# DF 4 Poster

Zeit: Samstag 08:30–16:30 Raum: Poster TU C

DF 4.1 Sa 08:30 Poster TU C

**Numerical Study of the Fabrication Tolerance in Photonic Crystal Devices** — •Javad Zarbakhsh, Farnaz Ghods Isfahani, and Kurt Hingerl — Christian Doppler Labor fuer Oberflaechenoptische Methoden, Institut fuer Halbleiter und Festkoerperphysik, Universitaet Linz, A-4040 Linz, Austria

We studied the fabrication tolerance and design flexibility of conventional Photonic Crystals(PC) structures. In fact, theoretically how flexible the PCs could be regarding to change of periodicity and the size of the elements to retain the favorable band gap width. Adhering to some constraints the changes in the photonic band gap width is negligible and the confine modes do not penetrate the PCs. The results of Finite Difference Time Domain (FDTD) are in agreement with the results of plain wave expansion (PWE). This brings another degrees of freedom for designing of the photonic crystal nanodevices.

DF 4.2 Sa 08:30 Poster TU C

**Photoconductivity measurements at the surface of titanium dioxide** — •Roger Amade[1], Sylvio Indris[1], Paul Heitjans[1], Andreas Haeger[2], Mina Finger[2], and Diethardt Hesse[2] — [1]Institut für Physikalische Chemie und Elektrochemie, Universität Hannover, 30167 Hannover, Germany. — [2]Institut für Technische Chemie, Universität Hannover, 30167 Hannover, Germany.

The electrical photoconductivity $\sigma_{ph}$ and conductivity $\sigma$ at the surface of a $TiO_2$ single crystal (rutile) was studied in a range of temperatures between 300 K and 573 K and under different ambient gases (oxygen and nitrogen) by means of impedance spectroscopy. The long times required (many hours) to reach steady state photoconductivity suggests the presence of slowly emptying traps. A single exponential could be used to fit the rise curves. In the dark, surface adsorbed oxygen gas acts as a recombination center increasing the decay rate of the photoconductivity. At about 473 K a maximum is observed in the equilibrium photoconductivity and a minimum in the rate constants of the rise and decay.

DF 4.3 Sa 08:30 Poster TU C

**Structure and latticedynamics in Bismuth Triborate, $BiB_3O_6$** — •W.-D. Stein[1], A. Cousson[2], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Laboratoire Léon Brillouin, C.E.A./ C.N.R.S., France

Bismuth Triborate, $BiB_3O_6$, is a particularly interesting material due to its outstanding non-linear optical properties [1,2], such as second harmonic generation and stimulated raman scattering. We are interested in the influence of the electron lone-pair on these effects, which is located at the bismuth-ion and was not included in the methods used to explain the measured features of optical nonlinearity [3]. We present a study of the structural properties with combined x-ray and neutron diffraction experiments at different temperatures. We find a temperature dependent shift of the bismuth ion with respect to the boron and oxygen ions which are not affected so much. This shift corresponds to a stronger localisation of this lone-pair. We also present our results of an inelastic neutron scattering experiment for determining the phonon dispersion curves. The effect of the lone-pair on the dispersion should be perceivable at the boundary of the brillouin zone, so that a neutron experiment was necessary to study their contribution.

[1] H. Hellwig *et al.* Solid State Comm. **109**, 249 (1999)
[2] A. Kaminskii *et al.* Opt. Comm. **206**, 179 (2002)
[3] D. Xue *et al.* Solid State Comm. **114**, 21 (2000)

DF 4.4 Sa 08:30 Poster TU C

**Theorie des Wärmeübertrags in einem UHV-Rasterthermomikroskop** — •Daniel Reddig, Svend-Age Biehs, Stefan Pieper und Martin Holthaus — Institut für Physik, Carl von Ossietzky Universität Oldenburg, D-26111 Oldenburg

Experimentelle Ergebnisse für den abstandsabhängigen Wärmestrom zwischen Sondenspitze und Probe eines UHV-Rasterthermomikroskops zeigen immer noch große Unterschiede zur bisherigen Beschreibung durch die Theorie. Auf unserem Poster zeigen wir, wie man über eine Bornsche Näherung die Greensche Funktion für die Anordnung eines sehr kleinen dielektrischen Körpers über einer dielektrischen Platte hinreichend gut approximieren kann. Die dadurch gewonnene recht einfache Greensche Funktion wird dann benutzt, um den Wärmestrom zwischen dem kleinen Körper und der Platte zu bestimmen. Die mit dieser Modellrechnung gewonnenen Ergebnisse liefern eine gute Beschreibung der Abstandsabhängigkeit des Wärmestroms in einem UHV-Rasterthermomikroskop.

