Reference:
[1] P.G. Collins et. al., Science 287, 5459 (2000); S. H. Jhi et. al., Phys. Rev. Lett. 85, 1710 (2000); P. M. Ajayan, et. al. Nature 441, 7095 (2006).
[2] L. D. A. Silva et. al., IEEE Trans. On Nanotech. 5, 517 (2006).

[12/05/10 - P160]
Trivalent and divalent rare earth ion in $Sr_4Al_{14}O_{25}$ - A Computer modelling approach, Marcos V. dos S. Rezende, Giordano F. da C. Bispo, Mário E. G. Valerio, *Universidade Federal de Sergipe* ■ $Sr_4Al_{14}O_{25}$ have a lot technologic application due to the long lasting phosphorescence when doped with trivalent and divalent rare-earth ions. The phosphorescence properties of this material depend on the incorporation of divalent Eu ions, and to obtain the rare earth with this valence the trivalent rare earth must be reduced using particular schemes. A few of such schemes have been used and developed and the most common one is to thermally treat the sample in reduced atmosphere using N_2/H_2 (95:5). In the present work, computer modelling methods employed in this work are based initially on well established approaches that use interatomic potentials to represent the interactions between ions, coupled with energy minimization and use is made of the Mott-Littleton method. The calculations were performed using the GULP code. The present work was divided in two parts. In the first one, the formation of extrinsic defects induced by trivalent rare-earth ions was modelled in 3 different temperatures. The results indicate that: i- at 0K and at 300K, some the trivalent ions preferentially substitutes at the Sr site with the charge compensation mechanism are clearly provided by interstitial oxygen ions and other preferentially substitutes at the Al^{3+} site. ii- at 1573K, on the other hand, all rare earth ions are likely to be incorporated at the Al sites. As a general behaviour, as the temperature increased, the tendency to accommodate the dopants at the Al sites also increased. In the next part, the reduction process RE^{3+} to RE^{2+} were considered either via the incorporation of the 2+ species during the preparation of the samples or via reduction of the incorporated RE^{3+} to the RE^{2+} after the preparation of the samples. Different atmospheres and different temperatures were also taken into account. Then, four schemes were considered. The results show that the incorporation of the divalent rare earth dopant is preferred to occur when during the sample growth in a reducing atmosphere. Comparing all rare earth, the lowest solution energies are obtained for the Eu^{3+} to Eu^{2+} process. All these theoretical results are in agreement with the experimental evidences including the unexpected abnormal europium reduction in air. (This work is supported by CAPES, CNPq and FINEP. MVSR acknowledge the PhD grant from CNPq).

[12/05/10 - P161]
STUDY OF THE DEFECT AGGREGATES IN $CaAl_2O_4 : Eu^{2+}$,R^{3+} THROUGH COMPUTER MODELLING TECHNIQUE, Marcos V. dos S. Rezende, Valdenilson S. Barbosa, Mário E. G. Valerio, *Universidade Federal de Sergipe* ■ The $CaAl_2O_4$ is a material that presents long lasting phosphrescence (LLP) when codoped with a Eu^{2+} and a trivalent ion forming R^{3+} aggregates . The creation of the calcium vacancies by R^{3+} codoping is one possible defect in this matrix. However, they seem not to be of equal importance since not all R^{3+} co-doping enhanced the persistent luminescence. Calcium vacancies can be an important defect in creating aggregates with the oxygen vacancy and the $[R_{Ca}]^+$ ion. The oxygen vacancy and the R^{3+} doping in Ca^{2+} site are both positively charged defect that can trap electrons and hence are of great importance on understanding the LLP mechanism in $CaAl_2O_4$. On the other hand, calcium vacancy is a negatively charged defect and can trap holes . In the present work we studied this system via computer modelling method based on interatomic potentials and energy minimisation. A potential set was developed that accurately reproduces the structure of $CaAl_2O_4$. The model includes pair wise interactions, Ca-O, Al-O and O-O. These potentials were used in defect calculations based on the Mott-Littleton approximation, embodied in the GULP code. Both intrinsic and extrinsic defects were studied including the ones possibly generated during radiation of the material. The intrinsic defects were the following: Schottky, Pseudo-Schottky, Anti-Schottky and Frenkel. The extrinsic defects were calculated by using different mechanisms leading to the formation of defects clusters $CaAl_2O_4 : Eu^{2+}R^{3+}$. For each mechanism, a solid state reaction was devised and the corresponding solution energy was calculated. The most favourable defect is the one with the lowest solution energy.

[12/05/10 - P162]
Model for Analysis of Biaxial and Triaxial Stresses by X-ray Diffraction Assuming Orthotropic Materials, Edson M. Santos, *Universidade Estadual de Feira de Santana*, Marcos T. D. Orlando, *Universidade Federal do Espírito Santo*, Milton S. R. Miltão, *Universidade Estadual de Feira de Santana*, Luis G. Martinez, *Instituto de Pesquisas Energéticas e Nucleares*, Alvaro S. Alves, *Universidade Estadual de Feira de Santana*, Carlos A. Passos, *Universidade Federal do Espírito Santo* ■ In this work we aim to develop expressions for the calculation of biaxial and triaxial stresses in polycrystalline anisotropic materials, and to determine their elastic constants using the theory of elasticity for continuum isochoric deformations; thus, we also derive a model to determine residual stress. The constitutive relation between strain and stress in these models must be assumed to be orthotropic, obeying the generalized Hooke's law. One technique that can be applied with our models is that of X-ray diffraction, because the experimental conditions are similar to the assumptions in the models, that is, it measures small deformations compared with the sample sizes and the magnitude of the tensions involved, and is insufficient to change the volume (isochoric deformation). Therefore, from the equations obtained, it is possible to use the $\sin^2\psi$ technique for materials with texture or anisotropy by first characterizing the texture through the pole figures to determine possible angles ψ that can be used in the equation, and

then determining the deformation for each diffraction peak with the angles ψ obtained from the pole figures. we give a proof of the consistency of these equations by comparing them with previously reported models for isotropic materials, and then we apply our model for biaxial stress using the experimental data obtained by Faurie *et al.* As a result, we can observe the magnitude of the elastic constants determined by our model.

