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Report:

Various nanocrystalline silicon (nc-Si) structures, examined over last years, have been shown to exhibit efficient light emission in the visible region of the spectrum [1,2]. It is associated with direct transition in Si quantum confined system. Silicon nanostructures doped with Er^{3+} have been found as a good candidate for an infrared efficient emitter at telecommunication wavelength (1535 nm). Indirect excitation of Er^{3+} ions via energy transfer mechanism from nc-Si to erbium is involved in this optical emission. The key parameter in energy transfer process, which assures the efficient IR luminescence, is the distance between nc-Si (activator) and Er sensitize. However, the mechanism is still unclear and under debate. Therefore, detailed studies on the nearest neighbourhood of Er in the SiO₂/Si multilayer structure would offer invaluable information on the system. XAFS spectroscopy, as an element selective technique, can provide specific information about local structure around the Er ions.

We have investigated local structure around the Er ions in the as deposited and annealed Er doped SiO₂/Si layers with various optical properties. The layers were fabricated by rf magnetron sputtering with nm-thick layers and subsequently annealed with different methods and temperatures. The EXAFS and XANES measurements were carried out at the Er L₃ edge. Since the samples were very diluted and gathering acceptable signal was very time

consuming, we focused only on two series, one with the samples with 1% of Er annealed at 900°C by RTP and/or FA method. The other series consist of the samples with 1, 3 and 5% of Er annealed at 1100°C by FA method. The samples were measured in a fluorescence mode with 12-element Ge detector. Additionally, reference Er_2O_3 powder sample was measured in a transmission configuration.

FEFF9.6 code was used in XANES simulations in order to check how sensitive the shapes of the spectra are for possible Er neighbourhoods. It had shown that there should be visible substantial differences depending on how the erbium atoms are built in the Si, SiO₂ or Er_2O_3 structures. However, in all investigated samples experimental XANES spectra have shapes similar to each other (see figure below, for clarity only one series is presented). This implies that the Er atoms are located in the same type of neighbourhood. Presence of the very intensive white line points out that there should be oxygen atoms in the first sphere. Comparing XANES spectra of the investigated thin layers with reference Er_2O_3 one can also notice that the second maximum shows different shape from the reference's one which implies that another structure is necessary to describe close neighbourhood of Er in the layers.

Preliminary EXAFS analysis confirms that the first sphere consist of oxygen atoms and does not differ very substantially between the samples (see inset in the figure below). The differences can be observed for the further spheres. It is also clearly visible that erbium do not form Er_2O_3 exclusions.



References:

[1] Y. Kanemitsu, J. Lumin. **100**, 209 (2002).

[2] R.J. Walters, G.I. Bourianoff, and H.A. Atwater, Nat. Mater. 4, 143 (2005).