

X-ray diffraction and colour centre studies on RbCl-RbBr mixed crystals

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Abstract. X-ray diffraction and colour centre studies have been carried out on RbCl-RbBr mixed crystals. The lattice constant closely follows the linear form of Vegard's law. The mean Debye-Waller factor shows a highly nonlinear composition dependence. The composition dependence of the F-band peak position is slightly nonlinear but that of the F-band half-width is highly nonlinear. The Ivey-Mollow relation holds for this system with an index of 2.5. The 'size effect' is found to have a dominant effect on the F-band width.

Keywords. Alkali halide mixed crystals; rubidium halides; lattice constants; Debye-Waller factor; colour centres.

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1. Introduction

The physical properties of alkali halide mixed crystals have been recently reviewed by Hari Babu and Subba Rao (1984) and Sirdeshmukh and Srinivas (1986). From these reviews it appears that no information is available regarding the RbCl-RbBr mixed crystal system. As a part of a continuing programme in this laboratory on studies of mixed crystals, x-ray diffraction and colour centre experiments have been carried out on this system which have yielded information on the composition dependence of the lattice constant (a), the Debye-Waller factor (B), the Debye temperature (θ), the F-band peak position (λ_{\max}) and the F-band halfwidth (W). The results are presented in this paper.

2. Experimental

2.1 Material preparation and characterization

Analar grade chemicals supplied by E Merck were used to obtain crystals of RbCl, RbBr and their mixed crystals. The powdered material was taken in a crucible and allowed to melt in an electric 'Bunsen' furnace. The melt was cooled very slowly by a regulated reduction of the energy input to the furnace. From the solidified mass, single crystals of dimensions $5 \times 5 \times 2 \text{ mm}^3$ could be cleaved out. As these dimensions were sufficient for the present studies, no effort was made to obtain larger crystals. Although the composition of the mixed crystals grown by the melt method will be generally close to the composition of the starting mixture, there can be some variation in the