DF 4.5 Sa 08:30 Poster TU C

**Wärmeabstrahlung einer Kugel** — •Stefan Pieper, Svend-Age Biehs, Daniel Reddig und Martin Holthaus — Institut für Physik, Carl von Ossietzky Universität Oldenburg, D-26111 Oldenburg

Die Berechnung der Strahlungswärmeverluste kleiner dielektrischer Körper hat im Rahmen der UHV-Rasterthermomikroskopie zunehmend an Bedeutung gewonnen. Auf unserem Poster wird gezeigt, wie Greensche Funktionen in sphärischer Geometrie berechnet und mit ihnen die Wärmeabstrahlung einer Kugel ins Vakuum numerisch exakt bestimmt werden kann. Untersucht werden die Material- und Abstandsabhängigkeiten des Wärmestroms sowie der Einfluß des Kugelradius' auf die Modenstruktur.

DF 4.6 Sa 08:30 Poster TU C

**Das fluktuierende Nahfeld einer dielektrischen Platte** — •Svend-Age Biehs, Stefan Pieper, Daniel Reddig und Martin Holthaus — Institut für Physik, Carl von Ossietzky Universität Oldenburg, D-26111 Oldenburg

Die Anwendung der Rytov'schen fluktuierenden Elektrodynamik auf einen unendlich ausgedehnten Halbraum mit einer gegebenen Permittivität, der an das Vakuum angrenzt, gibt das bekannte Kirchhoff-Plancksche Strahlungsgesetz und damit für den Fall des Schwarzen Strahlers das Stefan-Boltzmann-Gesetz zurück. Ein Vorteil der Rytov'sche Formulierung besteht darin, dass zusätzlich der Einfluss der evaneszenten Moden auf die Energiedichte im Nahfeld des dielektrischen Körpers untersucht werden kann. Betrachtet man endlich ausgedehnte Körper, findet man eine Modifikation des Kirchhoffschen Strahlungsgesetzes und der Energiedichte im Nahfeld des Körpers in Abhängigkeit von seiner Größe. Dieser Endlichkeitseffekt wird für den Fall einer dielektrischen Platte diskutiert.

DF 4.7 Sa 08:30 Poster TU C

**All-electron and pseudopotential calculations for PZT** — •Igor Chaplygin, Sibylle Gemming, and Gotthard Seifert — Institut für Physikalische Chemie und Elektrochemie, TU Dresden, D-01062 Dresden

Perovskites of the $PbZr_{(1-x)}Ti_xO_3$ (PZT)type are the most important ferroelectric materials. The main aim of the current study, carried out in the framework of the DFG project "Ferroic functional elements: physical basics and concepts", was the comparison of the results obtained using a pseudopotential code (ABINIT) with those of precise full-electron calculations. The latter were obtained using the FPLO (full-potential local-orbital) calculation scheme. Both schemes are based on density functional theory in local-density approximation. The structural and electronic ground state properties of PZT were studied for $x$=0.00,0.25,0.50,0.75, and 1.00. Several types of the atomic pseudopotentials were tested. We found that the Teter extended norm-conserving pseudopotential gives most reliable results for all compositions, the lattice constant being slightly underestimated compared with that given by FPLO. The pseudopotential code was used for the optimization of the crystal structure. The resulting ground state crystal structures are in good agreement with experiment and other theoretical calculations.

DF 4.8 Sa 08:30 Poster TU C

**Messung und Modellanpassung nichtlinearer Eigenschaften einer Metall-Ferroelektrikum-Silizium Struktur** — •M. Diestelhorst[1], K. Barz[1], H. Beige[1], B. Mereu[2] und M. Alexe[2] — [1]Martin-Luther-Universität Halle-Wittenberg, Fachbereich Physik Friedeman-Bach-Platz 6, Halle, 06108 — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, Halle, 06120

Untersuchungen an Metall-Ferroelektrikum-Silizium (MFS) Strukturen sollen die Anwendbarkeit eines Modells überprüfen, welches aus der allgemeinen Theorie des MOS-Kondensators abgeleitet wurde. Die untersuchte Probe besteht aus einer 300nm dicken ferroelektrischen Schicht ($Bi_4Ti_3O_{12}$), aufgebracht auf der $SiO_2$-Schicht eines p-Si-Wavers. Wird die Probe als nichtlineare Kapazität eines seriellen Schwingkreises ver-

wendet, zeigt sich eine Amplituden-Frequenz-Charakteristik, deren Verlauf mit bestehenden Modellrechnungen verglichen werden soll. Dazu wurden Netzwerkanalysen des Schwingkreises und Kapazitäts- Spannungsmessungen der Probe durchgeführt und ausgewertet.

