Seminář odd. 26
Tenkých vrstev a nanostruktur

Fyzikální ústav AVČR, Cukrovarnická 10, Praha 6

datum: 28. 3. 2012 čtvrtek

čas: 15:00

místnost: knihovna, budova A, 1.p.

TÉMA

Clathrates with group IV materials: novel photo-absorption materials for solar cells

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Clathrates are the materials composed with cage frameworks such as E20, E24 and E28, (E: group IV elements). According to the combinations of the cages, the clathrates are classified into type I, type II and so on. The clathrates generally encapsulate a molecule/atom inside each cage as a guest which is believed to be crucial for the formations of the cage structures. The inclusions of the guests in the cages induce peculiar characteristics in clathrates such as superconductivity and low thermal conductivity with high electrical conductivity.

Our research group in Gifu University focused on guest free Si or Ge clathrate, and their alloyed one as photo absorption materials of solar cells. According to a theoretical work, the guest free SiGe clathrates have band gaps which are tunable in the range from 1.2 to 1.9 eV depending on the atomic ratio of Si/Ge [1]. In addition, higher photo-absorption coefficients are expected because the type II Si/Ge clathrate have band structures with direct gap. We considered that such properties are suitable for future high-performance solar cells composed with environmentally friendly materials. However, there is no report on the clathrate solar cells due to existences of many thing to be achieved such as the synthesis of clathrates as single phase, preparations as film/bulk crystal forms, complete removal of guests and establishment of synthesis techiniques for alloying of Si and Ge clathrates.

In our work, Na doped Si/Ge clathrates are synthesized via thermal decompositions of Zintl phase NaSi/NaGe, respectively. As-prepared clathrates which include Na as the guests, have metallic characteristics because ionization of Na provides free electrons. In the case of type II structure, Na concentrations in the clathrates can be varied by conducting a post-thermal annealing after the synthesis. We are conducting developments of their synthesis techniques and analyzing them as semiconductors. I will talk about our resent work to achieve clathrate solar cells in near future.

[1] Moriguchi et al., Phys. Rev. B 62, (2000) 7138

odborný garant: *RNDr. Antonín Fejfar, Csc.*