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A Critical Study of Pressure Induced Phase Transition

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Different phase of oxygen under high pressure

The occurrence of three solid phase of oxygen at room temperature and the intense colors of these phases have been studies (109) up to 40 GPa pressure cell have been used to obtain absorption and reflectance spectra.

X-ray diffraction studies have been made of cubic (3*C*) and hexagonal (6*H*) polytypic of SiC under pressures to 105 and 95 GPa, respectively, using a diamond-anvil cell and an imaging plate technique. 3*C*-SiC undergoes a phase transition into the rock salt-type structure at 100 GPa or higher accompanied by a volume reduction of 20.3%. The 6*H* polytypic of SiC remains stable to the highest pressure studied, with a premonition of a phase transition above 90 GPa. Equation-of-state data for the two polytypic have been found to be essentially the same to 95 GPa, yielding the bulk modulus 260(9) GPa and its pressure derivative 2.9(0.3).

The structural changes are described in terms of a collective restoring of the initially tilted AlO_6 octahedra towards the ideal cubic perovskite structure without tilting. Up to 40 GPa, the pressure dependence of the volume of the pseudo-cubic phase is described by a third-order Birch-Murnaghan equation of state with parameters V_0 = 54.57(4) Å^3, KT = 190(5) GPa and K' = 7.2(4).

So far we were concerned with citing the literature pertinent to the electronic structure of GdN, and it is clear that there has been no consensus on its electronic structure. As for the type of magnetic-order and -properties of GdN, many have reported on its ferromagnetic order with a curie temperature of only 58 K [8], [17], [18], [19]. Some authors have found a change from insulating to metallic behavior at Tc = 58 K [18]. Others reported on its semi-conducting behavior in both the paramagnetic and ferromagnetic states [20]. A study by Ludbrook [21] showed that GdN was ferromagnetic below 70 K with a saturation moment of 7 μB/ion.

In this study, we present first-principles calculations; using the well known electronic structure code FPLO.09, of the electronic, magnetic and elastic properties, and possible pressure-induced crystallographic phase transitions in GdN. Our calculations were done using the LSDA and GGA schemes, with the 4f shell considered as a semi-core shell. The first purpose of our study is to investigate the relative stability of the three known crystallographic phase of GdN, namely: the RS, ZB, and CsCl structures. We have used the geometric optimization method, i.e., doing self-consistent calculation of the energy–volume dependence of the unit cell for different crystal structures; in order to find out the most energetically-favorable phase. The most stable structure we found is the magnetic RS structure. A second aim of this work is to check the metallicity status of each phase, in particular to investigate the presence of half-metallicity by calculating the electronic structure in both spin directions. Our motive for such an investigation was the diverse conclusions reported in the literature regarding this property as we have already pointed out. We have found out that only the ZB structure exhibits half-metallicity, whether the approximation used is the LSDA or the GGA, in contrast to the RS and CsCl structures which behave differently. Another important aim of this work is studying the effect that a hydrostatic pressure may have on the magnetic moment, energy gap and stability of the three crystal structures of GdN. We have predicted a strong pressure dependence of the total magnetic moment of the three phases and energy gap of the RS structure. In addition, three possible phase transitions are found namely from ZB to RS, RS to CsCl, and ZB to CsCl.

We study numerically and analytically first- and second-order phase transitions in neuronal networks stimulated by shot noise (a flow of random spikes bombarding neurons). Using an exactly solvable cortical model of neuronal networks on classical random networks, we find critical phenomena accompanying the transitions and their dependence on the shot noise intensity. We show that a pattern of spontaneous neuronal activity near a critical point of a phase transition is a characteristic property that can be used to identify the bifurcation mechanism of the transition. We demonstrate that bursts and avalanches are precursors of a first-order phase transition, paroxysmal-like spikes of activity precede a second-order phase transition caused by a saddle-node bifurcation, while irregular spindle oscillations represent spontaneous activity near a second-order phase transition caused by a supercritical Hopf bifurcation. Our most interesting result is the observation of the paroxysmal-like spikes. We show that a paroxysmal-like spike is a

single nonlinear event that appears instantly from a low background activity with a rapid onset, reaches a large amplitude, and ends up with an abrupt return to lower activity. These spikes are similar to single paroxysmal spikes and sharp waves observed in electroencephalographic (EEG) measurements. Our analysis shows that above the saddle-node bifurcation, sustained network oscillations appear with a large amplitude but a small frequency in contrast to network oscillations near the Hopf bifurcation that have a small amplitude but a large frequency. We discuss an amazing similarity between excitability of the cortical model stimulated by shot noise and excitability of the Morris-Lecar neuron stimulated by an applied current.

