Abstract

Materials play an important role in human life. They are either naturally occurring or synthesised in laboratories. There is great dearth for the synthetic analogues as many times natural materials do not meet the modern industrial needs, which always look for specialised performance. This can only be overcome by producing the synthetic analogues tailored for certain specific requirements. There is a continuing need to create new materials with improved performance associated with energy conversion, energy storage, interaction with electromagnetic fields and their behavior with temperature and pressures to which they are subjected to. Hence there is a quest for tailoring materials for specialised requirements and to understand the process involved therein.

This work is aimed at synthesising and characterising a class of material which are naturally occurring but rather slips into a field of least understood but highly explored group called silver chalcogenides, which constitute well known coinage metal - Silver, with that of rather infamous chalcogen group containing sulphur (S), Selenium (Se) and Tellurium (Te). Transition-metal chalcogenides have attracted huge attention of material scientists over past few decades for their great application potential and interesting properties in the field of optic sensors, transmission materials, solar cells, magnetic memory devices etc.

The three main minerals, Acanthite (Ag₂S), Naumannite (Ag₂Se) and Hessite (Ag₂Te) of Silver chalcogenides, were successfully synthesized by adopting simple and single step approach of ‘soft Solution Processing’. Attempts were also made to stabilise high temperature forms of silver chalcogenides by employing hydrothermal Roy-Tuttle test tube type autoclaves in the high P-T condition. Morphological studies revealed that the size development of homogenous phase of the silver chalcogenides is dependent on the duration and the amount of solvent used.
There are very few attempts and greater inconsistency associated with the reported values of the band gap energy of silver chalcogenides. Because of this reason bandgap energy of polycrystalline silver chalcogenides was determined. It is significant to note that there is a direct relationship between bandgap energy and density of the material. The bandstructures were constructed for the entire low temperature silver chalcogenide samples. Soft solution synthesis method of forming naumannite is one of the best approaches in obtaining constant bandgap energy. The necessity of working with suitable DFT functional algorithm for simulating the energy bandgap structure for each member of silver chalcogenide is established.