DF 4.9 Sa 08:30 Poster TU C

**X-ray induced polarisation degeneration in ferroelectric thin films** — •A. Solbach[1], J.L. Cao[1], U. Böttger[2], U. Ellerkmann[2], P. Gerber[2], P.J. Schorn[2], R. Waser[2] und U. Klemradt[1] — [1]II. Physikalisches Institut B, RWTH Aachen, Germany — [2]Institut für Werkstoffe der Elektrotechnik 2, RWTH Aachen, Germany

X-rays are an important tool for sample characterisation and the influence of x-rays is in general negligible. However, in conjunction with ferroelectric thin films and in-situ studies of electrical properties this assumption has to be reconsidered.

The influence of 11 keV x-rays on the electrical properties of ferroelectric $Pb(Zr_{0.3}Ti_{0.7})O_3$ (PZT) thin film capacitors has been studied using synchrotron radiation from HASYLAB bending magnet beamline E2. The 220 nm thick films were deposited by chemical solution deposition on a $Pt/TiO_2/SiO_2/Si$ substrate. The Pt top electrode was 70 nm thick.

The capacitors (370 $\mu$m × 370 $\mu$m) have been irradiated at grazing incidence ($\alpha_i = 0.7°$) with various doses up to 1200 kGy at ≈ 54 kGy/h. The x-ray dose does have an influence on the electrical properties, depending on the polarisation state during irradiation. The remanent polarisation and the coercitive voltage are decreased by 40% and the effect of imprint is enhanced. Subsequent continuous switching was able to recover 75% of the remanent polarisation as compared to unirradiated samples.

DF 4.10 Sa 08:30 Poster TU C

**Effects of the fabrication process and thermal treatment on $Pb(Zr_{0.3}Ti_{0.7})O_3$ thin films** — •Jiang-Li Cao[1], A. Solbach[1], T. Weirich[2], J. Mayer[2], U. Böttger[3], P.J. Schorn[3], P. Gerber[3], R. Waser[3], and U. Klemradt[1] — [1]II. B Physikalisches Institut, RWTH Aachen — [2]Gemeinschaftslabor für Elektronenmikroskopie, RWTH Aachen — [3]Institut für Werkstoffe der Elektrotechnik 2, RWTH Aachen

The effects of the fabrication process and annealing treatment on the structure of $Pb(Zr_{0.3}Ti_{0.7})O_3$(PZT) thin films prepared by chemical solution deposition on Pt/Ti oxide electrodes were investigated. By using atomic force microscopy (AFM) and transmission electron microscopy (TEM), the microstructures of the samples were examined. The density, surface and interface roughness as well as the thickness of each layer were determined using x-ray specular reflectivity. The structure of the PZT thin films was found to be influenced by the thermal history to a great extent. The Pt surfaces become roughening after the annealing treatment. A density decrease of the Pt bottom and top electrodes upon annealing was observed. The x-ray reflectivity and TEM observations revealed a sublayer structure of the PZT ceramic induced by the different annealing treatment. Based on the results obtained, the influences of the thermal-induced structure changes on the electrical properties were examined.

DF 4.11 Sa 08:30 Poster TU C

**Structural and electrical characterization of multiferroic $BiFeO_3$ thin films** — •Claus-Henning Solterbeck, Mohamed Bouazza, Serguei Iakovlev, and Mohammed Es-Souni — Institute for Materials and Surface Technology, University of Applied Sciences, Kiel

Pure and Gd-doped polycrystalline $BiFeO_3$ thin films were fabricated by chemical solution deposition. The microstructural characterization was performed by X-ray diffractometry, electron microscopy, and atomic force microscopy. The films show a preferred out-of-plane orientation of (100) (pseudocubic). Annealing in oxygen instead of air leads to smaller roughness and grain size.

