Loughborough University

# (24MPC321)
# FUNCTIONAL MATERIALS

Semester 2 2024/25 In-Person Exam paper

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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) Explain what happens to a semiconductor when it is doped to create a p-type material over the undoped material, make use of band diagrams and explain the role of states in the gap and temperature. [6 marks]

   (b) CdTe is doped with As to create a p-type material for use in a photovoltaic device.

   (i) The material is diffusion doped with a surface concentration $\phi_{\text{surface}} = 1 \times 10^{18}\,\text{cm}^{-3}$ at a temperature of $650\,^{\circ}\text{C}$. Calculate the time taken to diffuse enough dopant atoms into the material to achieve $0.1$ % of the surface concentration to a depth of $0.1\,\mu\text{m}$. Use the graph in figure 1 to determine the diffusion constant. [6 marks]

   (ii) Calculate the concentration gradients at the surface and at $0.1\,\mu\text{m}$ at the time given in your solution to part (b), if you don't have a solution take a time of $180\,\text{sec}$. [8 marks]

2. (a) Show that the density of states for a two-dimensional semiconductor has no dependence on the energy of the carriers. [11 marks]

   (b) The time independent version of Schrödinger's equation in 1D is given by:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

   $\hbar$ is Planck's constant, $h$, divided by $2\pi$, $m$ is the mass of the electron. Show that the solution of a 1D particle in a box where $V(x) = 0$ for $0 \leq x \leq L$ and $\infty$ elsewhere is:

$$\psi(x) = A\sin kx \text{ with } k = \frac{n\pi}{L}$$

   [9 marks]

3. (a) If the effective mass of an electron in Si is $2.37 \times 10^{-31}\,\mathsf{kg}$ calculate the thermal velocity of the electrons at room temperature $(300\,\mathsf{K})$. [3 marks]

   (b) If the mean free time between electron collisions in Si semiconductor at room temperature $(300\,\mathsf{K})$ is $0.1\,\mathsf{ps}$, estimate the mean free path. [4 marks]

   (c) In n-type doped Si the dopant concentration varies linearly from $1 \times 10^{20}\,\mathsf{cm}^{-3}$ to $2 \times 10^{17}\,\mathsf{cm}^{-3}$ over $0.1\,\mathsf{cm}$, considering the material at room temperature $(300\,\mathsf{K})$.

      (i) Calculate the concentrations of the electrons and holes in this sample at the maximum and minima concentrations. State any assumptions used in your calculations. [6 marks]

      (ii) If the diffusive current density is given by $J_{\mathsf{diff}} = qD_n\frac{dn}{dx}$, calculate the current density at $T = 300\,\mathsf{K}$ if the electron diffusion coefficient is $D_n = 22.5\,\mathsf{cm}^2\,\mathsf{s}^{-1}$. [7 marks]

4. (a) Neodymium magnets are ferromagnets with composition $Nd_2Fe_{14}B$, their unit cell is tetragonal with dimensions $8.78\,\text{Å} \times 8.78\,\text{Å} \times 12.12\,\text{Å}$ and contains 4 formula units. There are 31.3 $\mu_B$ per formula unit.

      (i) Calculate the density of the material in units of $\mathsf{g}\,\mathsf{cm}^{-3}$. [4 marks]

      (ii) Calculate the number of Bohr Magnetons per unit cell for $Nd_2Fe_{14}B$. [2 marks]

      (iii) Calculate the saturation flux density for $Nd_2Fe_{14}B$. [5 marks]

   (b) Compare this to ferromagnetic Nickel, its unit cell is face centred cubic with a cell dimension of 3.52 Å. There are 0.6 $\mu_B$ per Ni atom. [9 marks]

   Useful data:
   The molar mass for the following elements in units of g/mol:
   Nd = 144.242
   Fe = 55.847
   B = 10.811
   Ni = 58.71

| 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. . .*

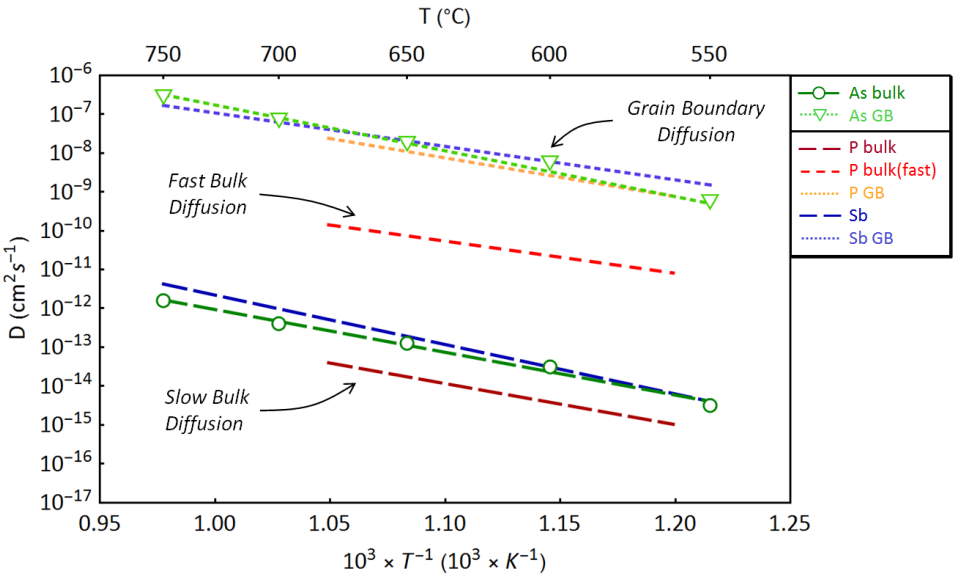


Figure 1: Graph showing the diffusivity of As in CdTe from E Colegrove *et al.* **2018** J. Phys. D: Appl. Phys. 51 075102.



*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 $k_B = 1.38 \times 10^{-23}\,\mathsf{J\,K}^{-1}$.
Bohr Magneton $= \mu_B = 9.27 \times 10^{-24}\,\mathsf{A\,m}^2$.
$F = 96.485 \times 10^3\,\mathsf{C\,mol}^{-1}$

Constant surface concentration diffusion concentration profile

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

where $\phi(x,t)$ is the concentration at a depth $x$ and time $t$, $\phi_{\mathsf{surface}}$ 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 $\mu_n$ and $\mu_p$ are the electron and hole mobilities respectively.

Useful differentiation formula:

$$\frac{d\,\mathrm{erfc}\,(x)}{dx} = -\frac{2}{\sqrt{\pi}}\exp\left(-x^2\right)$$