Ab initio calculation of electronic properties for dangling bond free nitridated silicon

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Abstract

Silicon oxynitride is used by the semiconductor industry as Gate oxide for mordern MOSFETs. For a low nitrogen concentration the theoretical calculation of electronic properties is difficult due to large unit cells and amorphous structures.
Using ab initio density-functional theory the influcene of electrical inactive nitrogen in a silicon oxid matrix was investigated. We report the calculated values of the total energies, density of states, band gap and dielectric constant for different concentrations of nitrogen. By classical MC and CPMD approximate unit cells were obtained for the amorphous structures. The exact value for the band gap was calculated by means of the GW-method and the dielectric response was calculated in the framework of first order pertubation theory as implemented in the ABINIT program.

Methods

classical MC [3] was used to get a starting point for the amorphous structures

- classical pair potenitals have been calculated with GAUSSIAN [4]

CPMD [1] geometry optimization of amorphous structures

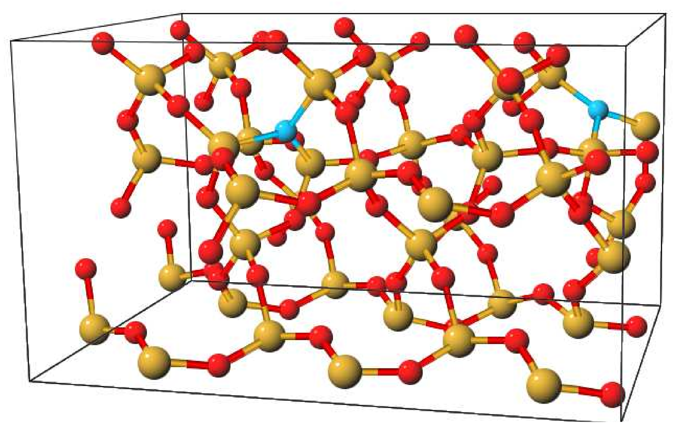
ABINIT [2] calculation of electronic properties

- **DFT-LDA** TM-Pseudopotentials[5], plainwave basisset ⟹ total energie, density of states
- **GW** correction of the LDA band structure ⟹ band gap
- **Response Function** ⟹ dielectric constant

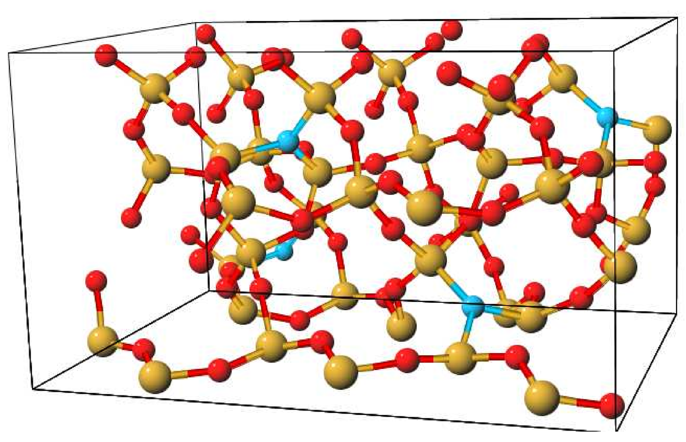
Conclusions

- first DFT calculation of dangling bond free SiO_xN_y with low nitrogen concentration
- an increasing amorphous charactor of the structure with increasing nitrogen content was observed
- detailed investigation of changes in the density of states
- it was shown that the GW Approximatian lead to good results for the band gap
- good agreement between experimental and theoretical results for dielectric constant