Emphasis was put on the electrical properties, which were characterized by measurements of the polarization, leakage current, and impedance as well as the piezoeletric coefficient. The films have a relatively weak ferroelectric polarization, $2\,P_r$, of approximately $1\,\mu C/cm^2$ and a low frequency dispersion of the dielectric constant. The resistance depends drastically on the atmosphere during crystallization with an increase by two orders of magnitude when annealing in oxygen. The piezoeletric coefficient $d_{33}$ of samples annealed in oxygen has a value of $12\,pm/V$.

Preliminary magnetic measurements are reported, too. $BiFeO_3$ has a small magnetic hysteresis with a coercitivity of 230 G.

DF 4.12 Sa 08:30 Poster TU C

**Ionic Motion in Ion Beam Sputtered Thin Film Glasses** — •Frank Berkemeier and Guido Schmitz — Institut für Materialphysik, Wilhelm–Klemm–Str. 10, 48149 Münster, Westfählische–Wilhelms–Universität Münster

Ion-conducting, amorphous thin films of a thickness between 50 nm and 1 $\mu$m are prepared using the ion beam sputter technique. A sodium borate glass of the composition $0.20\,Na_2O \cdot 0.80\,B_2O_3$ serves as the target. The glass layers are deposited on a silicon substrate between two sputtered silver electrodes. Temperature-dependent electrical measurements on the glass films performed by impedance-spectroscopy and direct-current technique reveal a specific dc-conductivity of the films independent of their thickness but about one order of magnitude higher than the dc-conductivity of the target material. The activation enthalpies of the dc-conductivity are found to be about $20\,kJ\,mol^{-1}$ less compared to that of the bulk material. Cross-section investigations obtained by TEM give inside in the surface reactions between the solid electrolyte and the silver electrode after the flow of an ionic current caused by impedance-spectroscopy or dc-measurements, respectively.

DF 4.13 Sa 08:30 Poster TU C

**Optical detection of ferroelectric domain orientation on the subwavelength scale** — •Thomas Härtling and Lukas Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Ferroelectric crystals are promising materials for applications in new information storage devices. These memories record information encoded in the direction of the remanent polarization of the material. Commercially available devices so far read and write information by addressing storage positions electrically. As optical methods of data transportation and processing advance, the challenge arises to read and write information in such devices optically allowing for higher working speed.

Here, we present a method which facilitates "optical reading"of the polarization state in a ferroelectric material. The process makes use of optical properties of nobel metal clusters dispersed on the surface of a ferroelectric material and their dependence on the surrounding medium. The process is able to resolve domain dimensions below the diffraction limit.

DF 4.14 Sa 08:30 Poster TU C

**Phase formation sequence during thin film solid-state reactions in the BaO-$TiO_2$ system** — •Andriy Lotnyk, Andreas Graff, Stephan Senz, and Dietrich Hesse — Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle, Germany

A $BaCO_3$ target is e-beam evaporated in a high vacuum system with an oxygen background pressure of $1 \times 10^{-2}$ Pa. The single crystal $TiO_2$ rutile substrate is heated between 300°C and 900°C. Reaction products are investigated by XRD and analytical TEM (EELS). A deposition at 500°C followed by solid-solid reaction at 600°C for 30 min produced the metastable intermediate $Ba_2TiO_4$ phase without any evidence of $BaTiO_3$ formation. It may be explained by Ti diffusion into the BaO thin film. The epitaxial relationship of the $Ba_2TiO_4$ (B2T) to the (110) rutile surface (T) is $(110)_{B2T} \parallel (110)_T$ and $[001]_{B2T} \parallel [001]_T$. The $Ba_2TiO_4$ phase is completely decomposed after two weeks of storage in air by reaction with $H_2O$ and $CO_2$. A gas-solid and solid-solid reaction at 700°C and 800°C leads to the formation of $BaTiO_3$ and $Ba_2TiO_4$. The orientation relationship of the $Ba_2TiO_4$ changes compared to the 600°C solid-solid reaction.

A gas-solid reaction at 900°C resulted in large pores between the substrate and the thin film. The film was converted almost completely to a Ti-rich phase covered by the remaining $BaTiO_3$. The Ti-rich phase was identified by pole figure analyses as $Ba_4Ti_{12}O_{27}$.

