European Science Foundation
Standing Committee for Physics and Engineering Sciences
(PESC)

ESF PESC EXPLORATORY WORKSHOP

2nd Workshop on *ab initio* phonon calculations

SCIENTIFIC REPORT

Cracow, Poland
6–8 December 2007

Convened by: Krzysztof Parlinski

EXECUTIVE SUMMARY

The "2nd Workshop on *ab initio* phonon calculations" has been hold in Cracow, Poland, in the period from **6 to 8 December, 2007**. The Workshop took place in the Lecture Hall of "prof. W.Danka", and Computer Rooms in the Pedagogical University in Cracow. There were 75 participants from 16 countries.

The Workshop was organised in the framework of the Ψ_k Programme on *Electronic Structure Calculations of Solids and Surfaces Network*, and sponsored by the Polish Academy of Science and the Pedagogical University. The organisation task has been carried out by the staff of Department of Materials Research by Computers of the Institute of Nuclear Physics, PAN, Cracow, and the Institute of Technics of Pedagogical University, Cracow.

During the Workshop recent advances of the density functional theory (DFT) as well as the methods of dynamical and thermodynamical properties calculation of crystalline systems were provided. The DFT approach allows to finds structure, electronic properties, and interatomic forces in temperature T=0K regime, while the dynamical matrix, which can be calculated within the DFT approach, define the phonons, and thermodynamical properties at finite temperature. During the Workshop computer tutorials gave an opportunity to learn how to obtain vibrational and thermodynamical quantities using presented methods.

SCIENTIFIC CONTENT

In the first day of the Workshop there were lectures, poster session and computer tutorials. Georg Kresse gave comments about the advantages of the direct method against the linear response method, where the last one has recently been implemented in VASP. The advantage of the direct method becomes essential for the systems and problems which require to consider large supercells. The novel features of VASP code which include the hybrid functional, with mixture of certain fraction of local exchange with the Hartree-Fock exchange was presented. Peter Blaha demonstrated several examples of using Wien2k+Phonon calculations to establish the phase transitions in complex crystalline systems. Helmut Schober showed the interconnection between ionic conductors, their atomic vibrations and the possibilities to study this systems by inelastic neutron scattering technique. Wilfried Wunderlich analysed bond-length spectrum in strontium titanate as a way for better understanding of the electron-phonon coupling in this material. Terry Frankcombe discussed the influence of anisotropy on the quantities derived within the quasiharmonic approximation. Krzysztof Parlinski showed several applications of the VASP+PHONON code to actinide compounds, graphene lattice, and surface vibrations. Mark Johnson described the application of *ab initio* phonon approach to systems with hydrogen bonds. He argued that these

bonds play a fundamental role in enzymatic catalysis. Michael Krisch gave an overview of the determination of the phonon dispersion relations in crystalline materials using inelastic X-ray scattering. Substantial progress was achieved for strongly correlated systems and materials under extreme pressure and temperature with respect to the study of the surface vibrations.

There were 23 oral contributions, which covered rather wide range of topics of computer simulations. The experimental data on lithium nitride, being a promising material for high capacity hydrogen storage, were presented in details. The anharmonicity of protons in sodium and potassium hydrogen disulfate was discussed on the basis of inelastic neutron scattering measurements including the overtones. The reason for expected low thermal conductivity in skutterudites, as a promising material for thermoelectric devices, was given. The new mechanism of Verwey phase transition in magnetite, involving two primary order parameters, one of which is strongly coupled to electronic states of X_3, has explained the variety of features observed for this material. It was shown that the nuclear inelastic scattering of synchrotron radiation is able to provide phonon density of state data not only for Fe^{57} isotope but also for Sm and Eu rare earth metals, for which the *ab initio* calculations are really challenging. The *ab initio* method has also been successfully applied to light actinides containing the f-electrons, Th and U, in which electron-phonon interaction seems to be essential.

It was demonstrated that the *ab initio* approach can be also applied to study the structure and magnetism of the Fe(210) grain boundary. This study could be the first stage of including phonons in such calculations and determine the complete spectral and thermodynamical properties of the grain boundary. Analysis of displacements associated with soft modes discovered in cubic antimonate rare earth metal phases, like RbSb, helped to establish the prototype phase. Moreover, a detailed *ab initio* analysis of phonon vibrations in GaN, doped with Mn impurities, proved that the spurious peak in Raman scattering spectra has a resonance character. The origin of martensitic transformation occurring in Ni_2MnGa crystals was determined from a soft mode along the [110] direction. Using quasiharmonic approximation a systematic and efficient stable shuffling structure was established. A proposition of predicting the phonon spectra of binary zincblende-type semiconductors as a function of concentration of constituents leads to an approach which gives results comparable to the measurements.

