

Nanoparticles with Core-Shell Structure for Photovoltaics: Morphology and Charge Transport

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Heterogeneous micro- and nanocrystals with so-called core-shell structure are of special interest due to their possible applications in photovoltaic devices including nanocrystalline layers for dye-sensitized solar cells and nanocrystalline Si:H films. The results reported in this contribution pertain to cubic microcrystals (MC) with a typical size between 50 and 500 nm in which core and shell grain has appropriately l and L dimension. Figure 1 (left) shows a schematic drawing of a cubic core-shell MC. The experiments were provided using model silver halide MC in which AgBrI core was covered with a thin (~ 10 -20 nm) shell layer of AgBr. The mismatch between lattice parameters in core and shell composition (~ 2 -3 %) resulted in creation the misfit dislocations in a surface layer of core-shell MC (Fig. 1, right image). Comparing with monograin structure, core-shell MCs show much higher photosensitivity and the increased values of surface conductivity. At the same time, little is known, how the core-shell structure influences the electronic properties of a semiconductor MC.

To investigate the relationship between the morphology and electronic properties of core-shell MC we have provided X-ray and dielectric dispersion (Maxwell-Wagner effect) studies of cubic MC with a structure of $\text{AgBr}_{0.97}\text{I}_{0.03}/\text{AgBr}$. To explain the high surface conductivity we present a phenomenological theory of dislocation-induced electronic transport in core-shell semiconductor MC.

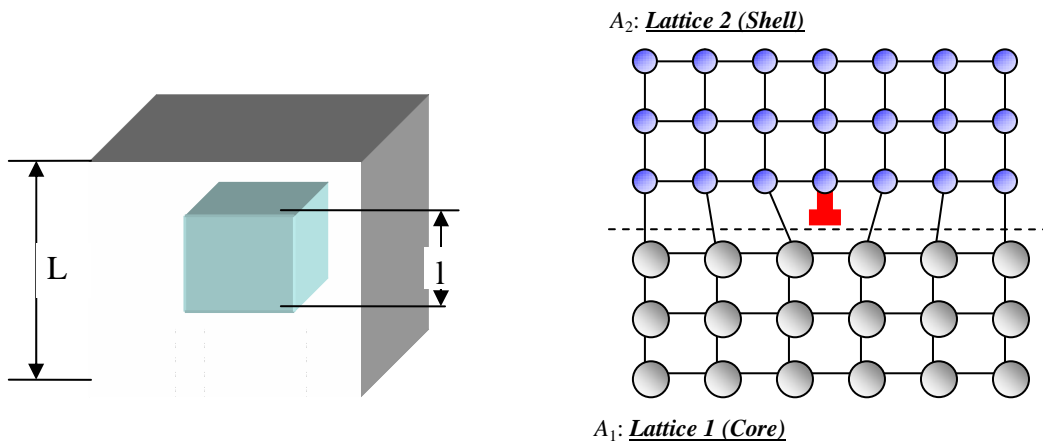


Fig. 1. Schematic representation of the internal structure of a cubic core-shell microcrystal (left). Creation of a misfit dislocation in the interfacial area between core and shell composition (right).

The X-ray powder diffraction data were obtained by using a RIGAKU D/MAX-B X-ray diffractometer. Figure 2 demonstrates a remarkable difference between X-ray diffraction intensities obtained for core-shell structure (a) and for a mixture of the appropriate monograin MCs (b). To calculate the relative intensities of X-ray diffraction patterns in a core-shell structure we have provided the theoretical simulation and obtained the appropriate formulas for different MC compositions. Figure 3 (c) presents the results of the theoretical simulation together with the experimental results obtained for $\text{AgBr}_{0.97}\text{I}_{0.03}/\text{AgBr}$ MCs.

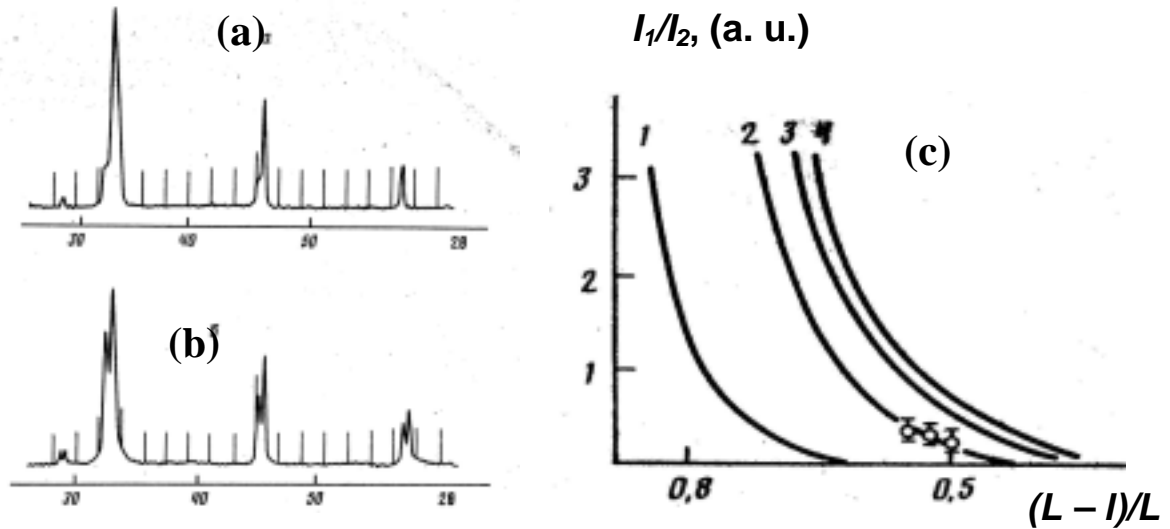


Fig. 2. X-ray diffraction patterns for $\text{AgBr}_{0.97}\text{I}_{0.03}/\text{AgBr}$ core-shell MC (a) and a mixture of monograin MCs with the same structure. Theoretical simulation of the relative X-ray intensities in a core-shell MCs (c).

Figure 3 shows the experimental curve for dielectric losses in core-shell microcrystals imbedded in a dielectric media. The calculation revealed that the value of dark conductivity in a surface subsystem (shell) is 2 orders of magnitude higher, than the one in the bulk (core).

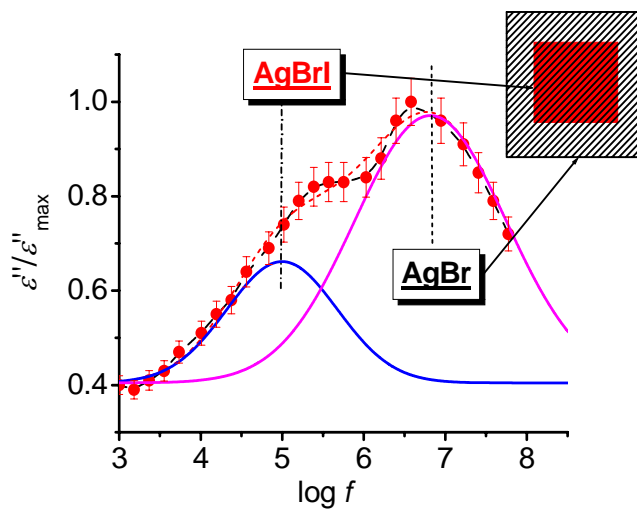


Fig. 3. Experimental results for normalized imaginary part of dielectric permittivity for core-shell AgBrI/AgBr MC, embedded in a dielectric media (points) and theoretical simulation of the appropriate contributions from the core and the shell subsystems.