DF 4.15 Sa 08:30 Poster TU C

**Dielectric Spectroscopy of Glass Behaviour in Mixed Betaine Phosphate/Betaine Phosphite Crystals** — •Juras Banys[1], Georg Voelkel[2], Carola Klimm[2], and Jan Macutkevic[1] — [1]Faculty of Physics, Vilnius University, Sauletekio 9, Vilnius 10222, Lithuania — [2]Fakultaet fuer Physik, Universitaet Leipzig, Linnestr 5, Leipzig D - 04103, Germany

The complex permittivity of mixed protonated and deuterated crystals BPx/BPI1-x (with x = 0.15 to 0.5) has been studied in a wide frequency range (20Hz-1MHz). The distribution of relaxation times have been obtained directly from dielectric spectra. The parameters of the double-well potentials of the hydrogen bonds, the local polarization distribution

function and the glass order parameter have been extracted from the distribution of relaxation times. An unusual result is that in contradiction to usual proton glasses the average of asymmetry A0 of the local potentials of the hydrogen bonds is nonzero, and does disappear only at low temperatures. The nonzero average of the local polarization asymmetry can be interpreted as result of a finite average cluster polarization which is averaged out at macroscopic scale. The cluster nature is unknown up to now. The new interesting result from dielectric spectroscopy is the vanishing of this cluster polarization at low temperatures. One could suspect that this disappearance of the cluster polarization is related with the real glass transition into the low-temperature nonergodic glass phase. One can conclude that the glassy behavior of the quasi-one dimensional protonated and deuterated mixed crystals BPx/BPI1-x is qualitatively different from that one in KDP-type orientational glasses.

DF 4.16 Sa 08:30 Poster TU C

**Investigation of Slow Li Diffusion in Amorphous Lithium Niobate by Multiple Time Spin-Alignment Echo NMR Spectroscopy** — •Martin Wilkening and Paul Heitjans — Universität Hannover, Institut für Physikalische Chemie und Elektrochemie

Recently, three-dimensional Li diffusion in amorphous $LiNbO_3$ was investigated by temperature (140 K $\leq T \leq$ 450 K) and frequency (23 MHz $\leq \omega_0/2\pi \leq$ 78 MHz) dependent spin-lattice relaxation NMR [1]. Measurements of the spin-lattice relaxation rate $T_1^{-1}$ had to be restricted to below 450 K in order to avoid crystallization of the sample. Thus, only the low-temperature flank of the diffusion induced peak of $T_1^{-1}$ was experimentally accessible yielding information about short-range Li diffusion. Long-range diffusion parameters below 450 K, however, can be probed, e. g., by multiple time stimulated-echo NMR spectroscopy, being sensitive to slow Li dynamics. Jump rates extracted from spin-alignment echo decays exhibit Arrhenius behaviour between 293 K and 413 K with an activation energy of 0.41(1) eV. This value is in good agreement with the activation energy of the not accessible high-temperature flank of the relaxation peak $T_1^{-1}(1/T)$. The latter one was predicted to be about 0.4 eV [1] taking into account the frequency dependence of the diffusion induced spin-lattice relaxation rates on the low-$T$ flank.

[1] M. Wilkening, D. Bork, S. Indris, and P. Heitjans, Phys. Chem. Chem. Phys. **4**, 3246 (2002).

DF 4.17 Sa 08:30 Poster TU C

**Mixed Alkali Effect in (Li, Na) Niobium Silicate Glasses – Probing Cation Dynamics by Impedance Spectroscopy and by Solid-Echo and Multiple-Time Spin-Alignment Echo $^7$Li NMR Spectroscopy** — •Muayad Masoud[1], Martin Wilkening[1], Rudolf Winter[2], and Paul Heitjans[1] — [1]Universität Hannover, Institut für Physikalische Chemie und Elektrochemie, Callinstraße 3-3a, 30167 Hannover, Germany — [2]University of Wales, Institute of Mathematical and Physical Sciences, Ceredigion SY23 3BZ, Wales, UK

Glasses with the composition $\frac{1}{3}[x\,Li_2O,(1-x)Na_2O]:\frac{1}{3}Nb_2O_5:\frac{1}{3}SiO_2$ $(0 \leq x \leq 1)$ were prepared by conventional quenching of the corresponding molten oxides. Conductivities $\sigma_{dc}$ probed by impedance spectroscopy exhibit a typical minimum at $x \approx 0.4$ whereas the corresponding activation energies (0.61(1) eV $\leq E_A^{\sigma_{dc}} \leq$ 0.91(1) eV) show a maximum at this composition (mixed alkali effect). In contrast to the $\sigma_{dc}$ measurements detecting the overall cation diffusion, with multi-pulse NMR techniques the Li and Na diffusion can be studied separately from each other. For instance, solid-echo $^7$Li NMR line narrowing showed an enhancement of Li diffusivity with both increasing temperature and Li content $x$. Consistently, lithium jump rates $\tau_{echo}^{-1}$, directly probed by recording two-time correlation functions via spin-alignment echoes, decrease exponentially with the introduction of Na ions. The corresponding activation energies $E_A^{echo}$ increase with increasing Na content.

