58th EHPRG

MEETING PROGRAMME

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Tuesday, September 8

Registration (8:30-16:45)

Oxides, MOFs and Inorganic compounds **(TEIDE** room**)**
Chair: J. Prchal

9:00-9:30 Invited: (E. Uykur) **High pressure infrared spectroscopy study on elemental tellurium: emergence of Weyl state and the high pressure polymorphs.**

9:30-9:45 (A. Celeste) **High pressure response of the mesoporous metal-organic framework MIL-101**

9:45-10:00 (A. Segura**) Pressure behavior of polar phonons in hexagonal and wurtzite boron nitride.**

Geophysics oriented **(TENO** room**)**
Chair: J. A. González

9:00-9:30 Invited (J.A. Sans) **New non-polar polymorph of Fe_2O_3 found at high-pressures**

9:30-9:45 (Qingyang Hu) **Reservoirs and behavior of hydrogen in Earth's lower mantle**

9:45-10:00 (M. Belov) **High pressure rhenium carbides: an *ab initio* description**

10:00-10:30 ***Coffee Break***

Chemistry at High Pressure (TEIDE Room**)**
Chair: R. Caracas

10:30-11.00 Invited (A. Otero de la Roza) **Unusual bonding and computational challenges under pressure.**

11:00-11:15 (A. Courac) **High pressure synthesis of new carbides of alkali and alkali earth metals.**

11:15-11:30 (K. F. Dziubek) **Stress-driven phase transitions in urotropine and other molecular cage compounds.**

11:30-11:45 (A. Grzelak) **Exploring the phase diagram of Ag/Cl_2 system by means of DFT and hybrid-DFT calculations.**

Pressure behavior of polar phonons in hexagonal and wurtzite boron nitride

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Keywords: high pressure, dielectric properties, lattice dynamics, polar phonons, FTIR, phase transition.

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This abstract report an investigation of the pressure behavior, up to 20 GPa, of the polar phonons in hexagonal (h) and wurtzite (w) boron nitride, by means of FTIR reflection and transmission measurements in diamond anvil cell.

The in-plane E_{1u} and out-of-plane A_{2u} infrared-active phonons of layered hexagonal boron nitride exhibit a highly anisotropic behavior. Infrared reflectivity spectra at normal incidence on high-quality single crystals show strict fulfillment of selection rules and an unusually long E_{1u} [transverse-optic (TO)] phonon lifetime. Accurate values of the dielectric constants at ambient pressure $\varepsilon_{0\perp}$ = 6.96, $\varepsilon_{\infty\perp}$ =4.95, $\varepsilon_{0\parallel}$ = 3.37, and $\varepsilon_{\infty\parallel}$ = 2.84 have been determined from fits to the reflectivity spectra, including interference fringe pattern.

The out-of-plane A_{2u} phonon reflectivity band is revealed in measurements on an inclined facet, and absorption measurements at an incidence angle of 30°, allowing us to observe both the transverse- and longitudinal-optic A_2u modes.

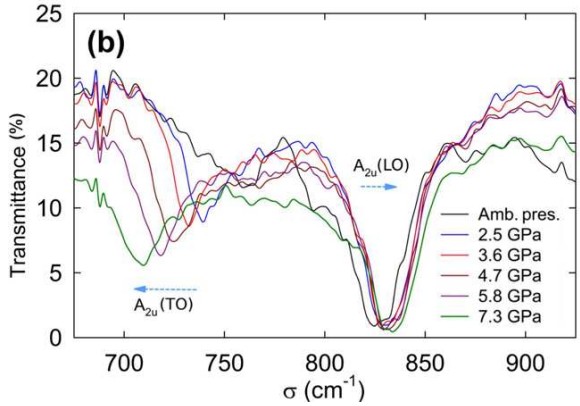

Figure 1: Pressure behavior of A_{1u} (LO and TO) in h-BN

Pressure coefficients and Grüneisen parameters for all infrared-active modes are determined and compared with ab initio calculations. While Grüneisen parameters are generally small in this layered crystal, the A_{2u}(TO) displays an exceptionally large and negative Grüneisen parameter that results in widening of the type I hyperbolic region with increasing pressure. Softening of the A_{2u}(TO) mode is induced by dynamical buckling of the flat honeycomb layers.

The layered hexagonal phase becomes unstable at 10 GPa and the transition to the wurtzite phase is completed at about 13 GPa. The phase transition is nonreversible and the optical features of the metastable wurtzitic phase are retained after a pressure cycle from 20.5 GPa down to ambient pressure. This allows the infrared-active optical phonons and the dielectric properties of the cold-pressed wurtzitic boron nitride sample to be studied over the whole range of pressures.

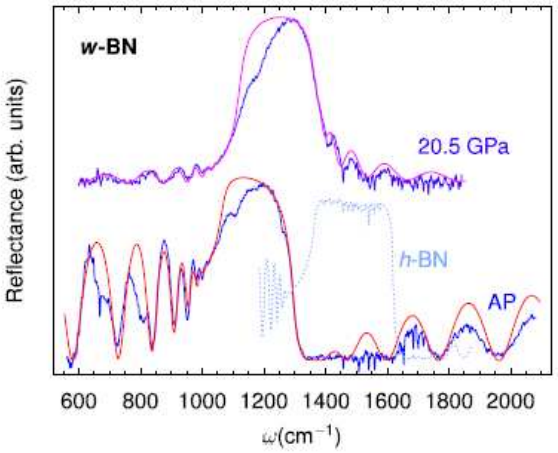

Figure 2. IR reflectance spectrum of w-BN at 20.5 GPa and ambient pressure, compared to the IR reflectance of h-BN.

Experimental permittivity values of ε_0 = 6.65 ± 0.03 and ε_∞ = 4.50 ± 0.05 are determined from fits to the reflectance spectra at ambient pressure. Accurate values of the refractive index in the mid-infrared and visible−ultraviolet regions are evaluated from the interference patterns.

Contrary to the h-BN case, the refractive index of w-BN decreases slightly with pressure, on account of the much lower compressibility of the close-packed structure. The pressure coefficients for the longitudinal optical and transverse optical modes are determined, and an overall good agreement with ab initio calculations is found.

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