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论文

从相变出发理解和计算变体间位向差

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摘要:

本文从相变出发, 结合母相对称性建立相变与变体位向差之间的定量联系, 详细介绍了如何计算相变矩阵和以之为基础的变体间位向差, 并以fcc→bcc相变系统为例, 运用相变矩阵和对称操作矩阵计算了N--W位向关系下变体间位向差, 结果与前人从位向关系出发计算结果一致. 本文方法有助于理解位向差的成因, 特别有助于开展对无理位向关系引起的变体间位向差的分析. 文中还进一步运用点群理论讨论了立方系N--W, K--S, Bain位向关系下独立存在的变体数目, 并且推导了相变矩阵与位向关系矩阵之间的转换关系.

关键词: 变体 相变晶体学 对称性 位向关系

THE UNDERSTANDING AND CALCULATION OF MISORIENTATION BETWEEN VARIANTS BASED ON THE PHASE TRANSFORMATION

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Abstract:

Misorientation between crystalline grains generated from a solid state phase transformation can be understood according to the orientation relationship (OR) between the parent and product phases, when such an OR is reproducible and unique. Due to the symmetry of the parent phase, the product phase can be related to the parent phase by various crystallographically equivalent variants of the same OR. When a pair of product particles with different variants meet at a grain boundary, the misorientation between the adjacent grains can be determined based on the OR and the symmetry of the parent phase. Misorientations for ideal rational ORs of phase transformations in some systems have been tabulated in literatures, and also, irrational ORs have been reported, with an increasing tendency because of the improvement of measurement technologies. This paper describes in details how to calculate the misorientation of different variants with a general OR. It starts from constructing the transformation matrix for the phase transformation with a rational or irrational OR, from either measurements or calculations. By applying the symmetry operators in the parent phase with the matrix manipulation, the misorientations between different variants have been derived. Since the misorentations are due to the symmetry of the parent phase, the determined values of misorientation nles between different vriants are firstly independent of the OR, but the misorientations axes are dependent on the OR. Nevertheless, the final results of the minimum rotation angles usually vary with the OR when the symmetry of the product phase is taken into consideration to derive misorientation angle/axis. The present approach elaborates the quantitative relationship between the OR of a phase transformation and the misorientation between product particles of different variants. It contributes to a better understanding of the cause of the misorientation, and provides simple formulas to determine the misorientations for a general OR. For simplicity, an example of applications of the present approach is given to an fcc→bcc phase transformation system with the N–W OR. The calculated results are consistent with thosgot from othr approaches. In additin, the nuber of indepndent variants with different ORs, such as the N–W, K–S, Bain ORs in the fcc/bcc system is analyzed, by following Cahn and Kaloji approacof uperimposing point groups of te parent and product phases. The relationship betweethe transformation matrix, the orintation relationship matrix and the correspondinmatrix in cuic systems is also discussed.

Keywords: variant crystalloraphy of phase transformation smmetry orientation relationship

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