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Computer simulation of pressure-induced structural transitions in MgO [001] tilt grain boundaries

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Abstract

Atomistic simulations using lattice and molecular dynamics were carried out on the {210}, {310}, and {410} tilt grain boundaries of MgO as a function of pressure up to 100 GPa at a single temperature of 600 K. The calculations show a significant change in the structure of the tilt grain boundaries as pressure increases. The results show that, beyond the previously identified reversible pressure induced collapse of the channel structure, an irreversible shear was identified that forms a mirror grain boundary, which does not possess well-defined dislocation cores and is consequently denser. These mirror boundaries are energetically more favorable than the symmetric boundaries at elevated pressures. As applied pressure approaches 100 GPa a reversible structural transition occurs causing the boundaries to shear perpendicular to the boundary plane forming highly dense structures that contained seven coordinate ions at the boundary and the presence of an edge dislocation-like structure. We suggest that differences between the boundary structures seen in the HREM studies with those predicted by simulations may result from stresses upon the crystal during preparation causing irreversible shearing.