In order to test the accuracy of the screened hybrid functional method, implemented recently in VASP code, calculations of phonon dispersion curves for cubic diamond, silicon, germanium and grey tin were performed. Still, phenomenological phonon dispersion curves of graphene with a model of two coordination spheres could be fitted to a few experimental data for graphite. The spin-orbit coupling has been especially considered for the one- and two-

dimensional cobaltates. There was a presentation of software able to analyse the infrared response such as transmittance, reflectance or emittance. The program called FOCUS, is available on the web.

The virtual crystal approximation, often applied to ideal substitutional disorder, can be essentially improved by considering the proper phonons. The accuracy of the *ab initio* phonon calculations within DFT, and the applicability of the quasiharmonic approximation have been discussed on the examples of a large set of fcc metals. Phonons were also calculated for two solid phases of oxygen. Ion bombardment with MeV kinetic energy allows to observe the structural modifications on insulator and semiconductor surfaces. Under de-excitation the phononic signal can be observed. It was shown that the atomic vibrations influence and modify the relaxations of crystal surfaces as a function of temperature. Analytical expressions for the diffusivity and effusivity of thin layers starting from the time-domain thermoreflectance were proposed. A correlation of a rapid increase of surface temperature in thin Bi film exposed to a fs-laser pulses, with a weak electron-phonon coupling leads to explanation of observed delay in rising the sample temperature. The electron-phonon scattering times for collisions with short-wavelength phonons in semiconductors were determined within the *ab initio* method.

At the end of the first day of workshop, there was a tutorial in the Computer Lab, where the participants could exercise the use of the Phonon program, using data of Hellmann-Feynman files already computed by VASP or Wien2k programs. This time was also used to exchange information, and learn methodological details, which routinely are not included in published articles. All participants obtained a CD with the Mini-Phonon program, which can be used to perform simple phonon calculations in combination with an *ab initio* program, and can help to illustrate phonon physics in student educational processes.

There were 29 posters. Special time was devoted to Poster session, but posters were displayed during the whole Workshop, also during the breaks, therefore, there was enough time to look at them carefully.

ASSESSMENT OF THE RESULTS, CONTRIBUTION TO THE FUTURE DIRECTION OF THE FIELD

A number of topics have been indicated as important areas for future research with increasing prospective potential. Phonons will still be used to search for soft modes and identify the structural phase transitions. Phonon calculations will facilitate the analysis of vibration in crystals, including molecular crystals, and estimate the phonon peak's intensities in inelastic neutron and X-ray scattering experiments. Knowledge of phonon vibrations allows to calculate, in an *ab initio* way, the thermodynamical functions important in prediction of phase transition, phase diagrams, and some chemical reactions.

The mentioned approach can be applied to bulk crystals, crystals with defects, surfaces and multilayers, hence one may study surface and interface phonons.

In comparing to the 1st Workshop a few new topics were implemented into the computer codes. *Ab initio* codes were supplemented by the more accurate hybrid functionals. There were contributions exclusively devoted to the consideration of the electron-phonon coupling. There was also some interest in study of atomic vibrations in substitutional disordered semiconductors.

Not much progress has been made in the following topics: There is still a need to calculate the anharmonic contributions to phonon shift and width, which go beyond the quasiharmonic approximation. This should allow to include anharmonic contributions to thermodynamical functions, and to compute thermal heat conductivity. There was not enough interest in study of *ab initio* vibrations in amorphous systems.

