MATEMAATIKA-LOODUSTEADUSKOND
FÜÜSIKAINSTITUUT
TEADUS- JA ARENDUSTEGEVUSE AASTAARUANNE 2013

1. Struktuur

Füüsikainstituut, Department of Physics
Instituudi direktor Pavel Suurvarik

- Rakendusfüüsika õppetool, Chair of Applied Physics, Jüri Krustok
- Teoreetilise füüsika õppetool, Chair of Theoretical Physics, Rein-Karl Loide

2. Teadus- ja arendustegevuse (edaspidi T&A) iseloomustus

2.1 Struktuuriüksusesse kuuluvad uurimisgrupid *(kõik uurimisgrupid näidatakse aruandes eraldi, järgides alltoodud ülesehitust).*
Uurimisgrupi nimetus *(eesti ja inglise keeles)* **ja juhi nimi**

- uurimisgrupi teadustöö kirjeldus *(inglise keeles*);
- uurimisgrupi aruandeaastal saadud tähtsamad teadustulemused *(inglise keeles);*
- uurimisgrupi kuni 5 olulisemat publikatsiooni aruandeaastal.

- **Chair of Applied Physics , Jüri Krustok**

Research topics in the Chair of Applied Physics are mainly related to semiconductor physics in close collaboration with department of Materials Science. Most studies involve optical and electrical characterization of absorber materials for solar cells. Low temperature photoluminecence spectroscopy, Raman spectroscopy, capacitance spectroscopy and modulation spectroscopy are the main experimental methods. Studied materials include $Cu_2ZnSn(Se_xS_{1-x})_4$, ZnO, TiO_2, $CuInS_2$ and CdTe. In addition some ferromagnetic materials were studied in co-operation with KBFI.

Main results:

Temperature dependent ER measurements (T=100–300 K) were performed with two different CdS/CdTe solar cells. All ER spectra were fitted using Aspnes third derivative functional form. Room temperature bandgap energies Eg=1.499 eV and Eg=1.481 eV for Cell 1 and Cell 2, respectively, were found. The low value of the broadening parameter Γ for both solar cells shows a good quality of CdTe absorber layers. The formation of CdTe1−xSx solid solution in the p–n junction region was detected for both solar cells.

Admittance and photoluminescence spectroscopy were used for investigating defect levels in CZTSe/CdS and Cu2ZnSn(Se0.75S0.25)4/CdS heterojunctions.Two defect states were observed in both materials by AS.The unstable defect state showed activation energies from 87meV to 100meV in CZTSe.This defect state was attributed to the interface states because possible change of interface properties with time could cause change of activation energy.The stable deep defect state in CZTSe was found to be at 74meV and this could belong to Cu_Zn acceptor defect.

Microphotoluminescence studies of Cu2ZnSnS4 polycrystals were performed. At room temperature, two photoluminescence (PL) bands were detected at 1.39 and 1.53 eV and attributed to band-to-tail (BT) and band-to-band (BB) recombination, respectively. At lower temperatures, band-to-impurity recombination always dominates. The results show that the model of heavily doped semiconductors applies to Cu2ZnSnS4 and that, in contrast to the ternary chalcopyrites, the BT recombination in Cu2ZnSnS4 has very low intensity. The laser power dependency of the PL intensity shows that the recombination mechanism of BT and BB bands exhibits an exciton-like behavior.
The optical properties of single-crystal SnS were studied by photoreflectance (PR) spectroscopy. Temperature-dependent PR spectra were measured in the range 20–200K. A room-temperature bandgap energy value of Eg=1.317eVwas estimated by fitting the temperature dependence of the bandgap energy obtained from the PR spectra.The vibrational properties of orthorhombic SnS were studied using Raman spectroscopy. Four vibrational modes were detected at 95,163,191,and218cm–1.

Publications:

- T. Raadik, J. Krustok, R. Josepson, J. Hiie, T. Potlog, N. Spalatu. Temperature dependent electroreflectance study of CdTe solar cells. Thin Solid Films, 535 (2013) 279–282.
- E. Kask, M. Grossberg, R. Josepson, P. Salu, K. Timmo, J. Krustok. Defect studies in $Cu_2ZnSnSe_4$ and $Cu_2ZnSn(Se_{0.75}S_{0.25})_4$ by admittance and photoluminescence spectroscopy. Materials Science in Semiconductor Processing, 16 (2013) 992-996.
- Khanduri, H., Chandra Dimri, M., Vasala, S., Leinberg, S., Lõhmus, R., Ashworth, T.V., Mere, A., Krustok, J., Karppinen, M., Stern, R. Magnetic and structural studies of $LaMnO_3$ thin films prepared by atomic layer deposition. Journal of Physics D: Applied Physics, 46 (2013) 175003.
- T.Raadik, M. Grossberg, J. Raudoja, R. Traksmaa, J. Krustok. Temperature- dependent photoreflectance study of SnS crystals. Journal of Physics and Chemistry of Solids 74 (2013) 1683–1685.
- M. Grossberg, P. Salu, J. Raudoja, J. Krustok. Micro-photoluminescence study of Cu_2ZnSnS_4 polycrystals. J. Photon. Energy, 3 (2013) 030599.

