relations between the spatial variations of the indium composition and those of the residual strain in InGaN films in InGaN/GaN multiple quantum wells (MQW) were simulated theoretically by this new method. The residual strains were found being able to be controlled significantly by selecting the pattern of composition fluctuation. The relation of the difference of the spatial pattern of the composition fluctuation to the dislocation density in InGaN/GaN MQW has been also discussed. In a typical case, $In_{0.5}Ga_{0.5}N$/GaN MQW structure with periodic composition fluctuation with period length less than 68 nm in InGaN layers seems to be able to be grown with no dislocation. In addition, the difference of the type of the short-range chemical ordering of the indium and gallium atoms, which must depend on the type of growth mode, was found to have a considerable influence on the stress distribution in InGaN films.

Keywords: *ab-initio* calculations, multilayer structures, residual stress strain

## P03.05.17

*Acta Cryst*. (2008). A**64**, C223

### Simulation of the para to ferroelectric phase transition in $BaTiO_3$: The role of domains

Stefano Leoni[1], Marek Pasciak[2]
[1]Max Planck Institute for Chemical Physics of Solids, Inorganic Chemistry, Noethnitzer Strasse 40, Dresden, Saxony, 01187, Germany, [2]Institute of Low Temperature and Structure Research, Polish Academy of Sciences, POBOX 1410, 50-950 Wroclaw, Poland, E-mail：leoni@cpfs.mpg.de

$BaTiO_3$ - one of the most extensively technologically used ferroelectric material - undergoes successive phase transitions on lowering temperature, form cubic, to tetragonal, to orthorhombic, to rhombohedral. Different mechanistic models have been invoked over the years, among them the displacive model and the oder-disorder model, both suffering from some important disagreement with experiments [1]. To shed light on the microscopic mechanisms, we have performed molecular dynamics simulations on the para-to-ferroelectric phase transition in $BaTiO_3$ as well as subsequent transitions that involve polarization rotation. Therein, all degree of freedom are treated explicitly, including positions, cell geometry and temperature. For an unbiased mechanistic analysis, we employ the path sampling scheme, designed for activated processes and successfully applied in many previous works. Two main results are obtained: first, a detailed picture of microscopic displacements leading to domains, which do sum up to the correct macroscopic polarization and correspond very well with experiments. Second, the relevance and even the necessity of antiferroelectric arrangements [1], that naturally derive from nucleating the ferroelectric phase within the paraelectric phase and outlast in the orthorhombic one. Combination of ferro and antiferro regions results in far-from-obvious domain structures [2]. Simulation under the effect of an external field allow assessing the response of the material from multidomain to single domain, whereby antiferro arrangements play a key role. [1] Q. Zhang, T. Cagin, W. A. Goddard III, PNAS 103, 14695 (2006), [2] M. Pasciak, S. Leoni, Mater. Res. Soc. Symp. Proc. 1034E (2007), in press, [3] M. Pasciak, S. Leoni, in preparation.

Keywords: ferroelectric physics, ferroelectric phase transitions, molecular dynamics simulations

## P03.06.18

*Acta Cryst*. (2008). A**64**, C223

### Exploration of structures of phosphorus and calcium at high pressure using metadynamics simulation

Hitose Nagara[1], Takahiro Ishikawa[1], Koichi Kusakabe[1], Naoshi Suzuki[2]
[1]Osaka University, Graduate school of engineering science, 1-3, Mchikaneyama-cho, Toyonaka, Osaka 560-8531, JAPAN, Toyonaka, Osaka, 560-8531, Japan, [2]Kansai University, Department of Pure and Applied Physics, 3-3-35 Yamate-cho, Suita, Osaka 564-8680, Japan, E-mail：nagara@mp.es.osaka-u.ac.jp

We predicted the structure of the phosphorus and calcium at high pressure which had been left unidentified after their powder X-ray diffraction patterns were reported. The X-ray experiment reported that the phosphorus has a new phase (P-IV) above the sc phase in the pressure region of 107GPa and 137GPa. After that some theoretical studies were made but they were not successful in predicting the structures of phosphorus which satisfactorily fit the X-ray pattern. We tried the first principles metadynamics simulation, which is a new theoretical method of finding the structures of local free energy minima. The structure of the P-IV we predicted was an incommensurately modulated structure[1] which was confirmed by an experimental group[2]. We then studied the calcium (Ca-IV and Ca-V) and found the structures of zigzag and helical modulations[3]. Both of the modulation periods were commensurate and the space groups of the structures are identified to be $P4_12_12$ and *Cmca*. These results will accelerate the study of the superconductivity of calcium in the phase V, of which the highest superconducting Tc in elements has been reported. We report the details of our studies of the exploration for those structures with some results of the studies for the origin of these modulated structures.

References:
[1]T. Ishikawa, H. Nagara, K. Kusakabe, and N. Suzuki, Phys. Rev. Lett. 96(2006), 095502.
[2]H. Fujihisa, Y. Akahama, H. Kawamura, Y. Ohishi, Y. Gotoh, H. Yamawaki, M. Sakashita, S. Tateya, and K. Honda, Phys. Rev. Lett. 98 (2007), 175501.
[3]T. Ishikawa, A. Ichikawa, H. Nagara, K. Kusakabe, M. Geshi, and N. Suzuki, Phys. Rev. B77, 020101(R), 2008.

Keywords: high pressure, simulation, metadynamics

## P03.06.19

*Acta Cryst*. (2008). A**64**, C223–224

### Cluster models for decagonal quasicrystals

Manabu Inukai[1], Kazuo Soda[1], Hidetoshi Miyazaki[1], Masahiko Kato[1], Shinya Yagi[1], Yoshihiko Yokoyama[2]
[1]Nagoya University, Department of Quantum Engineering, Graduate School of Engineering, Furo-cho, Chikusa-ku, Nagoya, Aichi, 464-8603, Japan, [2]Tohoku University (Katahira, Aoba-ku, Sendai, Miyagi, 980-8577, Japan), E-mail：inukai.manabu@g.mbox.nagoya-u.ac.jp

The model clusters specifying the sites for the constituent transition metals in the decagonal Al-Co-Ni and Al-Co-Cu quasicrystals have been proposed by comparing their electronic structures obtained by the x-ray emission and photoemission spectroscopic measurements [1] with those calculated by the discrete variational Xa potential (DV-Xa) method [2] on the basis of the reported electron microscopic data [3]. The experimentally observed electronic structures can be well explained by those of the model clusters. Their electronic structures show the pseudogap across the Fermi level in the Al partial density of states, which agrees well with a band structure calculation for the