0.00000107
0.46	0.515345	0.96	0.174576	1.46	0.038946	1.96	0.005574	2.46	0.000503	2.96	0.000028	3.46	0.00000099
0.47	0.506255	0.97	0.170130	1.47	0.037627	1.97	0.005336	2.47	0.000477	2.97	0.000027	3.47	0.00000092
0.48	0.497250	0.98	0.165769	1.48	0.036346	1.98	0.005108	2.48	0.000453	2.98	0.000025	3.48	0.00000086
0.49	0.488332	0.99	0.161492	1.49	0.035102	1.99	0.004889	2.49	0.000429	2.99	0.000024	3.49	0.00000080

Table of $\operatorname{erfc}(x)$

continued. . .

Formulae Sheet and Useful Constants

The intrinsic carrier density for silicon is $N_i = 1.45 \times 10^{10}\,\mathsf{cm}^{-3}$.
Avogadro constant is $N_A = 6.022 \times 10^{23}$.
The charge on an electron is $q = 1.602 \times 10^{-19}\,\mathsf{C}$.
Vacuum permeability is $\mu_0 = 1.257 \times 10^{-6}\,\mathsf{N\,m}^{-2}$.
Boltzmann constant is $k_B = 1.38 \times 10^{-23}\,\mathsf{J\,K}^{-1}$.
$F = 96.485 \times 10^3\,\mathsf{C\,mol}^{-1}$

The total amount of dopant that we have put into the system is:

$$Q(t) = 1.13\,\phi_{\text{surface}}\sqrt{Dt}$$

where $Q(t)$ is the amount of dopant at time t, ϕ_{surface} is the surface concentration and D is the diffusion constant. Constant surface concentration diffusion concentration profile

$$\phi(x,t) = \phi_{\text{surface}}\,\text{erfc}\left(\frac{x}{\sqrt{Dt}}\right)$$

where $\phi(x,t)$ is the concentration at a depth x and time t, ϕ_{surface} is the surface concentration and D is the diffusion constant.

The conductivity in a semiconductor is given by:

$$\sigma = qn\mu_n + qp\mu_p$$

and the resistivity by

$$\rho = \frac{1}{qn\mu_n + qp\mu_p}$$

where n is the electron carrier density, p is the hole carrier density and μ_n and μ_p are the electron and hole mobilities respectively.

The theoretical capacity of an electrode is:

$$C_t = \frac{nF}{3600M}$$

where n is the number of Li ions, F is the Faraday constant and M is the molar mass.

The polarisation per unit cell is given by

$$P = \sum_i q_i d_i$$

where q_i is the charge on the ion and d_i is its displacement.