DFT simulation of the physical properties of the newly discovered $Ti_3Co_5B_2$-type novel borides $Mn_{3-x}\{Rh,Ir\}_5B_2$ using HPC in addition to X-ray single crystal and TEM data evaluation

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Boron has unique chemical properties and with it's ability of reactions with metals boron yields to a large class of metal borides with high melting points and super hardness [1,2]. Some metal borides are superconductors and there are many borides with extraordinary magnetic properties [3].

While investigating the phase relations in the Mn-{Rh,Ir }-B system we have discovered for both systems a ternary compound, $Mn_{3-x}\{Rh,Ir\}_5B_2$. The crystal structure of both compounds were determined from X-ray single crystal data to be isotypic with the $Ti_3Co_5B_2$-type (space group $P4/mbm$, No. 127). Remarkably, both cases exhibit a significant defect at the Mn 2a sites, which is at the origin of the unit cell. The absence of a superstructure related to these defects is confirmed by transmission electron microscopy studies, in fact Mn atoms and their corresponding vacancies randomly share the 2a sites in a small unit cell.

The aim of this presentation is to show that we can model this randomly occurring vacancies of Mn atoms in the above mentioned crystallographic positions with large supercell simulations. We initially perform a full relaxation of the lattice parameters and ionic positions for the unit cell with no vacancies followed by supercell calculations with cells as large as $2 \times 2 \times 3$, which results in a 240 atoms structure. The effect of the Mn vacancies is then simulated by running calculations with some Mn atoms removed from the 2a site (out of 24).

To run simulations on such big supercells we needed the aid of high-performance computing (HPC) and, therefore, did our calculations on the Vienna Scientific Cluster (VSC). We have run several tests with the Vienna ab-initio simulation package VASP, which we have used for our density functional theory (DFT) approach to find out the optimal adjustments for the parallelism settings. The results of this investigation will be presented here.

References

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