

Andriy Zhugayevych, Research Highlights for 2000-2010

Chemistry Department, University of Houston, TX (October 22, 2010)

Midgap electronic states in amorphous pnictides and chalcogenides

Amorphous pnictide and especially chalcogenide semiconductors (As, Se, As₂Se₃, Ge₂Sb₂Te₅ etc.) exhibit significant photo- and current-induced changes whose nature is not well understood thus limiting the potential applications of the phenomenon. It is generally believed that these changes are intimately related to midgap electronic states localized on coordination defects and their pairs. In a series of papers we propose a novel approach for the description of the midgap states by taking into account the secondary bonding which is argued to be significant in pnictides and chalcogenides and results in the coordination defects linearly extended over several front and back bonds. Front-back bond switching makes the defects mobile which is the underlying mechanism of photo- and current-induced structural changes.

Efficient perturbation theory for disordered systems

It is an old idea [E. Feenberg, Phys. Rev. 74, 206 (1948)] that the perturbation series for the resolvent of a matrix can be rearranged so as to exclude the multiple scattering. Surprisingly that result was left undeveloped and used formally. In our work reported at Conference on Applied Physics (Kiev, Ukraine, 2007) we study this technique in detail. We observe that the believed improvement in convergence of the rearranged series is generally not valid, but is valid for sparse matrices, though the complications introduced by the rearrangement make its brute-force use inefficient. Nevertheless the constructive use of the method is possible: for matrices with i.i.d. random variables on their diagonal the rearrangement enables to take the average explicitly (note that some off-diagonal disorder, e.g. random bond model, can be reformulated as diagonal one).

Dynamic correlation function of a lattice gas

Many dynamic properties of a lattice system is encoded in its equilibrium two-point two-time correlation function¹. Its calculation is nontrivial in contrast to the static case for which various series methods exist. In particular, the BBGKY approach developed for a classical gas is not directly transferable to a lattice gas because the equation for one-particle distribution function involves not only two-particle but also higher order distribution functions. In our paper [Phys. Rev. B 74, 035418 (2006)] we extend the low-temperature expansion method to include the time-dependence and the transient configurations. The obtained correlation function is accurate within few percent for the temperatures up to 0.7 of the critical temperature T_c . Yet our work is not finished since our present approach does not give an algorithm to calculate the dynamic correlation function to any order of $\exp(-T_c/T)$.

Kinetics of the phosphorescence decay of a porous silicon

The kinetics of the phosphorescence decay of a porous silicon in a wide temperature range is anomalously slow (the integral over the extrapolated signal diverges). This phenomena is observed in some conjugated polymers, but the existing explanation as the tunneling recombination of geminate electron-hole pairs requires an unnatural distribution of activation energies for porous silicon: wide, flat, with depression at small energies. In my PhD thesis I demonstrate that this is a generic feature of the disordered systems with significant initial separation of the recombining particles: it is their multiple retrapping which is responsible for the depression of the distribution of activation energies. Part of these results are presented in [Physics of Low-Dimensional Structures, 7/8, 25 (2003)] and [Int. J. Nanotechnology 3, 65 (2006)].

Inverse problem for the luminescence

The analysis of the luminescence response is one of the easiest tools for studying the physical properties of materials. In particular, much information can be obtained by deconvoluting the time curve of the luminescence decay. The deconvolution is nontrivial, except the case of the multi-exponential decay, since the numerical inverse-Laplace transformation is mathematically incorrect problem. In my PhD Thesis I discuss the subject in detail and derive the inversion formulas for the case of the power-law decay, observed for example in some conjugated polymers and nanostructured silicon as an after-glow or phosphorescence. This method applied for porous silicon [Low Temperature Physics 28, 706 (2002)] is consistent with the measurements of the thermally stimulated luminescence complementing the latter at small activation energies.

¹For a lattice gas it is $\langle \delta n_x(t) \delta n_y(0) \rangle$, where $\delta n_x(t)$ is the fluctuation of the number of particles in point x at time t . Its coarse grained version for an atomic monolayer adsorbed at a solid surface can be probed by STM.