FINAL PROGRAM

Wednesday, December 1, 2007

17:00– 20:00	Registration
19:00–	Informal reception at Demel Hotel

Thursday, December 2, 2007

9:00 – 9:10	Welcome
9:10 – 9:50	Georg Kresse *VASP: linear response and hybrid functionals*
9:50 – 10:30	Peter Blaha *Electronic structure, atomic forces, structural relaxations and phonons by WIEN2k*
10:30– 11:00	Coffee break
11:00– 11:40	Helmut Schober *Dynamic instability at the origin of oxygen ion conduction in solid oxides at ambient temperature*
11:40– 12:20	Wilfried Wunderlich *Phonons in $SrTiO_3$ analyzed by difference bond-length spectrum*
12:20– 12:40	Daniel J. Bull *Vibrational modes in light-metal imides and amides for hydrogen storage*
12:40– 14:10	Lunch at Demel Hotel

14:10– 14:50 Terry J. Frankcombe
Anisotropic phonon effects in complex metal hydrides

14:50– 16:20 Poster Session

15:30– 16:00 Coffee break

16:20– 17:00 Krzysztof Parlinski
Lattice dynamics with PHONON

17:00– 19:00 Tutorial Session

Friday, December 3, 2007

9:00 – 9:40 Mark Johnson
Inter-molecular hydrogen bonds; from temperature-driven proton transfer in molecular crystals to denaturation of DNA

9:40 – 10:00 Nina Verdal
Strong hydrogen bonds in trialkali hydrogendisulfates studied with inelastic neutron scattering and periodic density functional theory

10:00– 10:20 Michael M. Koza
Vibrational dynamics of nano-cage based thermoelectric materials — skutterudites, clathrates and osmates

10:20– 10:50 Coffee break

10:50– 11:30 Michael Krisch
Recent advances in inelastic x-ray scattering from phonons

11:30– 11:50 Przemysław Piekarz
Mechanism of the Verwey phase transition in magnetite

11:50– 12:10 Svetoslav Stankov
Lattice dynamics of Sm and Eu metallic films by nuclear inelastic scattering of synchrotron radiation

12:10– 12:30 Johann Bouchet
Lattice dynamics of the light actinides

12:30– 14:00 Lunch at Demel Hotel

14:00– 14:20 Adam Kiejna
Effect of impurities on grain boundary cohesion in iron

14:20– 14:40 Stefaan Cottenier

Phonon information as a useful ingredient in the search for the high pressure phase of RSb

14:40– 15:00 Wojciech Gebicki

Lattice dynamics and Raman scattering of GaN:Mn crystals

15:00– 15:20 Tilmann Hickel

Determination of symmetry reduced structures by a soft-phonon analysis in magnetic shape memory alloys

15:20– 15:40 Andrei Postnikov

Impurity vibration modes in diluted semiconductor alloys

15:40– 16:10 Coffee break

16:10– 16:30 Kerstin Hummer

Lattice dynamics of the group IV semiconductors: An ab initio study using screened hybrid density functionals

16:30– 16:50 Leonid A. Falkovsky

Phonon dispersion in graphene

16:50– 17:10 Hua Wu

Orbital physics in the 1D cobaltates and 2D ruthenate

17:10– 17:30 Domingos De Sousa Meneses

Software for retrieving the phonon response from infrared spectra

18:40 Bus departure from Za Kolumnami Hotel

18:50 Bus departure from Demel Hotel

19:00– Dinner in Modlnica

Saturday, December 4, 2007

9:00 – 9:20 Olivier Pagès

Phonon behavior in semiconductor alloys: A unified picture

9:20 – 9:40 Blazej Grabowski

From ab initio to materials properties: Accuracy and error bars of DFT thermodynamics

9:40 – 10:00 Duck Y. Kim

Lattice vibration in the phase transition of solid oxygen: ϵ- and ζ-phase

10:00– 10:20 Orkhan Osmani

Ab initio calculations of phononic temperatures by relaxation of hot electrons

10:20– 10:50 Coffee break

10:50– 11:10 Pawel Scharoch

Understanding the temperature dependent surface multilayer relaxation of Al(110): An ab initio approach

11:10– 11:30 Jean-Luc Battaglia

Thermal diffusivity and effusivity of thin layers based on thermoreflectance with femtosecond laser pulse

11:30– 11:50 Anja Hanisch

Thermal boundary resistance and discrete phonon spectrum of ultrathin Bi(111) heterolayers on Si(001): An ultrafast time resolved electron diffraction study

11:50– 12:10 Jelena Sjakste

Ab initio method for the electron-phonon scattering times in semiconductors

12:10– Closing

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STATISTICAL INFORMATION ON PARTICIPANTS

The 75 participants were comming from 16 countries: Austria (3), Belgium (2), Czech (7), Finland (1), France (13), Germany (8), Japan (2), Lithuania (1), Mexico (1), Poland (26), Russia (2), Slovakia (1), Spain (1), Sweden (2), UK (2), USA (3).