[12/05/10 - P163]
Potassium on bilayer graphene: Band gap opening and selective adsorption, Flávia de Araújo Solon, Jorge Luiz Brito de Faria, *Instituto de Física - IF/UFMT*, Rodrigo B. Capaz, Marcos G. Menezes, *Instituto de Física - IF/UFRJ* ■ Graphene is a two-dimensional carbon material that takes the form of a planar lattice of sp^2 bonded atoms. Since the monolayer graphene was isolated in 2004, ultrathin carbon systems have attracted tremendous attention. The properties of electrons in graphene are fundamentally different from those deriving from the Schrodinger equation. In particular the quantum Hall effect is quantized with integer plus half values and can even be observed at room temperature. Monolayer graphene has a vanishing Fermi point at the Brillouin-zone corner and low-energy quasiparticles with a linear spectrum, $\varepsilon(\vec{k}) = \pm v|\vec{k}|$ which obey a massless Dirac equation.

The electronic bandgap is an intrinsic property of semiconductors and insulators that determines their transport and optical properties. A tunable bandgap (as such, it has a central role in modern device physics and technology and governs the operation of semiconductor devices) would be highly desirable because it would allow great flexibility in design and optimization of devices such as p-n junctions, transistors, photodiodes and lasers. In particular if it could be tuned by applying a variable external electric field.

Bilayer graphene has an entirely different (and equally interesting) band structure. Most notably, the inversion symmetric AB-stacked (Bernal) bilayer graphene is a zero-bandgap semiconductor in its pristine form. But a non-zero bandgap can be induced by breaking the inversion symmetric of the two layers. Indeed, a bandgap has been observed in a one-side chemically doped epitaxial graphene bilayer. In our work, we consider potassium adsorption to induce the symmetry breaking. Also, we studied the valence band structure of a bilayer of graphene and demonstrated that through selective control of the carrier concentration in the graphene layers, one can easily tune the band structure near the Dirac crossing. Finally, by comparing the adsorption energies for AB- and AA-stacked graphene bilayers, we demonstrate that the Moire pattern formed by rotated graphene layers provide a new template for the selective adsorption of atoms or clusters that can be used to self-organize arrays of metallic or magnetic clusters.

[12/05/10 - P164]
Computer modelling of defect structure and rare earh doping in MWO_4 (M = Ca, Sr, Ba, Pb), Jomar B Amaral, Marcos V S Rezende, Mario E G Valerio, *Departamento de Física - Universidade Federal de Sergipe* ■ Currently, the tungstates MWO_4 (M = Ca, Sr, Ba, Pb), have been used in various applications such as optical fiber, moisture sensors, catalysts, solid state lasers, microwave applications and in particular as scintillators for detection of ionizing radiation. This study aims to investigate in these matrices the intrinsic and extrinsic defects (when doped with rare earth elements) so their applications can be well understood and optimized. Computer modelling is a useful technique for determination of the defect properties of materials and the location of dopant ions. For M = Ca, Sr and Ba, the intrinsic defect is most likely the pseudo Schottky MO pair and for $PbWO_4$ the oxygen Frenkel defect is the main intrinsic disorder. The formation energies and solution energies were then calculated for the extrinsic defects, via solid state reactions. The formation energies are also used in a set of equations that can predict the effect of solubility and concentration of dopants in these matrices. For M = Ca, Sr or Pb, the main defect is the rare earth (Ln^{3+}) entering in the M^{2+} site accompanied by a M^{2+} vacancy as charge compensation defect. For $BaWO_4$, the Ln^{3+} occupies the Ba^{2+} site but compensated by oxygen at an interstitial site. In all matrices the concentration of dopants is around 1 mol per cent. Some of these theoretical results are in agreement with experimental results and others still need confirmation. This work is partially supported by CNPq and CAPES.

[12/05/10 - P165]
Computer modelling of defect structure and rare earh doping in YVO4, Ricardo D Santos, Jomar B Amaral, Marcos V R Santos, Romel M Araujo, Paulo J R Montes, Mario E G Valerio, *Universidade Federal de Sergipe* ■ The YVO4 has been studied because of their interesting optical properties. It was shown that the Nd: YVO4, when pumped by a transversely diode laser produces light in a continuous regime. This kind of pumping makes possible to take advantage on the high absorption coefficient of the crystal. The YVO4 doped with trivalent rare earth ions have luminescence properties that point to potential use in optical devices. Computer modelling methods, based on energy minimisation and the Mott-Littleton [1] method, with interactions represented by interatomic potentials, have been used for determination of the defect properties of materials and the location of dopant ions. Such calculations enable predictions to be made of the sites occupied by dopant ions, and the form of charge compensation adopted, if needed. The formation energies and solution energies were then calculated for the extrinsic defects, via solid state reactions. The formation energies are also used in a set of equations that can predict the effect of solubility and concentration of dopants in these matrices. Some of these theoretical results are in agreement with experimental results and others still need confirmation. This work is partially supported by CNPq and CAPES.
[1] Mott, N.F. and Littleton, M.J., Trans. Faraday Soc. 34, 485 (1983).

[12/05/10 - P166]
First-principles Study of Stacking Faults in Ice Ih, Domingos Lopes da Silva Junior, Maurice