CHAPTER I

GENERAL INTRODUCTION, SCOPE, CONTENTS AND AIM OF THE PRESENT WORK
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1.1 Introduction:

The physical properties of solids are controlled by the nature and concentration of lattice defects present in the solids. The investigation of the changes in the physical properties with controlled variation of lattice defects is of considerable interest from theoretical as well as experimental point of view. The lattice defects are vacant lattice sites, interstitial atoms, foreign atoms, dislocations etc. the concentration of which may vary from sample to sample depending on its thermal and mechanical history and also on the impurity content. These lattice defects lead to perturbation in the perfect lattice of a crystal. This in turn can lead to localised energy levels which may take part in the electronic processes inside the solid. The situation is further complicated by the dynamic character of such imperfections as they are comparatively mobile and can undergo changes by their mutual interactions. Thus it becomes desirable to develop a proper understanding of the nature and the properties of lattice imperfections in solids.
When a solid is irradiated with ionising radiations like X-rays, apart from the defects already present, separation of electric charges leading to local variation in charge density from that available in normal crystal, may also occur in some cases. X-ray irradiation generally produces electrons and holes in solids like alkali halide crystals which get trapped at special lattice positions (like negative ion and positive ion vacancies) forming colour centres which give new absorption bands in the normally transparent spectral region (Fig. 1.1); colour centres thus formed are an important class of point defects in ionic crystals.

The concepts in defect solid state are developed from an intensive study of the colour centre 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. These studies on colour centres and electronic properties of alkali halide crystals have become an established line of research for understanding in general the influence of lattice defects on the physical properties of solids. The importance of this is indicated by the phenomenal growth of experimental and theoretical investigations on colour centres.

The colouration of pure crystals is generally characteristic not only of the process of colouration but is also strongly influenced by the nature of the impurities and the
FIG. 11 BAND PICTURE OF AN ALKALI HALIDE, SHOWING ENERGY LEVELS AND SOME OPTICAL ABSORPTION DUE TO EXCITONS, IMPURITIES AND COLOUR CENTRES (SCHEMATIC)

previous history regarding thermal, mechanical etc. treatment the sample may have undergone. These colour centres are destroyed by heating when the electrons or their counterparts, holes, are freed from their trapped states and recombine with each other; then the material is normally 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 trap depths available in the particular specimen. The dielectric, magnetic etc. properties of the solid (as a matter of fact, all the electronic properties of the solid) are also expected to undergo corresponding changes during the bleaching process. Excellent reviews of this field by Pohl\textsuperscript{1}, Mott and Gurney\textsuperscript{2}, Seitz\textsuperscript{3}, and Schulman and Compton\textsuperscript{4} show the useful information obtained in alkali halides.

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 received some attention\textsuperscript{5,6}.

1.2 Scope of the Present Work:

Thus it can be seen that the data on optical, electrical etc. properties collected over the past several