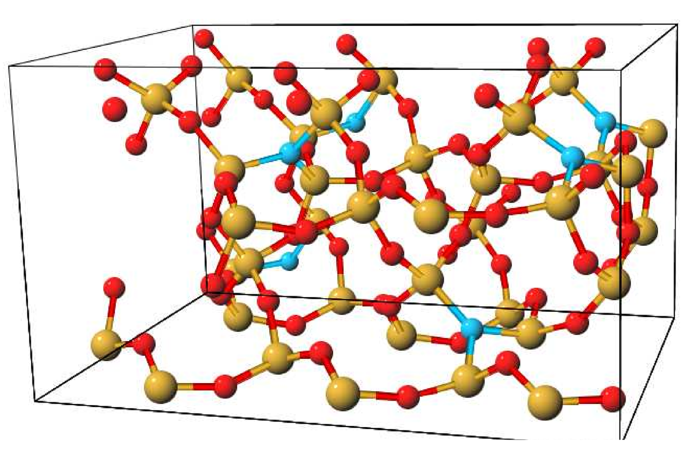
Structure Models



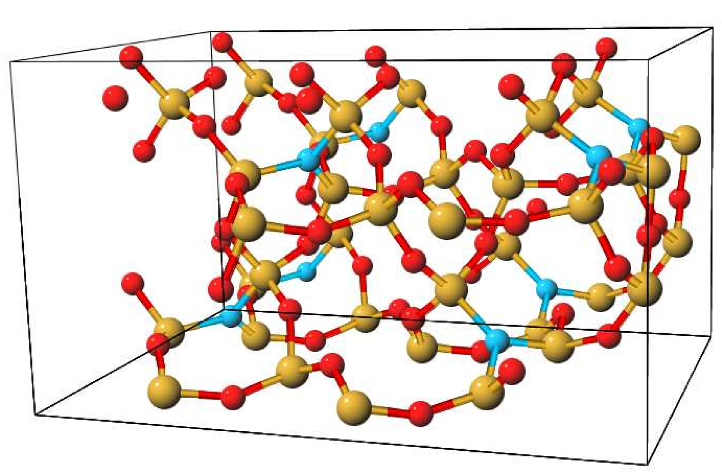
$N_{2\%}$



$N_{4\%}$



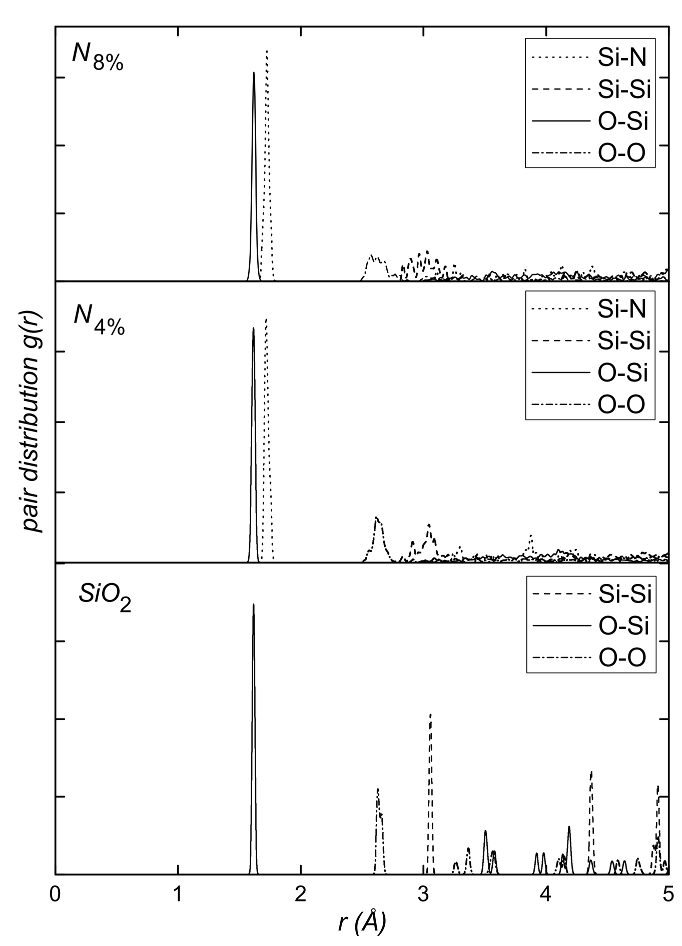
$N_{6\%}$



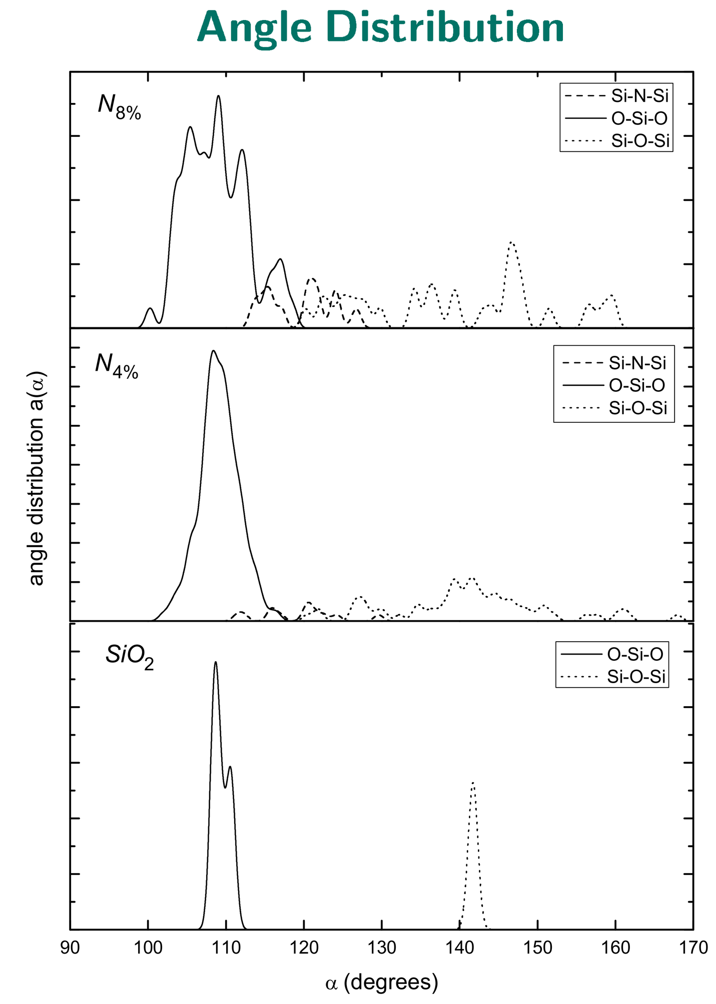
$N_{8\%}$

System	Number of atoms	N (%)
α-SiO_2	9	0
Si_2N_2O	20	40.0
β-Si_3N_4	14	57.1
$N_{2\%}$	107	1.87
$N_{4\%}$	106	3.77
