

Characterization of $\text{Cs}_2\text{NaAlF}_6:\text{Cr}^{3+}$ single crystals

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Abstract –The intense fluorescence observed for $\text{Cs}_2\text{NaAlF}_6:\text{Cr}^{3+}$ shows that this system is a very good candidate for tunable radiation source applications. In low temperature photoluminescence measurements were observed a near-infrared band attributed to the zero-phonon transition ${}^2E({}^2G) \rightarrow {}^4A_2({}^4F)$ while at room-temperature the emission is assigned to the ${}^2T_2({}^2F) \rightarrow {}^4A_2({}^4F)$ transition. Polarized Raman spectra of $\text{Cs}_2\text{NaAlF}_6$ indicate that the guest ion causes only small perturbations to the host lattice. Magnetic measurements show that the Curie magnetic moments rise with decreasing temperature.

In doped insulating materials, the physical properties are related to point defects that arise during the compound's formation process by the insertion of interstitial impurities into the host lattice. In samples doped with transition-metals such as Cr, Fe, Co, Ni and Mn, the most important optical features are broad emission and absorption bands in the visible and near-infrared region. These bands allow the materials to function in a wide class of applications ranging from room temperature solid state lasers to special paper sheets to oriented dosimeter chips for radiological protection. $\text{Cs}_2\text{NaAlF}_6:\text{Cr}^{3+}$ crystallizes in a hexagonal structure having R3m symmetry, with $Z = 6$ (Fig. 1). In this space group the Al occupies octahedral 3a or 3b position (with the local symmetry D_{3d}), while the Na anion is resides in the 6c position (with the local symmetry C_{3v}). Previous investigation of $\text{Cs}_2\text{NaAlF}_6:\text{Cr}^{3+}$ samples with various Cr^{3+} concentrations demonstrated pure phase samples whose X-ray diffraction patterns were indexed with the same space group. In low temperature photoluminescence measurements of $\text{Cs}_2\text{NaAlF}_6:\text{Cr}^{3+}$ were observed a near-infrared band attributed to the zero-phonon spin-forbidden transition ${}^2E({}^2G) \rightarrow {}^4A_2({}^4F)$ while at room-temperature the emission is assigned to the ${}^2T_2({}^2F) \rightarrow {}^4A_2({}^4F)$ transition. Two non-equivalent octahedral sites were identified through time-resolved measurements and lifetime fluorescence bands are measured. The incorporation of Cr^{3+} ions into the Al site of $\text{Cs}_2\text{NaAlF}_6$ results in the formation of local $[\text{CrF}_6]^{3-}$ centers which couple to the host lattice through electron–phonon (el–ph) interactions. Polarized Raman scattering spectra of $\text{Cs}_2\text{NaAlF}_6$ with a Cr^{3+} content of 0.1, 0.5 and 3.0 at% have been studied at both room temperature and 16 K. A shoulder located near the very intense band assigned to the $\text{AlF}_6^{3-} A_{1g}$ mode indicates that the guest ion causes only small perturbations to the host lattice. Magnetic susceptibility measurements performed on the 0.1, 0.5, 3, 10 and 50 at% samples show that for particular concentrations the Cr^{3+} ions are not isolated, but participate to inter and/or intra-cluster magnetic exchange. The heat capacity measurements (Fig.2) were performed to thermal characterization of the luminescence for $\text{Cs}_2\text{NaAlF}_6:\text{Cr}^{3+}$ system.

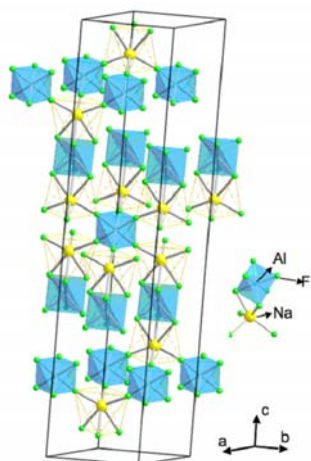


Figure 1: Crystal structure for $\text{Cs}_2\text{NaAlF}_6$. The transparent polyhedra represents NaF_6 and the semi-transparent frame the $\text{Al}(\text{Cr})\text{F}_6$ polyhedra.

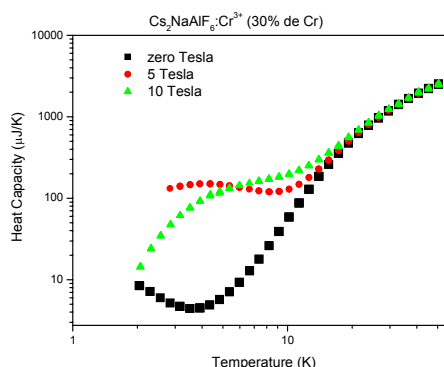


Figure 2: Heat capacity measurements of $\text{Cs}_2\text{NaAlF}_6$ with a Cr^{3+} content of 30.0 at% as a function of temperature at different magnetic fields.