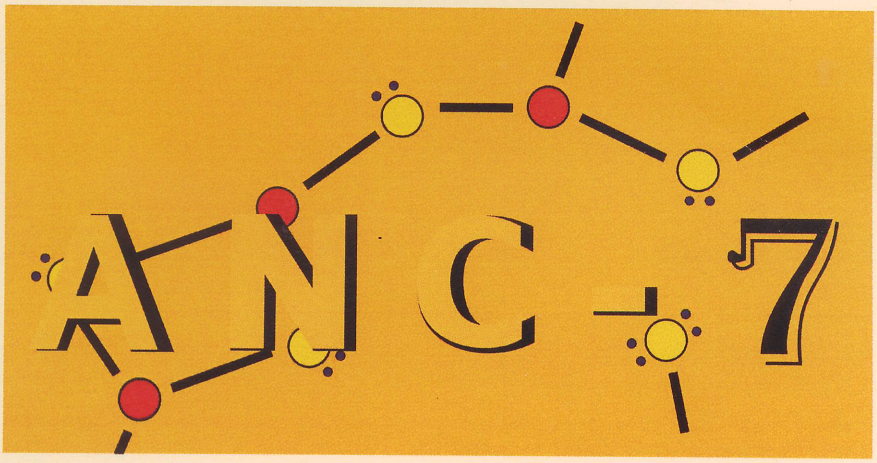

Abstract Book

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changes upon relaxation from a liquid to a solid glassy state were identified. The process of the LTPM into the HTPM polymorphoids transformation (LTPM→HTPM) occurs above the $T_{w\text{-}rev}$ temperature, on the cooling melt. Below the $T_{w\text{-}rev}$ temperature is the HTPM → LTPM reverse process. The paper discusses the structure and relaxation of such ICSs as $As_{40}Se_{60}$ and $As_{50}Se_{50}$, as well as their intermediate compounds, including the area without polymorphoid compositions. The photostructural transformations were analyzed in vitreous $As_{40}Se_{60}$ and $As_{50}Se_{50}$ .It showed that their physical and chemical nature were directly related to the interconversion of the HTPM and LTPM polymorphoids. The glass aging mechanism is a process of the HTPM into LTPM polymorphoids transformation. The aging process does not take place in absence of polymorphoids.

Oxidized surfaces studied by energy dependent luminescence in graphen-like two dimentional GeS , β-GeS_2 crystals and glassy GeS_2 after long-term ageing

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We report for the first time the results of experimental studies of room temperature photoluminescence (PL) on surface of crystalline c-GeS with 3 coordinated Ge on sulfur and β-GeS_2 with 4 coordinated Ge on sulfur after long-term aging. PL of c-GeS exhibit the excitation-dependent photoluminescence with increasing intensity of PL bands up to Eex = 4.6 eV . At Eex = 4.6 eV the PL of c-GeS exhibits a strong broad violet band centered at 3.15 eV. An analogous intense violet PL band at UV excitation is known for rutile-like GeO_2. Excitation-dependent photoluminescence of β-GeS_2 have IR, visible and UV peaks (shoulders) at 1.6, 1.85, 1.95, 2.12, 2.25, 2.37, 2.55, 2.7, 2.8, 2.95, 3.0, 3.20, 3.4 eV. In contract with PL spectra of c-GeS, excitation-dependent PL spectra of β-GeS2 exhibit increasing intensity up to Eex = 2.75 eV. For this Eex the strong broad green band centered at 2.37 eV appear. Such behavior of PL spectra of β-GeS_2 is typical for GeO_2 with quartz-like structure. Peaks observed at different positions and with different intensities in the energy dependent PL spectra could be related to the presence of different types of defects in natural oxides formed on the samples surface.
The positions of PL bands in excitation-dependent photoluminescence of aged and freshly fractured g-GeS_2(TiVj) prepared with different rate of quenching (Vj) and melt temperature (Ti) are compared and analyzed together with PL spectra of β-GeS_2.

Time-dependent density functional theory modeling of excited state AsS network forming clusters

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One of the open questions in Chalcogenide glasses is an atomistic understanding of how these glasses (and thin films derived from them) change when exposed to photons with energy greater than the bandgap of the material. Understanding these photostructural transformations might stimulate major progress in a diverse list of fields such as photonics, memory devices, and micro/nanolithography. As a first avenue of study we will present results of time-dependent density functional theory calculations of some modest sized AsS structures reminiscent of the structures believed to be present in AsS thin films. The atomic positions of these structures were first optimized using density functional theory. These structures were then re-optimized using time-dependent density functional theory; during this optimization the atoms are allowed to move under the