$N_{6\%}$	105	5.71
$N_{8\%}$	104	7.69
$N_{12\%}$	17	11.8
$N_{25\%}$	16	25.0

Pair Distribution



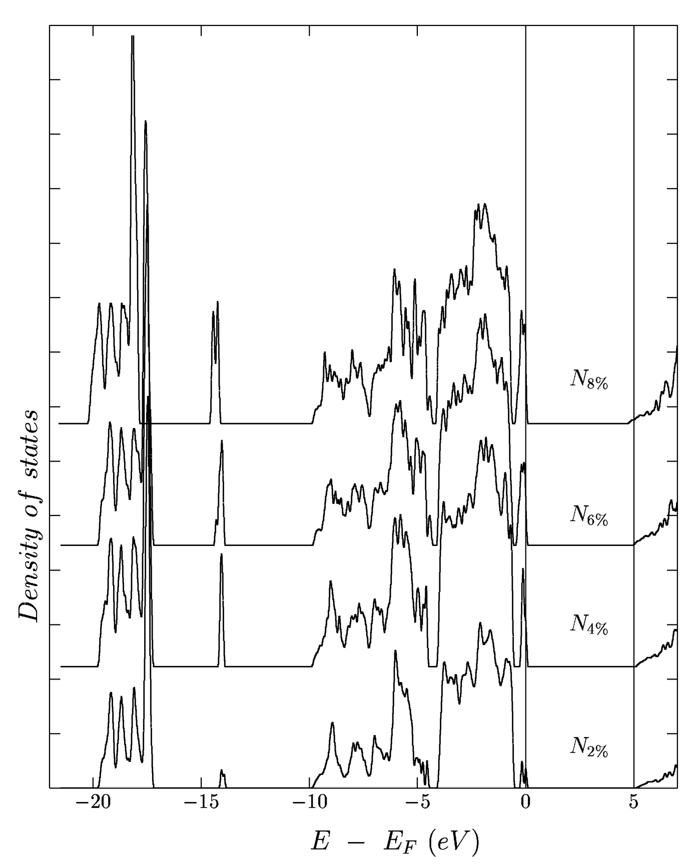
Angle Distribution



- both the pair and the angle distribution indicate the amorphous character of the structures
- all structures are dangling bond free
- distribution of nitrogen is homogeneous

