o.m13.p19 **Spectral distribution of the photoemission quantum efficiency and reflection for Tl-As-S crystals in far ultraviolet.** T.N. Shchurova, N.D. Savchenko, A.A. Spesivykh,V.M. Bentsa, *Uzhgorod State University, 13 Kapitulna St., Uzhgorod, 88000, Ukraine.*
Keywords: synchrotron radiation, photoemission quantum efficiency, quantum transitions.

The incorporation of thallium atoms into As-S network gives rise to the chemical bonds rearrangement resulting in the increase of conductivity for the obtained crystals of Tl-As-S family.

In this work the electronic structure determined from photoemission and optical data in the synchrotron radiation energy range from 11.0 to 21.0 eV for Tl_3AsS_3, Tl_3AsS_4, $TlAsS_2$ single crystals has been considered. Reflection spectra and spectral distribution of the photoemission quantum yield have revealed in this energy range an effective 6*s* and 5*d* electronic excitation of thallium atoms. An electron energy level diagram for thallium atoms in As-S matrix accounting for crystalline field polarization energy has been built. The observed spectral features at 15.2, 16.1, 14.35 eV have been interpreted as transitions from $5d^96s^26p5^0$, $5d^96s^26p8^0$ and $5d^{10}6s7p\ ^1P_1$ states, respectively, to the principal $5d^{10}6s^2\ ^1S_0$ state of thallium ion. The charge of the thallium ion in As-S alloys is close to +1. In As-S network thallium atoms bind together $(As_xS_y)^{-n}$ molecular complexes by ionic-covalent bonds into chained and layered networks.

The free 6*p* state of thallium ion is considered to take part in the formation of the bottom of the conduction band, reducing the forbidden band width, that results in the conductivity increase.

o.m13.p20 **Continuous Distortion of Periodic Surfaces as a Model for Phase Transitions.** S. Leoni, S.P. Piotto, R. Nesper, *Laboratory of Inorganic Chemistry, ETH Zurich, Switzerland.*
Keywords: distortion, periodic surfaces, phase transitions.

In the last years, the design of nano- and meso-scaled materials and the requirements for a control on the behaviour and properties of very complex systems under a wide range of conditions, has motivated extensive theoretical work, particularly in properly modeling phase transitions and in their energetic monitoring. Furthermore, a clear understanding of the palette of competing shapes and of their relative energetic situation for a particular system is the starting point for its control. Because of the cooperative mechanism of such phase transitions, a description of the evolution of a system in terms of deformation of a continuous, underlying surface of minimal curvature is very appropriate. The flexibility of the PNS [1,2] and Exponential Scale [3] approaches have provided for the description of a wide collection of topological phase transitions, and for the elucidation of the feasibility of a transformation. The ductility of such functions has allowed for the construction of mathematical models for systems like surfactants, aggregates and for an account of the different topologies, from lamellar to hexagonal to cubic. To the wide relevance of the low-genus minimal surfaces P, D and the Gyroide, particularly in a self-assembly context, corresponds an intensive effort in elucidating their geometric relation. The Bonnet-Transition, an isometric transformation, offers a solution for the interconversion, but shows non-continuous intermediates. Recently, an approach based on lower symmetry distortion of the cubic minimal surfaces has appeared [4].

Starting from our experience in the topological modeling of complex systems and in the elucidation of topological pathways for solid-solid reconstructive phase transitions [5], we have implemented a method for estimating the variation of curvature parameters like the Gaussian and mean curvatures along a topological phase transition. Our approach generates a discrete approximation of a surface in form of a triangular mesh.

With the help of the approximated surfaces the calculation of Gaussian and mean curvature as well as the surface energy becomes possible. The bending energy of a regular surface is estimated applying the model of the Helfrich Hamiltonian [6]. Increasing the resolution of the mesh, limiting values for the curvature have been computed.

In spite of its extreme simplicity, our method allows for a good and quick estimate of parameters that correlate in a very sensible way to topological changes, and provide starting parameters for energy calculation.

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