DF 4.18 Sa 08:30 Poster TU C

**Strukturelle Phasenübergänge mit Protonenordnung in $TlH_2PO_4$** — •In-Hwan Oh, Stefan Mattauch und Gernot Heger — Institut für Kristallographie der RWTH Aachen, 52056 Aachen

$TlH_2PO_4$ gehört zu den $X(H,D)_2PO_4$-Verbindungen der KDP-Familie (X = K, Rb, Tl, Cs), die sich durch interessante ferroische Eigenschaften auszeichnen. Charakteristisch ist eine reiche Polymorphie mit vielen Phasenübergängen, die durch H/D-Ordnung in Wasserstoffbindungen hervorgerufen werden. Protonierte und deuterierte Verbindungen zeigen einen Isotopen-Effekt ($T_C$-Werte bzw. Polymorphismus unterschiedlich). Durch Neutronenbeugung an Einkristallen kann die H/D-Verteilung detailliert untersucht werden. Die Kristallstruktur der orthorhombischen Hochtemperaturphase von $Tl(H,D)_2PO_4$ (RG P 2/c $2_1$/a $2_1$/n) ist gekennzeichnet durch $n(H,D)_2PO_4$-Doppelschichten, die durch Wasserstoffbindungen verbrückt sind. Alle drei unterschiedlichen O-(H,D)-O Bindungen sind fehlgeordnet. Die (H,D)-Verteilung lässt sich entsprechend einem Doppelminimumpotential beschreiben. Die ferroelastische Phase von $TlH_2PO_4$ unterhalb von 350 K (RG P 1 $2_1$/a 1) zeigt eine partielle Protonenordnung mit einer asymmetrischen O-H$\cdots$O-Bindung. Mit sinkender Temperatur verstärkt sich diese Asymmetrie und bei 230 K wird der Übergang zu einer antiferroelektrischen Struktur (RG P $\bar{1}$) erreicht, die eine komplette Protonenordnung aufweist.

DF 4.19 Sa 08:30 Poster TU C

**Broadband Dielectric Spectroscopy of Water confined in MCM-41 Molecular Sieve Materials** — •Banys Juras[1], Kinka Martynas[1], Meskauskas Agnius[1], Poeppl Andreas[2], Voelkel Georg[2], Boehlmann Winfried [2], Umamaheswari Venkatesan [2], and Hartmann Martin[3] — [1]Faculty of Physics, Vilnius University, Sauletekio 9, 2040 Vilnius, Lithuania — [2]University of Leipzig, Faculty of Physics and Geoscience, Linnéstr. 5, D-04103 Leipzig, Germany — [3]Department of Chemistry, Chemical Technology, University of Kaiserslautern, Erwin-Schrödinger-Str. 54, D-67663 Kaiserslautern, Germany

Dielectric properties of water adsorbed in pure siliceous and aluminum containing mesoporous MCM - 41 materials have been investigated in the frequency range 20 Hz to 1 MHz. The dielectric spectra revealed three dispersion regions, liquid like free water in the center of the mesopores, an intermediate water layer with reduced mobility, and an interfacial water layer at the inner surface of the mesopores. The latter displays features of the glassy state of a hydrogen-bonded system although the temperature dependence of the mean relaxation time follows the Arrhenius law. The analysis of the relaxation time distribution by means of a double well potential indicates a strong dependence of the water hydrogen bond strength in the interfacial layer on the framework aluminum concentration. Typical saddle point have been obtained for the relaxation time at higher temperatures.

