Nanocomposites and nanomaterials

Raman scattering study of crystal multilayer structures with quantum dots

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The results of the theoretical and experimental study of Raman scattering (RS) in multilayer structures with quantum dots (QDs) are reported. The model is proposed for description of RS spectra of the above structures takes into account the real crystal structure of both the QD and surrounding matrix, as well as a QD-matrix interaction. The secondary quantization and Green function (GF) method are used in the model, because the spectral dependence of the scattering intensity can be expressed via the imaginary part of the GF.

For QDs embedded in a crystalline matrix, with close enough values of the lattice constant *a* of QD and matrix (for example Ge/Si $\Delta a/a$ ~0.04), and QD size d >> *a*, a new unit cell can be introduced. It includes, for example, Ge QD and partly a surrounding Si matrix. This new cell is sufficiently large enough and contains many initial unit cells. Thereby we obtain a new crystal with a new lattice parameter, $a \rightarrow La, L = \{L_x, L_y, L_z\}$.

The model presented in our study allows an analysis of the RS features for all types of phonons within the framework of microscopic approach, using only the common parameters of real crystals (including phonon frequency, atomic mass and lattice constant). This problem was partially considered by us earlier [1]. It is obvious, that in the SL with QDs the number of optical phonons increases because a new reciprocal lattice vector, b_L, is smaller than the primary one, $b = 2\pi / a \rightarrow b_L = 2\pi / La$. Each primary optical branch is transformed into several optical branches and each acoustical branch is transformed into several optical ones, and one acoustical band (sometimes such conversion is considered as folding of phonon branch). Therefore, for example, the structure of low-frequency bands in RS will result in many new optical phonons arising due to formation of new (larger) crystal unit cells.

The results obtained show that the crystal structures of the superlattice with QDs can be described as a mixed crystal with a specific distribution of “impurities” (Ge-atoms) organized in large “molecules” (QDs). A qualitative correlation in position and intensity distribution of bands for calculated and experimental Raman spectrum for multilayer Ge/Si QD crystal structure is observed and the doublet character of bands is explained.

[1] V.O. Yukhymchuk, V.M. Dzhagan, A.M. Yaremko, M.Ya. Valakh, EPJ, **B74** (2010) 409