Determination of the band diagram of disordered meta-materials

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Summary:

The solar energy harvesting is of great importance in the renewable energy problematics. Among the third generation of inorganic solar cells, tandem cells are an interesting mean to increase the conversion of photons to electric charges by adapting the bandgap of a meta-material in order to harvest a larger portion of the solar spectra [1, 2].

Such meta-materials are made of semiconductor nanocrystals (NCs) embedded within an insulating layer. The material choices, the NC size and shape, as well as the NC density in the insulating die, influence the electrical characteristics of the meta-material in a non trivial way (energy bandgap, carrier mobilities, effective masses, ...). In the case of ordered layers of NCs, 3D Kronig-Penney-like models [3–5], or even *ab-initio* calculations [6, 7], allow to address numerically the characterization of this kind of meta-materials on the bases of an orthorhombic organization.

In practice, the nanocrystal arrangement inside the insulating die is disordered. In order to obtain more relevant information for these materials, the aim of the present work is to study numerically other organizations (e.g. hexagonal) and more appropriate unit cells to account for the disorder. The student will have to elaborate models within the effective mass approximation and the resolution of the Hamiltonian will be processed in a finite element solver used in the team. Skills in computer science will be a valuable asset for this theoretical work.

References

[1] Cho, E.-C.; Green, M. A.; Conibeer, G.; Song, D.; Cho, Y.-H.; Scardera, G.; Huang, S.; Park, S.; Hao, X. J.; Huang, Y.; Dao, L. V. *Advances in OptoElectronics* **2007**, *2007*, 69578.

[2] Conibeer, G.; Green, M.; Cho, E.-C.; König, D.; Cho, Y.-H.; Fangsuwannarak, T.; Scardera, G.; Pink, E.; Huang, Y.; Puzzer, T.; Huang, S.; Song, D.; Flynn, C.; Park, S.; Hao, X.; Mansfield, D. *Thin Solid Films* **2008**, *516*(20), 6748 – 6756.

[3] Lazarenkova, O. L.; Balandin, A. A. *Journal of Applied Physics* **2001**, *89*(10), 5509–5515.

[4] Lazarenkova, O. L.; Balandin, A. A. *Phys. Rev. B* **2002**, *66*(24), 245319.

[5] Jiang, C. W.; Green, M. A. *Journal of Applied Physics* **2006**, *99*(11).

[6] Seino, K.; Bechstedt, F.; Kroll, P. *Phys. Rev. B* **2012**, *86*, 075312 1–7.

[7] Seino, K.; Bechstedt, F.; Kroll, P. *Mat. Sci. Eng. B* **2012**, *177*, 1098–1102.