DF 4.20 Sa 08:30 Poster TU C

**Nanoindentierungen an $SrTiO_3$ Einkristallen zum Beginn der plastischen Deformation** — •Andre Belger, Beate Bergk und Peter Paufler — Institut für Strukturphysik der Fachrichtung Physik, TU Dresden , D-01062 Dresden, Germany

Mit einem Nanoindenter Hysitron TriboScope wurden mittels konischem Indenter (Öffnungswinkel 60°) mit sphärischer Spitze (Spitzenradius 400 nm) Eindruckversuche an {100}, {110}- und {111}-orientierten Oberflächen von einkristallinem $SrTiO_3$ (Lieferant: Crys Tec) bei Raumtemperatur durchgeführt. Die Kraft - Eindringtiefen - Kurven weisen nach anfänglicher reiner elastischer Verformung oberhalb von 500 $\mu$N Tiefensprünge bei konstanter Kraft (‚pop-in') auf die mit irreversibler Verformung verbunden waren. Nach der Entlastung zeigten sich an der Oberfläche der Einkristalle im Einklang mit der jeweiligen Oberflächensymmetrie scharfe Gleitbänder entlang von Geraden, die sich vom Eindruck ausgehend mit zunehmender Last in den Kristall ausbreiteten. Diese Oberflächenspuren können auf Gleitebenen des Typs {011} oder {100} zurückgeführt werden. Aus der Auftragung der ‚pop-in'-Tiefe $\Delta h$ über dem Kontaktdruck $p$ bei Beginn der plastischen Vorformung konnte durch Extrapolation $\Delta h \Rightarrow 0$ ein kritischer Kontaktdruck von 22 GPa für (111)- und 20 GPa für (110)-Indentierung bestimmt werden. Der Anstieg $\delta(\Delta h)/\delta p$ ist für die Probe mit (111) Orientierung (2.62nm/GPa) etwa 40 % größer als für die (110) Probe (1.84nm/GPa). Die Entlastung nach dem ‚pop-in' erfolgt entgegen der Erwartung nicht rein elastisch, sondern ist bei nachfolgender Belastung mit Energiedissipation verbunden. Dies deutet auf eine druckinduzierte Phasenumwandlung hin.

DF 4.21 Sa 08:30 Poster TU C

**DIELECTRIC RELAXATION IN STRONTIUM TITANATE CONTAINING A- AND B- SUBSTITUTIONS** — •Andrey Sotnikov[1,2], Elena Smirnova[2], Wolfgang Hässler[1], Manfred Weihnacht[1], and Vladislav V. Lemanov[2] — [1]Leibniz Institute for Solid State and Materials Research Dresden, Dresden, Germany — [2]A.F.Ioffe Physical-Technical Institute, St. Petersburg, Russia

Over the many years a number of ferroelectrics and high permittivity systems closely related to ferroelectrics showing a strong dielectric relaxation, have been studied. Some of them were solid solutions based on Sr-

TiO3 and KTaO3 incipient ferroelectrics. In the present work, we studied systematically the effect of A-, B- and complex A- and B- simultaneous substitution in SrTiO3 on dielectric relaxation processes. For this purpose ceramic samples of strontium titanate containing Pb(2+), Ba(2+), Zr(4+), and Pb(2+)Zr(4+) were prepared. Dielectric spectra were measured between 0.1 Hz and 1 MHz in a wide temperature range from 4.2 K to 400 K. A well-developed dielectric relaxation of different types (from simple Debye-type to relaxor-type with broad distribution of relaxation times) were observed. The main features and possible mechanisms of the relaxation are discussed.

DF 4.22 Sa 08:30 Poster TU C

**Broadband dielectric spectroscopy of 0.4PZN-0.3PMN-0.3PSN ceramics** — •Juras Banys[1], Jan Macutkevic[1], Algirdas Brilingas[1], Karlis Bormanis[2], Andris Sternberg[2], and Vismant Zauls[2] — [1]Faculty of Physics, Vilnius University, Lithuania — [2]Institute of Solid state Physics, University of Latvia, Latvia

Dielectric properties of 0.4PZN/0.3PSN/0.3PMN ceramics in the frequency range 20 Hz to 100 THz and temperature range 20 K to 500 K ranges are reported. At higher temperatures dielectric dispersion occurs in microwave and THz range. At low temperatures anomalous broadening of dielectric dispersion has been observed. Distribution of relaxation times has been calculated directly from dielectric spectra. Over the temperature of the maximum permittivity, the distribution of the relaxation times is symmetrically shaped. At lower temperatures, the distribution of relaxation times becomes asymmetrically shaped. On further cooling the second maximum appears.