THEORETICAL STUDY OF MAGNETIC PROPERTIES OF THE 1:12 ALLOYS

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Since the discovery of $Nd_2Fe_{14}B$, the best permanent magnet to date, magnets containing the combination of rare earth elements and Fe attract high scientific interest. The iron-based compounds are specifically attractive as they have large magnetic moments due to the high concentration of Fe, rather high coercivity and high Curie temperature. One of the best candidates are the 1:12 compounds with the $ThMn_{12}$-type structure. It has been shown that light rare earths and iron cannot form a stable binary 1:12 compound, so a third element must be added to stabilize the ternary $RE(Fe,M)_{12}$ phase, where M=Ti, V, Si, Mo and etc. Such substitution results in a significant decrease in the saturation magnetization of the compound because the M atom does not carry a magnetic moment and causes a reduction of the magnetic moments of surrounding Fe atoms. Further, the change in the structure due to the substitution of iron by other elements can influence magnetocrystalline anisotropy and Curie temperature of the alloy. A number of attempts to stabilize the compounds with the decreasing concentration of M element have recently been made. Most of the known 1:12 compounds are stable when they have 10 atoms of Fe and 2 atoms of an impurity in the unit cell ($REFe_{10}M_2$). An example is $SmFe_{10}V_2$. However, $NiFe_{11}Ti$ is known to be stable even with one Ti atom per formula unit. Recent experiments show that it is also possible to stabilize the 1:12 phases with reduced concentrations of V or Ti.

In this work the magnetic properties of the 1:12 compounds were studied theoretically from first principles. Starting from the known stable $NiFe_{11}Ti$, $SmFe_{11}Ti$ and $SmFe_{10}V_2$ phases we tried to improve the magnetic properties by reducing the content of Ti and V respectively. The phase stabilities of $NdFe_{11-x}Ti_x$ and $SmFe_{10-x}V_x$ were calculated and compared to the available experimental data. This work is supported by the European Research Project NOVAMAG (EU686056) and STandUP for energy (Sweden).