

CHAPTER - I

GENERAL INTRODUCTION, SCOPE, CONTENTS AND AIM OF THE PRESENT WORK

1.1 INTRODUCTION

Real solids contain a number of lattice defects like vacancies, interstitials, impurities, dislocations etc; the nature and concentration of such defects may vary from sample to sample depending on its thermal and mechanical history and also on its impurity content. The physical properties of solids are found to be considerably influenced by these defects. The investigation of the changes in the physical properties with controlled variation of lattice defects is of considerable importance from theoretical as well as experimental point of view. Such a study paved the way for application of some of these materials in technology. Apart from these defects, separation of electric charges leading to local variation in charge density (from that available in normal crystals) may also occur in some cases; such defects can be easily induced by irradiation with ionising radiations like X-rays. X-ray irradiation generally gives rise to internal photoelectrons which may get trapped at the special lattice sites having localised potential barriers and does not, in most cases, cause any displacement of the constituent atoms or ions from their natural lattice positions. The imperfections, produced by X-ray irradiation in a material, are therefore, considered simple in structure and so the physical properties of solids on X-ray irradiation has become the subject matter of many investigations¹⁻⁴.

The concepts in defect solid-state are developed from an intensive study of the colouration phenomena in the alkali halides which are in many ways considered ideal solids for experimental and theoretical investigations because they have simple cubic structures, are obtainable in a reasonable degree of chemical purity and are amenable for growth in large single crystals. However, many experimentally observed properties of these materials could not be explained without assuming that the real crystals fall short of the ideal, highly ordered structure. They contain structural imperfections of various types, viz., vacant lattice sites, interstitial ions, impurities and dislocations. Vacant lattice sites and interstitial ions along with a small number of dislocations present in real crystals are generally formed during the growth process itself. Vacancies and/or interstitial ions can also be produced by chemical impurities which are intentionally added to the host of material or are intrinsically present in it. For example, foreign atoms of the same or different valency existing in the crystal even in a few parts per million concentration give evidence of their presence by introducing new electronic levels and new absorption bands (Fig. 1.1). Such disturbances in the electronic configuration of a material may bring about changes in its physical properties like dielectric, magnetic, mechanical etc.

X-ray irradiation of an alkali halide crystal produces new absorption bands in the normally transparent spectral region; these bands are due to colour centres which are electrons and

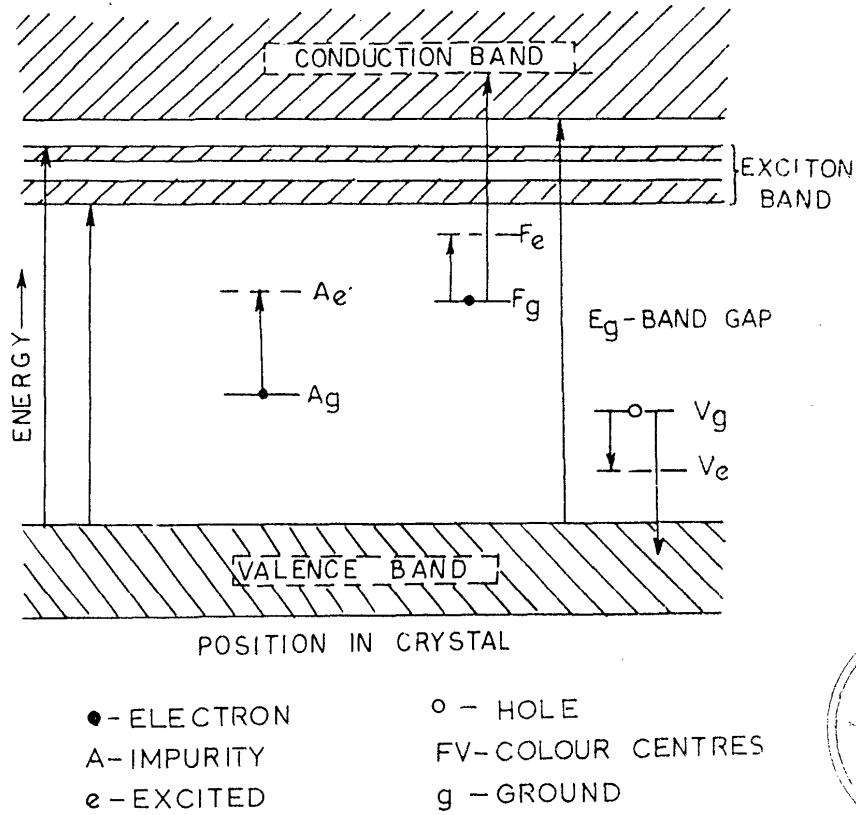


FIG. 1.1 BAND PICTURE OF AN ALKALI HALIDE, SHOWING ENERGY LEVELS AND SOME OPTICAL ABSORPTIONS DUE TO EXCITONS, IMPURITIES AND COLOUR CENTRES (SCHEMATIC)

(J.H. Schulman and Compton, "Colour Centres in Solids," Pergamon Press Inc., New York, 1963)

holes trapped at special lattice sites. In pure crystals, generally the colouration is characteristic not only of the process of colouration but is also strongly influenced by the nature of the impurities and the previous history regarding thermal, mechanical etc. treatment the sample may have undergone. These colour centres are destroyed by heating when the electrons or their counterpart, holes, are freed from their trapped states and recombine with each other. (the material is then generally reduced to its original state. The bleaching process is often found to be accompanied by emission of light (called thermoluminescence) the intensity of which passes through a number of maxima at particular temperatures. These characteristic temperatures can be related to the trap depths available in the particular specimen. The dielectric, magnetic and in fact all the electronic properties of the solid, are also expected to be influenced during the bleaching process. Excellent reviews of this field by Pohl⁵, Mott and Gurney⁶ , Seitz¹ Schulman and Compton³ show the useful information obtained on alkali halides.

T
X

Thus, for obvious reasons, research on imperfection-determined properties was mainly confined to the alkali halides; such studies in other materials are also of great interest as they offer a testing ground for the concepts developed from studies in alkali halides. Similar work on alkaline earth halides^{7,8} and other solids^{9,10} received some attention.

1.2 SCOPE OF THE PRESENT WORK

It is evident from the above considerations that the