Simulation of photonic behaviour of CdTe/PbTe periodic structures

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Low-dimensional CdTe/PbTe heterostructures are widely known for their potentially applicable optical [1] and thermoelectrical [2] properties. Use of molecular beam epitaxy method in combination with appropriate temperature and time of annealing of CdTe/PbTe multilayer structures allows to easily obtain samples containing PbTe (CdTe) quantum dots or nano-pilars. Their well controllable spatial dimensions and periodic distribution together with over two times higher refractive index of PbTe ($n_{PbTe} = 5.75$) in comparison to CdTe ($n_{CdTe} = 2.75$) makes light see CdTe/PbTe heterostructures as a new meta-material, which creates potential for obtaining composite crystal with photonic gap.

In this paper we concentrate on numeric prediction of photonic behaviour of nanocomposite consist of periodically distributed PbTe (CdTe) dots in CdTe (PbTe) matrix using an open-source software *Meep* (MIT Electromagnetic Equation Propagation). *Meep* exploits the *finite-difference time-domain* (FDTD) method for simulation of light propagation in any electromagnetic system [3]. We have used it to calculate the experimentally useful transmission and reflection spectra for CdTe/PbTe periodic crystals with different sizes and spatial distribution of dots. Due to large contrast of refraction indexes, photonic behaviour was already observed for virtual crystals containing relatively low number of about 100 dots.



Fig 1. Transmission spectra of CdTe/PbTe virtual crystal

We have found, that in the case of 50 nm PbTe dots periodically dispersed in CdTe, investigated heterosystem exhibit photonic gap in region of wavelength between 600 and 900 nm (see Fig.1). Further, doubling the period of the crystal up in direction of light propagation causes arising the additional gap between 1200 and 1400 nm. Moreover, removal of few dots from randomly chosen positions in the crystal results in appear of impurity-like levels in photonic gap. We compare these results with that obtained for inverted structure of CdTe dots in PbTe matrix. Our simulations clearly showed, that real, periodic CdTe/PbTe structures should exhibit most of the features expected for photonic crystal.

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[2] Szot M. et al. Cryst. Growth Des. 11, 4794 (2011)

[3] A.F. Oskooi, et al., Computer Physics Communications, 181, 687-702 (2010)