Contribution ID: 4 Type: 口头报告

β-Ga2O3 倾转界面及其电子结构关联性研究

摘要

本研究探讨了单斜晶系 β-Ga2O3（超宽禁带半导体材料）中原子尺度晶体倾斜、缺陷形成与电子结构变化之间的关联，该材料在高功率电子器件和抗辐射应用领域具有重要价值。通过结合高空间分辨率（~2 Å）与能量分辨率（~40 meV）的扫描透射电子显微镜-电子能量损失谱（STEM-EELS）、像差校正 STEM 及密度泛函理论（DFT）计算，我们直接观测到辐照诱导微结构缺陷处的纳米尺度带隙窄化现象（从 4.86 eV 降至 3.98 eV）。实验采用重离子辐照（6 MeV Au3+，1×1015 离子/平方厘米）沿 [010] 晶带轴引入原子级镶嵌式倾斜结构，导致沿块体边界形成排列的镓空位线/团簇。X 射线衍射摇摆曲线展宽与原子分辨率成像共同证实，这些缺陷会引起各向异性晶格畸变。DFT 模拟表明，镓空位（VGa1 和 VGa2）会降低材料带隙，并使载流子迁移率限制因素从本征极性光学声子（POP）散射转变为电离氧原子散射。具体而言，与八面体配位的 VGa2 空位（带隙 4.42 eV，有效质量 0.21 m_0）相比，四面体配位的 VGa1 空位会引发更显著的带隙缩减（3.96 eV）和更低的有效质量（0.10 m_0）。面内倾转界面结构通过破坏长程声子极化，抑制 POP 散射并提升电子迁移率。本工作建立了原子尺度结构形变与电子性能退化之间的直接联系，为极端环境下 β-Ga2O3 的缺陷调控合成与性能优化提供关键理论依据。研究结果凸显了纳米尺度缺陷工程在定制先进功率电子器件与抗辐射半导体材料中的重要作用。

关键词

宽禁带半导体，扫描透射电子显微镜，电子能量损失谱，马赛克倾转，电子结构，离子辐照

Abstract

Crosslinking structural transformation mechanism at nanoscale to the corresponding anisotropically electronic properties is essential to both the atomic-level controlled synthesis and extreme-conditional applications of the ultrawide bandgap semiconductors. Here, we report the first direct observation of bandgap variation at certain microstructural flaws in monoclinic crystal β-Ga2O3 via scanning transmission electron microscopy-electron energy loss spectrum (STEM-EELS) technology with both high energy and spatial resolution. Atomic-scale tilt of the Mosaic blocks relative to [010] zone axis is demonstrated to cause specific point defects accumulation at block boundaries, resulting in the formation of vacancy lines (or clusters) and then the crystal deformation induced flaws. These as-formed tiny Mosaic tilts observed from both in-plane and out-of-plane geometry are correlated to the corresponding electronic structure obtained by density functional calculations, indicating the carrier mobility limits transferred from intrinsic polar optical phonon scattering to the ionized oxygen atoms

scattering in the defective monoclinic crystal. These findings provide a new insight on these anisotropic defect formation induced electronic structural variation, paving the way for precise synthesis and development of high-performance ultra-wide bandgap materials.

Keywords

Ultra-wide bandgap semiconductors, STEM-EELS, Mosaic Tilts, Electronic structures, Ion irradiation

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Session Classification: 核技术及应用、医学物理与工程

Track Classification: 口头报告: 核技术及应用、医学物理与工程