TOPOLOGICAL THEORY OF LINE-DEFECTS ON CRYSTAL SURFACES, AND THEIR INTERACTIONS WITH BULK AND INTERFACIAL DEFECTS

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INTRODUCTION

Important surface processes are known to be mediated by surface defects; for example, crystal growth proceeds by the motion of steps (see Zangwill[1] for a review). Recent advances in surface science, particularly through new experimental techniques, are revealing the existence of a diversity of line defects in addition to steps, and it is anticipated that these may also significantly influence surface processes. In view of these developments, it is therefore appropriate to formulate a theory which can be used to enumerate the distinct types of defects that can arise on any given crystal surface in its unrelaxed and reconstructed conditions. This can be done on the basis of symmetry theory for unrelaxed surfaces, and also for reconstructed cases if the nature of the relaxation is known. Thus, the primary objective of this work is to present a theory which can predict the nature of all admissible defects on surfaces. In addition, we discuss the interaction of such surface defects with bulk and interfacial defects.

Defects in crystalline materials are constrained to adopt particular forms. They can be treated using topological methods, and are thereby found to be characterised by symmetry operations of the underlying crystal. A well known example of such topological characterisation is the assignment of a Burgers vector to a dislocation in the bulk of a crystal. This parameter expresses an intrinsic

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geometrical property of the discontinuity, and is completely independent of the defect's core structure and line direction. In the following section we review this characterisation process, and subsequently generalise the essential idea involved to the case of surface defects. The distinctive types of defects that can arise in the bulk of a single crystal are then reviewed briefly in these terms.

In order to identify all of the admissible defects that can arise at surfaces and interfaces, it is necessary to summarise the space groups which describe the permissible symmetries of crystal surfaces and interfaces. This is done in the fourth and fifth sections of the paper, and in the sixth section we discuss defects on unrelaxed and relaxed crystal surfaces, using the (001) surface of Si as an illustration. Interfaces resemble surfaces in some respects, but, on the other hand, exist inside crystals. Therefore, in the discussion of interfacial defects in the following section, it is convenient to consider these in two categories, namely surface-like and bulk-like defects. The final section of the paper is a summary of the crystallographic origin and topological properties of all the various line defects which can arise at surfaces, in the bulk, and at interfaces, and includes an account of the interactions between defects of different types.

In the present work, we use the notation adopted in the International Tables for Crystallography[2], for the mathematical representation of symmetry operations. Using matrix form, a symmetry operator, $\mathfrak{W}$, is written $(\mathbf{W},\mathbf{w})$, where $\mathbf{W}$ is the orthogonal part (e. g. rotation, or mirror reflection) and $\mathbf{w}$ represents any associated displacement (due to nonsymmorphic elements, or the location of an element, or both). Pure translation operations have the form $(\mathbf{I},\mathbf{t})$, where $\mathbf{I}$ represents the identity operation and $\mathbf{t}$ the translation vector. When referring to the ith operator in a space group, we write $\mathfrak{W}_i = (\mathbf{W}_i,\mathbf{w}_i)$, and in the general case this will comprise both a translation and rotation or reflection.

CHARACTERISATION OF DISCONTINUITIES

The topological properties of a line of discontinuity in a material are intinsic geometrical aspects which are completely independent of its line direction. In crystalline materials, these properties are constrained to have particular forms because of the medium's symmetry. The object of the present section is to outline this topological characterisation using a framework which encompasses