Theory and computation

Our calculation is a first-principles study of GdN compound in the RS, ZB, and CsCl structures, within the framework of density functional theory. The equilibrium lattice constant, magnetic moment, energy gap, phase transition pressure, bulk modulus and its pressure derivative are calculated by the full-potential nonorthogonal local-orbital minimum basis method (FPLO) [25], [26] using both LSDA [27] and GGA [28] approximations. The bulk modulus and its pressure derivative have been computed using the Murnghan equation of state [29]. We have used the same set of parameters in our computation to ensure unbiased comparison between the results obtained from LSDA and GGA approximations. The magnetic properties of rare earth compounds are determined from the highly localized 4f-states while the other electronic properties are determined by the itinerant s-d electrons [30]. We have treated the f-shell as semi-core state. The calculation parameters are: the k-mesh subdivision: 24 × 24 × 24, the accuracies of the density and total energy are 10−6 and 10−8 Hartree, respectively. The space groups and the positions of atoms in the three phases are tabulated in Table 1. The spin and charge density maps were done using the WIEN2K code [31].

Table 1. The space groups and the atomic positions in the three phases of GdN.

Phase	Space group	Gd-position	N-position
RS	#225	0 0 0	½ ½ ½
ZB	#216	0 0 0	¼ ¼ ¼
CsCl	#221	0 0 0	½ ½ ½

These pressures are confirmed by calculating the enthalpy dependence on the pressure (Fig. 3). A phase transition is possible when the enthalpies of two crystal structures are equal. The pressure at which the two enthalpies are the same is the transition pressure. For example, the pressure-enthalpy curves of the CsCl and RS crystal structures (Fig. 3) intersect at a pressure of 113GPa, at which the enthalpies of these two different crystal structures are equal.

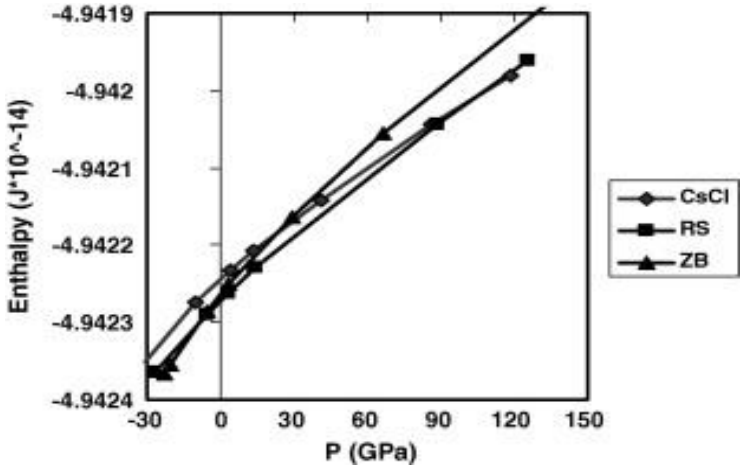

Fig. 3. The enthalpy vs. the pressure using the GGA approximation, for the three crystal structures.

Conclusion

Our geometry-optimization calculation indicates that the magnetic phases, of the three crystal structures of GdN, are more energetically stable than their non-magnetic counterparts. The most stable of the three phases, however, is the magnetic RS structure. Both of the LSDA and GGA approximation have predicted half-metallicity in the ZB structure; with an energy gap of 1.24 and 1.01 eV in the spin-down channel for both approximations respectively. The total magnetic moment of ZB structure is 7 μB at ambient pressure. Our new data, of the spin density map of this phase, supports our calculation that only Gd atom carries the spin magnetic moment of this compound. On the contrary, the electronic structure of CsCl clearly shows the absence of any energy gap in either spin direction; indicating the metallicity of this crystal structure. The rock-salt structure however, behaves differently in that it exhibits half-metallicity in the GGA approximation, but shows metallicity in the LSDA approximation.

1. molecular probes as defects in a pure crystal can of courses, influence its phase transition , particularly by nucleation of a new phase . such effect may be of interest in themselves .

2. Other kinds of SHB measurment ,performed by using hydrostatic pressure e.g pressure cycling experiment can be applied to tackle difrent problem of defect in a PT , etc

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