100 points

Minor-1

CML102

28th Aug 2015

1. Plot E vs k diagram and the DOS vs E diagram for a free electron in a 1D nanowire. Write the relevant equations. **[10+10+10]**

2. A researcher wanted to make green emitting ($\lambda_{em} = 540$ nm) CdSe nanocrystals. She used the Brus equation to evaluate the desired particle size. The nanocrystals grow at 1 monolayer per minute in the zinc blende structure under these synthesis conditions. The growth direction is [111] and the lattice parameter, a i.e. the cube edge length, is 0.6 nm.

   a. What size did she calculate?
   b. How long did she carry out the reaction?
   c. Approximately, what is the color of emission that she obtained?
   d. Why is this discrepancy observed between the calculation and experiment?
   e. What needs to be done in order to achieve green emission?

$$E_g(d) - E_g(bulk) = \frac{h^2}{2m^* d^2} - 1.8\frac{e^2}{2\pi\epsilon\epsilon_0 d}$$

   The zinc blende structure is similar to the diamond structure. You can assume Se at 000 and Zn at ¼ ¼ ¼ . A monolayer is made up of a complete Cd and Se layer. The bulk value for the energy gap is $E_g(bulk) = 1.74$ eV. Use the following parameters: effective mass of electrons/holes $m_e^* = 0.13m_0$, $m_h^* = 0.4m_0$, mass of free electrons ($m_0 = 9.1095 \times 10^{-31}$ kg); dielectric constant $\epsilon_{CdSe} = 5.8$, permittivity constant $\epsilon_0 = 8.854 \times 10^{-12}$ C^2 N^{-1} m^{-2} , Planck's constant $h = 6.63 \times 10^{-34}$ J s, 1 eV $= 1.602 \times 10^{-19}$ J. **[15+10+5+5+5]**

3. The Scherrer equation provides an estimate of the diameter of the particle, $d = \frac{4}{3}\frac{0.9\lambda}{\beta\cos\theta}$. The XRD peak at $2\theta = 28^\circ$ has an FWHM (β) equal to 5°. Estimate the particle diameter. **[10]**

4. Plot FC and ZFC curves for an antiferromagnetic material with a brief explanation as to why the differences are seen in the two cases. **[20]**

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