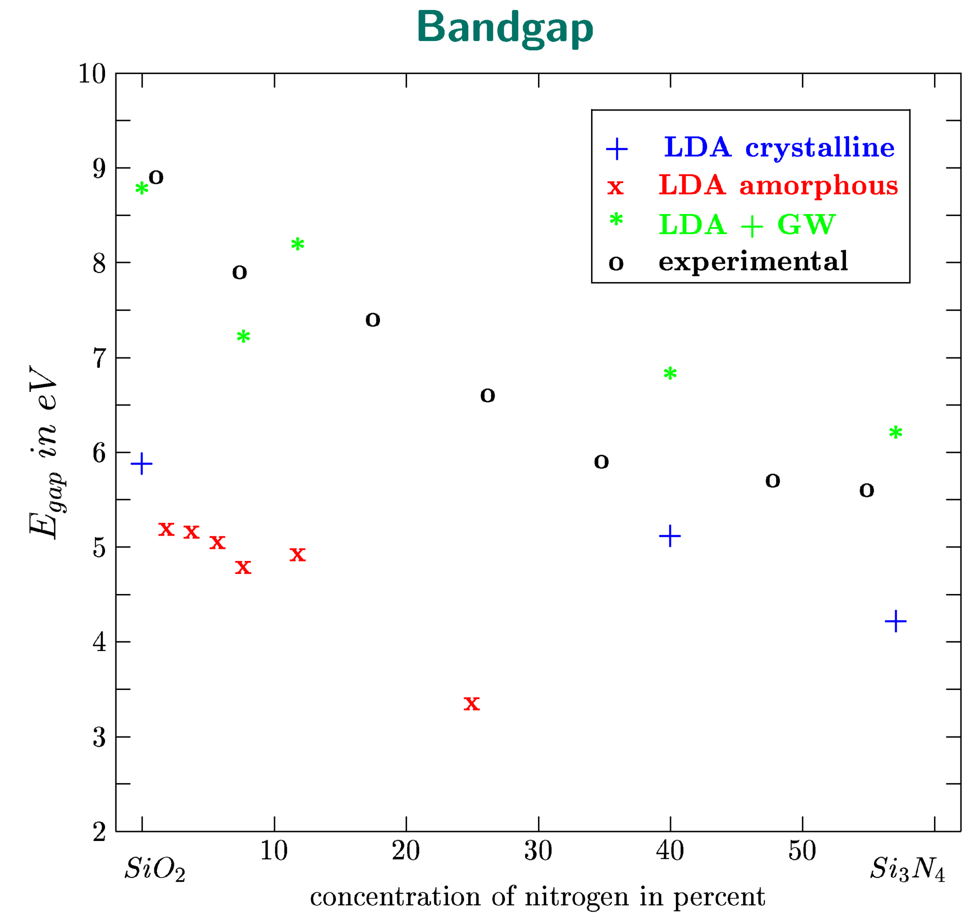
Electronic Properties

Density of States



- new states inside the orignal band gap of α-quarz at top of the valence band
- the bottom of the conduction band remains unchanged
- energy level of the N 2s states is about -14eV

Bandgap

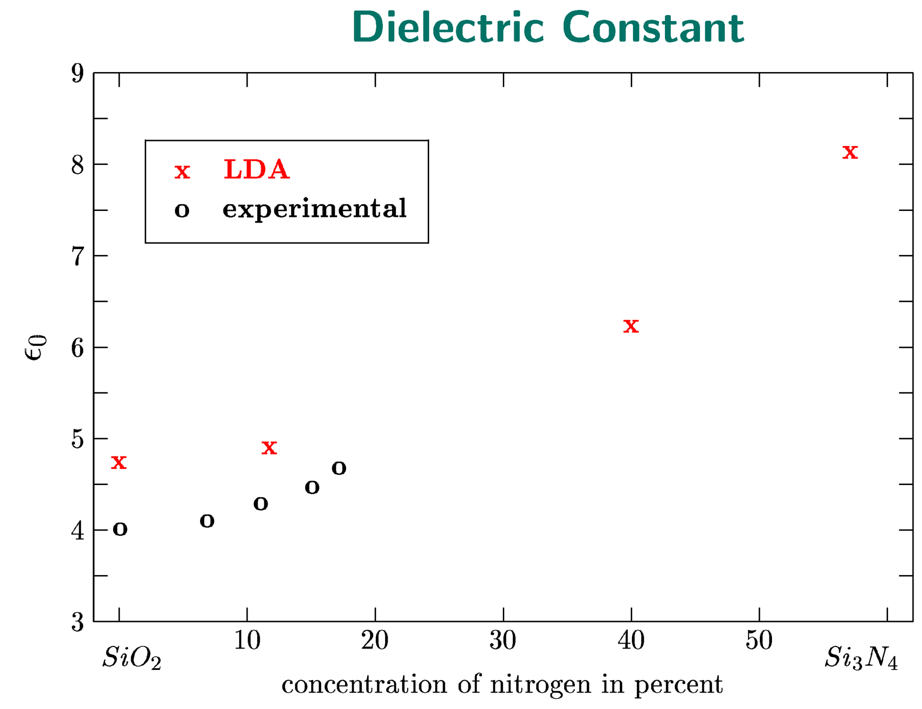


- the LDA is known to underestimate the band gap of semiconductors
- the band gap for the amorphous structures is smaller as the one for the crystalline phases
- GW Method leads to good agreement with experimental results

Total Energie

	$\alpha - SiO_2$	Si_2N_2O	$\beta - Si_3N_4$	$N_{2\%}$	$N_{4\%}$	$N_{6\%}$	$N_{8\%}$
Total Energy (Ha)	-113.4	-186.3	-110.7	-1331.2	-1302.1	-1273.1	-1237.6
Energy per valence electron	-2.36	-1.94	-1.73	-2.34	-2.325	-2.306	-2.275

Dielectric Constant



- the LDA is known to overestimate the dielectric constant
- the change of the dielectric constant is in conjunction with experimental results for a thin silicon oxynitride layer as gate insulator in a nmos transistor

References

[1] CPMD code, Copyright IBM (1900-2006), Copyright MPI für Festkörperforschung Stuttgart (1997-2001) (URL http://www.cpmd.org)
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