Report on the research activity of
Dr. Hab. Juris PURANS
performed at the CNR-IFN, Istituto di Fotonica e Nanotecnologie. UoS di Trento
STM program (12 April -17 may 2010)

Proponente: **Dr. Francesco Rocca**

Fruitore: **Dr. Hab. Juris Purans**

Istituto di afferenza del Fruitore: **Institute of Solid State Physics, University of Latvia**

Kengaraga street 8, LV-1063 Riga LATVIA

Descrizione dettagliata dell'Istituzione ospitante:

CNR-IFN, Istituto di Fotonica e Nanotecnologie. UoS di Trento.

Via alla Cascata 56/c , 38123 POVO (Trento) FAX: 0461314875 .

Numero di codice del dipartimento (v. All.2) **Cod:7: Materiali e Dispositivi**

Titolo del programma: **Femtometer accuracy EXAFS studies: isotopic effect in the first, second and third coordination shells of germanium**

Obiettivi. Recently, we measured temperature-dependent EXAFS on the two isotopes ^{70}Ge and ^{76}Ge (Purans et al. PRL **100** 055901 (2008) and Highlight ESRF 2009). The analysis of the first coordination shell has evidenced the effects of isotopic mass change on the low-temperature differences of EXAFS Debye-Waller factors. The full analysis of nearest neighbors distances with femtometer accuracy will be extended up to the second and third coordination shells.

Resoconto dell'attività svolta:

At first, we have extended the data analysis and discussion beyond the results previously obtained only for the first coordination shell of Ge: temperature-dependent EXAFS on the two isotopes ^{70}Ge and ^{76}Ge (Purans et al. PRL 100 055901 (2008) and Highlight ESRF 2009). We have extended our analysis to the second and third coordination shells, where a contribution of the so-called multiple-scattering (MS) effects into EXAFS signal is expected. The DW factors have been obtained for two isotopes of ^{70}Ge and ^{76}Ge using the best fit procedure of the EXAFS signals within the MS approximation in the temperature range from 20 to 300 K. The determined temperature dependencies of the DW factors have been used to calculate the characteristic frequencies within the Einstein model. The obtained values of the characteristic frequencies are in good agreement with those expected from a variation of the isotopic mass. Moreover, new results on classical molecular dynamics simulations have been discussed. The simulations have been performed by Dr. A.Kuzmin and PhD. student J.Timoshnko on a big-computer cluster at Riga for crystalline germanium with the aim to estimate the thermal effects within the first three coordination shells and their influence

on the single-scattering and multiple-scattering contributions to the Ge K-edge extended x-ray absorption fine structure (EXAFS).

Second, we have focused the activity on ending together the final version of a large paper on ReO_3 – material that show low temperature negative thermal expansion that extends the data analysis. We have completed the analysis of XAFS and XRD measurements previously done at ESRF (Grenoble, F) on different ReO_3 samples in the low (only XAFS) and high (XAFS and XRD) temperature regions. Two sets of XRD and XAFS measurements were done on the same time from 300 K to 650 K step of 50 K.

More generally, this visit is an important event of long term cooperation.
This short term visit to Trento has aimed also at increasing the synergies of research groups of Trento (IFN-CNR and Dept. of Physics) and Riga University, acting in a common research area of the Solid State Physics, with complementary methods and competencies. The possibility of detecting relative distance variations smaller than 10 femtometers by means of a conventional transmission EXAFS apparatus and a standard procedure of data analysis have been demonstrated by our experiments. We are currently developing and applying our approaches to understand the local origin of the negative thermal expansion (measured usually only by XRD) on some interesting crystalline materials.

The visit has been the occasion for a more wide common discussion about some other scientific topics that we are developing together: in particular the continuation of a previous FP6-STREP Project "X-TIP" where we demonstrated the possibility to collect with the spatial resolution about 50 nm typical of a SNOM Microscope the X-ray Optical Luminescence excited as a function of X-ray energy at a focused Synchrotron Beamline. We plan in the next future to apply for a new EU grant on this topics, that is very promising in the field of studying with local probes the nanostructured materials.

Firma del Fruitore

RIGA (Lettonie), 16 July 2010