

s6.m21.o3 **Structural Phase Transition and Charge-Ordering Effect in η - $\text{Na}_{1.286}\text{V}_2\text{O}_5$.** Fabienne Duc and Patrice Millet, *Centre d'Elaboration de Matériaux et d'Etudes Structurales, UPR CNRS 8011, 29 rue Jeanne Marvig, BP 94347, 31055 Toulouse Cedex 04, France. E-mail: fduc@cemes.fr*

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Charge ordering in mixed-valence transition metal oxides is a subject of great interest in solid state physics, very likely related to many electronic and magnetic properties that these compounds display. Within the transition metal oxides systems, vanadates offer an enormous playground of compounds where different valence states can coexist, and which may eventually give rise to quantum spin antiferromagnetic orderings. Recently, the detailed study of the V^{4+} -rich zone of the sodium-vanadium-oxygen phase diagram has led to the structural characterization of the vanadium oxide bronze η - $\text{Na}_{1.286}\text{V}_2\text{O}_5$ [1-2] (also denoted by the stoichiometric formula $\text{Na}_9\text{V}_{14}\text{O}_{35}$). The structure of the latter (space group $P2_1/c$) is built up of layers consisting of VO_5 square pyramids sharing edges and corners with their apical oxygens pointing up and down alternately to form double strings in the [100] direction. These double strings are isolated in the [001] direction via VO_4 tetrahedra and have a stair-like shape with a step every ten VO_5 square pyramids. This compound has been reported to exhibit [2] a spin-gap behaviour, although its magnetic susceptibility curve could not be fitted by theoretical equations for spin-gap systems. It is presently considered as a new type of low-dimensional system.

This contribution will give an overview of recent results [3] obtained by low temperature x-ray diffraction on the η - $\text{Na}_{1.286}\text{V}_2\text{O}_5$ phase. The x-ray data clearly reveal the existence, around 100 K, of a structural second-order phase transition, stabilizing a superstructure associated with charge ordering.

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s6.m21.o4 **Phonon and Defect-Induced Effects in Resonant "Forbidden" Reflections.** V.E. Dmitrienko,^a E.N. Ovchinnikova,^b K. Ishida,^c J. Kokubun,^e A. Kirfel,^d S.P. Collins,^e D. Laundy,^f A.P. Oreshko,^b Y. Joly^g and D. Cabaret^h, ^a*Institute of Crystallography, 59 Leninskii pr., 119333 Moscow, Russia*, ^b*Moscow State University, Physical Department, 119992, Moscow, Russia*, ^c*Tokyo University of Science, Noda, Chiba 278-8510, Japan*, ^d*Mineralogisch- Petrologisches Institut der Universität Bonn, D-53115 Bonn, Germany*, ^e*Diamond Light Source, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon, OX11 0QX, UK*, ^f*Daresbury Laboratory, Warrington, WA4 4AD, UK*, ^g*Laboratoire de Cristallographie, F-38042 Grenoble, France*, and ^h*Laboratoire de Mineralogie-Cristallographie, case 115, Tour 16, 4 place Jussieu, F-75252 Paris, France. E-mail: dmitrien@ns.crys.ras.ru*

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In this report, we present a survey of atomic displacement effects on the anisotropy of x-ray resonant scattering and discuss thermal-motion-induced (TMI) and point-defect-induced (PDI) "forbidden" reflections [1-5]. To this purpose, tensor structure factors and unusual polarization properties of both types of reflections are calculated. Owing to their resonant character, the TMI and PDI reflections allow for separate studies of both impurity and host atoms of different types. The considered phenomena can provide a very sensitive tool to assess point defects because only those atoms produce contributions to the PDI reflections that are "distorted" by defects and have appropriate absorption edges.

Strongly temperature dependent TMI reflections were recently observed in Ge [3,4] and in ZnO [5]. Owing to interference with the temperature-independent contribution, their intensities can increase and decrease with temperature. In Ge crystals, the contributions from vibrations parallel and perpendicular to atomic bonds were separated [4]. Drastic changes of the diffraction spectra were found in ZnO, contrary to the rather small changes observed for Ge. Using two different theoretical approaches [6,7] we present *ab initio* simulations of the temperature dependence and of diffraction spectra for Ge and ZnO.

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