Phase evolution of $V_{1-x}Fe_xO_2$, (x=0, 0.5, 0.75, 1.0 %) system as a function of temperature

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Vanadium dioxide (VO_2) is a strongly correlated material that has attracted much attention over the last years, as it exhibits a remarkable Metal-Insulator Transition (MIT) at $T_{MIT}\approx$ 68°C, which is accompanied by a reversible Structural Phase Transition (SPT) between the monoclinic (M1) insulating phase and high-temperature rutile (R) metallic phase [1]. At T_{MIT}, a dramatic change of the electrical resistance and a strong modification of the optical transmittance in the near infrared region take place. Displacing T_{MIT} at lower or higher values is a very challenging issue. The main method that has been widely investigated is the introduction of carriers or strain by elemental doping. High valence dopants (Nb^{5+}, $Mo^{6+,}$ W^{6+}) is expected to reduce the T_{MIIT} while low valence dopants (Al^{3+}, Cr^{3+}, Fe^{3+}) is expected to increase it [2-4]. Up to now the phase diagram of the $V_{1-x}Fe_xO_2$ system remains controversial, especially in the low concentration region x≤1%.

We have investigated the phase evolution of $V_{1-x}Fe_xO_2$, (x=0, 0.5, 0.75, 1.0 %) system by in-situ X-Ray Powder Diffraction (XRPD) and Diffuse Reflectance in infrared region in the temperature range 25-90°C to resolve the unclear characteristics of the phase diagram in the low concentration region. The XRPD patterns have been analysed by the Le Bail method using the JANA2006 software [5]. The appearance of the insulating M1 and the metallic R as well as the intermediate triclinic (T) and monoclinic (M2) phases could be monitored in the above temperature range while diffuse reflectance measurements as a function of temperature showed the MIT. The phase diagram of the $V_{1-x}Fe_xO_2$ system in the low concentration region (Fig.1(a)), could be thus unambiguously resolved. We have also observed that the stabilized by Fe dopant intermediate M2 and T phases have been vanished after further annealing the samples under N2/vacuum at high temperature 800 °C (Fig.1(b)). The results will be discussed in respect to Vanadium – Oxygen (V-O) defects [6].

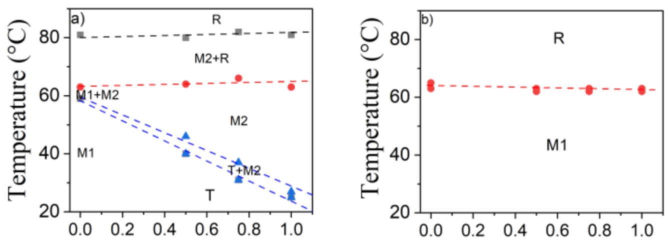

Figure 1: Phase diagram of $V_{1-x}Fe_xO_2$, (x=0, 0.5, 0.75, 1.0 %) before (a) and after (b) annealing under N2/vacuum at 800°C.

References

[1] Z. Tao et al, Phys. Rev. Lett. 109, 166406, (2012).
[2] R. Zhang et al, Ceram. Int. 42, 0272-8842, (2016).
[3] J.-L. Victor et al, J. Phys. Chem. Lett. 12, 7792-7796, (2021).
[4] E. Strelcov et al, Nano Lett. 12, 6198−6205 (2012).
[5] V. Petricek et al, Z. Kristallogr. 229(5), 345-352 (2014).
[6] S. Joshi et al, Sci. Rep. 10, 17121 (2020).

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