Chair of Theoretical Physics, Rein-Karl Loide

– The main reseach topics are related to molecular dynamics (MD) simulations of the nanomaterials (nanotubes, graphene) and studied the physical properties of alkaline-earth metals hydroxides by density functional theory (DFT) method. The studies were performed in collaboration with the Institute of Physics of the Tartu University and Department for Solar Energy of the Institute for Energy Technology (Norway).

Main results:
Numerically studied of graphene nanoribbons (GNRs) and carbon nanotubes (CNTs) structures and have found two types of them: 1) CNT and GNR structures formed by van der Waals forces with the distance close to 0.35 nm; 2) CNT and GNR structures interconnected by short (0.17 nm) and strong chemical bonds. It appeared that the latter bonds essentially perturb conjoined carbon C_6 rings. The reason of the perturbation is the pseudo-Jahn-Teller effect.
MD simulations of recoil processes following the scattering of X-rays or neutrons have been performed in ionic crystals and metals. At small energies (<10eV) the recoil can induce intrinsic localized modes (ILMs) and linear local modes associated with these modes. The existence of highly mobile ILMs in Ni, Nb and Fe is shown.
The DFT simulations is used for comparative study on structural energetics, electronic structure, dielectric and optical properties, and chemical bonding features of alkaline-earth metals hydroxides by example of Mg(OH)2 and Ca(OH)2. The investigation employ both PBE-GGA and range-separated hybrid functional schemes. The existing of high-energy excitons in both materials is founded.

Publications:

- V Krasnenko, V Boltrushko, M Klopov, V Hizhnyakov. Conjoined structures of carbon nanotubes and graphene ribbons. Physica Scripta xx –yy ilmumas.
- V. Hizhnyakov, M. Haas, A. Shelkan and M. Klopov. Theory and MD simulations of intrinsic localized modes and defect formation in solids. Physica Scripta xx –yy ilmumas.

– Photogrammetrical study of lunar surface photographs made by the crew of Apollo 12 during their 2 extravehicular activities (EVA). We composed a 3D scene based on views from different camera station locations and find locations and dimensions of natural and artificial objects on the lunar surface. The object of the work is to compose a precise map of the landing site that would include relative positions of the Lunar Module, ALSEP instrument package, Surveyor automatic spacecraft etc. The are also planning to compose a profile map of the 200-meter Surveyor crater. It is the first accurate photogrammetric study of the Apollo 12 landing site and it continues our work on photogrammetrical map of the Apollo 11 landing site.

  Main results:

  Results of photogrammetrical study of Apollo 11 landing site, based on photographs made by the crew during the Extravehicular Activity (EVA), were prepared for publication, the corresponding article was sent to Journal of the British Interplanetary Society. Current status: feedback from anonymous referee is awaited.

  Photogrammetrical study of Apollo 12 landing site based on EVA photographs was mostly completed. As a result, a camera station map including locations of 298 camera stations was obtained for the first time. Photogrammetrically determined locations of artifacts and surface features were compared with photographic locations in Lunar Reconnaissance Orbiter Camera images, a perfect agreement was found Current status: after estimation of accuracy of the measurements, an article would be prepared.

– Algebraically one of possible representations of Indian sacred diagram Sriyantra. The object was to compose a full system of equations describing the diagram, to find their mathematical solution and to prove its uniqueness. We challenged the statement of mathematical complexity of the figure (A.P.Kulaichev, Sri Yantra and its Mathematical Properties. Indian Journal of History of Science. 1984, Vol. 19(3), pp 279-292) and proved that an accurate solution may be found without use of complicated techniques.

  Main results:

  One of possible representations of Indian sacred diagram Sriyantrawas studied. The full set of algebraic equations describing the yantra was put out and studied analytically and numerically, the algebraic solution was found and its uniqueness was proved. The corresponding article was prepared for Indian Journal of History of Science. Current status: feedback from anonymous referee is awaited.

2.2 Loetelu struktuuriüksuse töötajate rahvusvahelistest tunnustustest.

2.3 Loetelu struktuuriüksuse töötajatest, kes on välisakadeemiate või muude oluliste T&A- ga seotud välisorganisatsioonide liikmed.

2.4 Soovi korral esitatakse aruandeaastal saadud T&A-ga seotud tunnustused (va punktis 2.3 toodud tunnustused), ülevaade teaduskorralduslikust tegevusest, teadlasmobiilsusest ning hinnang oma teadustulemustele.