Chapter 4
Line Profiles Caused by Planar Faults

ABSTRACT

The planar faults in crystalline materials yield characteristic broadening of X-ray line profiles. The diffraction peak shape caused by intrinsic and extrinsic stacking faults and twin boundaries formed on close packed {111} planes in face centered cubic (fcc) crystals are calculated. The Bragg reflections consist of subreflections that can be categorized by specific selection rules for the hkl indices. The breadth and the position of the subreflections relative to the exact Bragg angle depend on their indices. For instance, if the sum of indices of a subreflection is a multiple of three, neither the position nor the breadth of this peak is influenced by planar faults. Other subreflections are broadened and shifted simultaneously due to intrinsic and extrinsic stacking faults. For both fcc and hexagonal close packed (hcp) crystals each subreflection caused by twin boundaries is a sum of symmetric and antisymmetric Lorentzian functions. The latter profile component is caused by the interference between the radiations scattered from the parent and twinned lamellae in the crystal. The antisymmetric Lorentzian function yields a shift of the subprofile center. For fcc materials this displacement of peak position is marginal since twin boundaries are formed on close packed {111} planes; however in hcp crystals, where twinning usually occurs on pyramidal planes, this effect should be taken into account in the line profile evaluation. The effect of anti-phase boundaries on line profiles of superstructure reflections for Cu_3Au is also discussed in this chapter.

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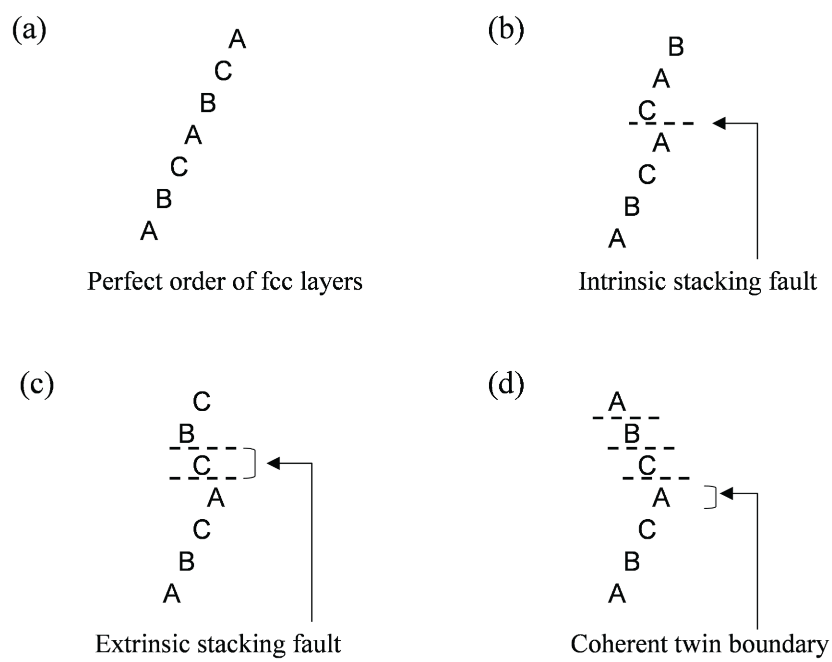
INTRODUCTION

Planar faults are two dimensional lattice defects in crystalline materials. As examples, Figure 1 shows three types of planar faults in face centered cubic (fcc) crystal structures, namely intrinsic and extrinsic stacking faults, as well as coherent twin boundary. These defects are formed on {111} planes in fcc crystals. When {111} planes are packed on each other in the three dimensional lattice, there are three different positions in the stacking sequence which are usually denoted by letters *A*, *B* and *C*. The perfect order of layers in an fcc lattice is ABCABC etc., which is altered when planar faults are formed. Figure 1 shows the stacking sequence for perfect order and the three types of planar faults. In the case of an intrinsic stacking fault a part of the lattice is shifted by vector

Figure 1. The stacking sequence of {111} planes for perfect order of layers and the three types of planar faults in fcc crystals: intrinsic stacking fault, extrinsic stacking fault and coherent twin boundary. The three different positions of {111} planes are denoted by letters A, B and C. The dashed lines indicate the shift by vector $\frac{1}{6}\langle 11\bar{2}\rangle$ *when the faults are formed.*



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